O*bject* ***O****riented* ***P****rogramming* *via* ***F****ortran 90/95*

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Contents

Preface

There has been an explosion of interest in, and books on object-oriented programming (OOP). Why have yet another book on the subject? In the past a basic education was said to master the three r's: reading, 'riting, and 'rithmetic. Today a sound education in engineering programming leads to producing code that satisfy the four r's: readability, reusability, reliability, and really-efficient. While some object-oriented programming languages have some of these abilities Fortran 90/95 offers all of them for engineering applications. Thus this book is intended to take a different tack by using the Fortran 90/95 language as its main OOP tool. With more than one hundred pure and hybrid object-oriented languages available, one must be selective in deciding which ones merit the effort of learning to utilize them. There are millions of Fortran programmers, so it is logical to present the hybrid object-oriented features of Fortran 90/95 to them to update and expand their programming skills. This work provides an introduction to Fortran 90 as well as to object-oriented programming concepts. Even with the current release (Fortran 95) we will demonstrate that Fortran offers essentially all of the tools recommended for object-oriented programming techniques. It is expected that Fortran 200X will offer additional object-oriented capabilities, such as declaring "extensible" (or virtual) functions. Thus, it is expected that the tools learned here will be of value far into the future.

It is commonly agreed that the two decades old F77 standard for the language was missing several useful and important concepts of computer science that evolved and were made popular after its release, but it also had a large number of powerful and useful features. The following F90 standard included a large number of improvements that have often been overlooked by many programmers. It is fully compatible with all old F77 standard code, but it declared several features of that standard as obsolete. That was done to encourage programmers to learn better methods, even though the standard still supports those now obsolete language constructs. The F90 standards committee brought into the language most of the best features of other more recent languages like Ada, C, C++, Eiffel, etc. Those additions included in part: structures, dynamic memory management, recursion, pointers (references), and abstract data types along with their supporting tools of encapsulation, inheritance, and the overloading of operators and routines. Equally important for those involved in numerical analysis the F90 standard added several new features for efficient array operations that are very similar to those of the popular MATLAB environment. Most of those features include additional options to employ logical filters on arrays. All of the new array features were intended for use on vector or parallel computers and allow programmers to avoid the bad habit of writing numerous serial loops. The current standard, F95, went on to add more specific parallel array tools, provided "pure" routines for general parallel operations, simplified the use of pointers, and made a few user friendly refinements of some F90 features. Indeed, at this time one can view F90/95 as the only cross-platform international standard language for parallel computing. Thus Fortran continues to be an important programming language that richly rewards the effort of learning to take advantage of its power, clarity, and user friendlyness.

We begin that learning process in Chapter 1 with an overview of general programming techniques. Primarily the older "procedural" approach is discussed there, but the chapter is closed with an outline of the newer "object" approach to programming. An experienced programmer may want to skip directly to the last section of Chapter 1 where we outline some object-oriented methods. In Chapter 2, we introduce the concept of the abstract data types and their extension to classes. Chapter 3 provides a fairly detailed introduction to the concepts and terminology of object-oriented programming. A much larger supporting glossary is provided as an appendix.

For the sake of completeness Chapter 4 introduces language specific details of the topics discussed in the first chapter. The Fortran 90/95 syntax is used there, but in several cases cross-references are made to similar constructs in the C++ language and the MATLAB environment. While some readers may want to skip Chapter 4, it will help others learn the Fortran 90/95 syntax and/or to read related publications that use C++ or MATLAB. All of the syntax of Fortran 90 is also given in an appendix.

Since many Fortran applications relate to manipulating arrays or doing numerical matrix analysis, Chapter 5 presents a very detailed coverage of the powerful intrinsic features Fortran 90 has added to provide for more efficient operations with arrays. It has been demonstrated in the literature that object-oriented implementations of scientific projects requiring intensive operations with arrays execute much faster in Fortran 90 than in C++. Since Fortran 90 was designed for operations on vector and parallel machines that chapter encourages the programmer to avoid unneeded serial loops and to replace them with more efficient intrinsic array functions. Readers not needing to use numerical matrix analysis may skip Chapter 5.

Chapter 6 returns to object-oriented methods with a more detailed coverage of using object-oriented analysis and object-oriented design to create classes and demonstrates how to implement them as an OOP in Fortran 90. Additional Fortran 90 examples of inheritance and polymorphism are given in Chapter 7. Object-oriented programs often require the objects to be stored in some type of “container” or data structure such as a stack or linked-list. Fortran 90 object-oriented examples of typical containers are given in Chapter 8. Some specialized topics for more advanced users are given in Chapter 9, so beginning programmers could skip it.

To summarize the two optional uses of this text; it is recommended that experienced Fortran programmers wishing to learn to use OOP cover Chapters 2, 3, 6, 7, 8, and 9, while persons studying Fortran for the first time should cover Chapters 1, 2, 3, and. Anyone needing to use numerical matrix analysis should also include Chapter 5.

A OO glossary is included in an appendix to aid in reading this text and the current literature on OOP. Another appendix on Fortran 90 gives an alphabetical listing on its intrinsic routines, a subject based list of them, a detailed syntax of all the F90 statements, and a set of example uses of every statement. Selected solutions for most of the assignments are included in another appendix along with comments on those solutions. The final appendix gives the C++ versions of several of the F90 examples in the text. They are provided as an aid to understanding other OOP literature. Since F90 and MATLAB are so similar the corresponding MATLAB versions often directly follow the F90 examples in the text.

Ed Akin, Rice University, 2002

Index

Chapter 1

Program Design

1.1 Introduction

The programming process is similar in approach and creativity to writing a paper. In composition, you are writing to express ideas; in programming you are expressing a computation. Both the programmer and the writer must adhere to the syntactic rules (grammar) of a particular *language*. In prose, the fundamental idea-expressing unit is the sentence; in programming, two units—*statements* and *comments*—are available.

Standing back, composition from technical prose to fiction should be organized broadly, usually through an outline. The outline should be expanded as the detail is elaborated, and the whole re-examined and re-organized when structural or creative flaws arise. Once the outline settles, you begin the actual composition process, using sentences to weave the fabric your outline expresses. *Clarity* in writing occurs when your sentences, both internally and globally, communicate the outline succinctly and clearly. We stress this approach here, with the aim of developing a *programming style that produces efficient programs that humans can easily understand*.

To a great degree, no matter which language you choose for your composition, the idea can be expressed with the same degree of clarity. Some subtleties can be better expressed in one language than another, but the fundamental reason for choosing your language is your audience: People do not know many languages, and if you want to address the American population, you had better choose English over Swahili. Similar situations happen in programming languages, but they are not nearly so complex or diverse. The number of languages is far fewer, and their differences minor. Fortran is the oldest language among those in use today. C and C++ differ from it somewhat, but there are more similarities than not. MATLAB's language, written in C and Fortran, was created much later than these two, and its structure is so similar to the others that it can be easily mastered. The C++ language is an extension of the C language that places its emphasis on object oriented programming (OOP) methods. Fortran added object oriented capabilities with its F90 standard, and additional enhancements for parallel machines were issued with F95. The Fortran 2000 standard is planned to contain more user-friendly constructs for polymorphism and will, thus, enhance its object-oriented capabilities. This creation of a new language and its similarity to more established ones are this book's main points: More computer programming languages will be created during your career, but these new languages will probably not be much different than ones you already know. Why should new languages evolve? In MATLAB's case, it was the desire to express matrix-like expressions easily that motivated its creation. The difference between MATLAB and Fortran 90 is infinitesimally small compare to the gap between English and Swahili.

An important difference between programming and composition is that in programming you are writing for two audiences: people and computers. As for the computer audience, what you write is "read" by interpreters and compilers specific to the language you used. They are *very* rigid about syntactic rules, and perform *exactly* the calculations you say. It is like a document you write being read by the most detailed, picky person you know; every pronoun is questioned, and if the antecedent is not perfectly clear, then they throw up their hands, rigidly declaring that the *entire* document cannot be understood. Your picky friend might interpret the sentence "Pick you up at eight" to mean that you will literally lift him or her off the ground at precisely 8 o'clock, and then demand to know whether the time is in the morning or afternoon and what the date is.

Humans demand even more from programs. This audience consists of two main groups, whose goals can conflict. The larger of the two groups consists of *users*. Users care about how the program presents itself, its *user interface*, and how quickly the program runs, how *efficient* it is. To satisfy this audience, programmers may use statements that are overly terse because they know how to make the program more readable by the computer's compiler, enabling the compiler to produce faster, but less human-intelligible program. This approach causes the other portion of the audience—programmers—to boo and hiss. The smaller audience, of which *you* are also a member, must be able to read the program so that they can enhance and/or change it. A characteristic of programs, which further distinguishes it from prose, is that you and others will seek to modify your program in the future. For example, in the 1960s when the first version of Fortran was created, useful programs by today's standards (such as matrix inversion) were written. Back then, the user interface possibilities were quite limited, and the use of visual displays was limited. Thirty years later, you would (conceivably) want to take an old program, and provide a modern user interface. *If* the program is structurally sound (a good outline and organized well) and is well-written, re-using the "good" portions is easy accomplished.

The three-audience situation has prompted most languages to support *both* computer-oriented and human-oriented "prose". The program's meaning is conveyed by *statements*, and is what the computer interprets. Humans read this part, which in virtually all languages bears a strong relationship to mathematical equations, and also read *comments*. Comments are *not* read by the computer at all, but are there to help explain what might be expressed in a complicated way by programming language syntax. *The document or program you write today should be understandable tomorrow*, not only by you, but also by others. Sentences and paragraphs should make sense after a day or so of gestation. Paragraphs and larger conceptual units should not make assumptions or leaps that confuse the reader. Otherwise, the document you write for yourself or others served no purpose. The same is true with programming; the program's organization should be easy to follow and the way you write the program, using both statements and comments, should help you and others understand how the computation proceeds. The existence of comments permits the writer to directly express the program's outline in the program to help the reader comprehend the computation.

These similarities highlight the parallels between composition and programming. Differences become evident because programming is, in many ways, more demanding than prose writing. On one hand, the components and structure of programming languages are far simpler than the grammar and syntax of any verbal or written language. When reading a document, you can figure out the misspelled words, and not be bothered about every little imprecision in interpreting what is written. On the other, simple errors, akin to misspelled words or unclear antecedents, can completely obviate a program, rendering it senseless or causing it to go wildly wrong during execution. For example, there is no real dictionary when it comes to programming. You can define variable names containing virtually any combination of letters (upper and lower case), underscores, *and* numbers. A typographical error in a variable's name can therefore lead to unpredictable program behavior. Furthermore, computer execution speeds are becoming faster and faster, meaning that increasingly complex programs can run very quickly. For example, the program (actually groups of programs) that run NASA's space shuttle might be comparable in size to Hugo's *Les Misérables*, but its complexity and immediate importance to the "user" far exceeds that of the novel.

As a consequence, program design must be extremely structured, having the ultimate intentions of performing a specific calculation efficiently with attractive, understandable, efficient programs. Achieving these general goals means breaking the program into components, writing and testing them separately, then merging them according to the outline. Toward this end, we stress *modular programming*. Modules can be on the scale of chapters or paragraphs, and share many of the same features. They consist of a sequence of statements that by themselves express a meaningful computation. They can be merged to form larger programs by specifying what they do and how they *interface* to other packages of software. The analogy in prose is agreeing on the character's names and what events are to happen in each paragraph so that events happen to the right people in the right sequence once the whole is formed. Modules can be re-used in two ways. As with our program from the 1960s, we would "lift" the matrix inversion routine and put a different user interface around it. We can also re-use a routine within a program several times. For example, solving the equations of space flight involves the inversion of many matrices. We would want our program to use the matrix inversion routine over and over, presenting it with a different matrix each time.

The fundamental components of good program design are

1. Problem definition, leading to a program specification
2. Modular program design, which refines the specification
3. Module composition, which translates specification into executable program
4. Module/program evaluation and testing, during which you refine the program and find errors
5. Program documentation, which pervades all other phases

The result of following these steps is an efficient, easy-to-use program that has a user's guide (how does someone else run your program) and internal documentation so that other programmers can decipher the algorithm.

Today it is common in a university education to be required to learn at least one foreign language. Global interactions in business, engineering, and government make such a skill valuable to one's career. So it is in programming. One often needs to be able to read two or three programming languages—even if you compose programs in only one language. It is common for different program modules, in different languages, to be compiled separately and then brought together by a "linker" to form a single executable. When something goes wrong in such a process it is usually helpful to have a reading knowledge of the programming languages being used.

When composing to express ideas there are, at least, two different approaches to consider: poetry and prose. Likewise, in employing programming languages to create software there are distinctly different approaches available. The two most common ones are "procedural programming" and "object-oriented programming." The two approaches are conceptually sketched in Fig. 1.1. They differ in the way that the software development and maintenance are planned and implemented. Procedures may use objects, and objects usually use procedures, called *methods*. Usually the object-oriented code takes more planning and is significantly larger, but it is generally accepted to be easier to maintain. Today when one can have literally millions of users active for years or decades, maintenance considerations are very important.

1.2 Problem Definition

The problem the program is to solve must be well specified. The programmer must broadly frame the program's intent and context by answering several questions.

- *What must the program accomplish?*
  From operating the space shuttle to inverting a small matrix, some thought must be given to *how* the program will do what is needed. In technical terms, we need to define the *algorithm* employed in small-scale programs. In particular, numeric programs need to consider well how calculations are performed. For example, finding the roots of a general polynomial *demands* a numeric (non-closed form) solution. The choice of algorithm is influenced by the variations in polynomial order and the accuracy demanded.

- *What inputs are required and in what forms?*
  Most programs interact with humans and/or other programs. This interaction needs to be clearly specified as to *what* format the data will take and *when* the data need to be requested or arrive.

- *What is the execution environment and what should be in the user interface?*
  Is the program a stand-alone program, calculating the quadratic formula for example, or do the results need to be plotted? In the former case, simple user input is probably all that is needed, but the programmer might want to write the program so that its key components could be used in other programs. In the latter, the program probably needs to be written so that it meshes well with some pre-written graphics environment.

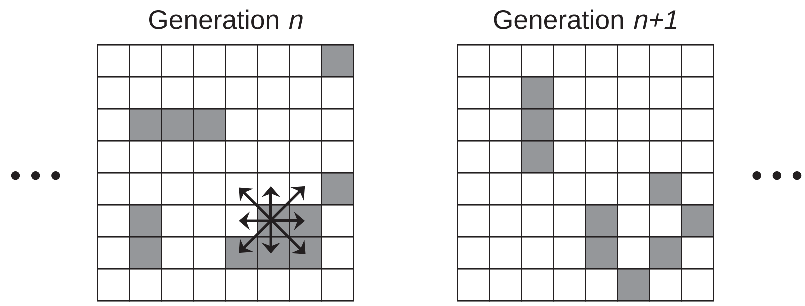


Figure 1.1: Here, the game is played on an 8×8 square array, and the filled squares indicate the presence of life. The arrows emanating from one cells radiate to its eight neighbors. The rules are applied to the n^{th} generation to yield the next. The row of three filled cells became a column of three, for example. What is going to happen to this configuration the next generation?

- *What are the required and optional outputs, and what are their formats (printed, magnetic, graphical, audio)?*
  In many cases, output takes two forms: *interactive* and *archival*. Interactive output means that the programs results must be provided to the user or to other programs. Data format must be defined so that the user can quickly see or hear the programs results. Archival results need to be stored on long-term media, such as disk, so that later interpretation of the file's contents is easy (recall the notion of being able to read tomorrow what is written today) and that the reading process is easy.

The answers to these questions help programmers organize their thoughts, and can lead to decisions about programming language and operating environment. At this point in the programming process, the programmer should know what the program is to do and for whom the program is written. We don't yet have a clear notion of how the program will accomplish these tasks; that comes down the road. This approach to program organization and design is known as *top-down* design. Here, broad program goals and context is defined first, with additional detail filled in as needed. This approach contrasts with *bottom-up* design, where the detail is decided first, then merged into a functioning whole. For programming, top-design makes more sense, but you as well as professional programmers are frequently lured into writing code immediately, usually motivated by the desire to "get something running and figure out later how to organize it all." That approach is motivated by expediency, but usually winds up being more inefficient than a more considered, top-down approach that takes longer to get off the ground, but with increased likelihood of working more quickly. The result of defining the programming problem is a *specification*: how is the program structured, what computations does it perform, and how should it interact with the user.

An Extended Example: The Game of Life

To illustrate how to organize and write a simple program, let's structure a program that plays *The Game of Life*. Conway's "Game of Life" was popularized in Martin Gardner's Mathematical Games column in the October 1970 and February 1971 issues of *Scientific American*. This game is an example of what is known in computer science as *cellular automata*. An extensive description of the game can be found in *The Recursive Universe* by William Poundstone (Oxford University Press, 1987).

The rules of the game are quite simple. Imagine a rectangular array of square cells that are either empty (no living being present) or filled (a being lives there). As shown in Fig. 1.1, each cell has eight neighboring cells. At each tick of the clock, a new generation of beings is produced according to how many neighbors surround a given cell.

- If a cell is empty, fill it if three of its neighboring cells are filled; otherwise, leave it empty.
- If a cell is filled, it
  dies of loneliness if it has zero or one neighbors,
  continues to live if it has two or three neighbors,
  dies of overcrowding if it has more than three neighbors.

The programming task is to allow the user to "play the game" by letting him or her define initial configurations, start the program, which applies the rules and displays each generation, and stop the game at any time the user wants, returning to the initialization stage so that a new configuration can be tried. To understand the program task, we as programmers need to pose several questions, some of which might be

- What computer(s) are preferred, and what kind of display facilities do they have?
- Is the size of the array arbitrary or fixed?
- Am I the only programmer?

No matter how these questions are answered, we start by forming the program's basic outline. Here is one way we might outline the program in a procedural fashion.

1. Allow the user to initialize the rectangular array or quit the program.
2. Start the calculation of the next generation.
   (a) Apply game rules to the current array.
   (b) Generate a new array.
   (c) Display the array.
   (d) Determine whether the user wants to stop or not.
      i. If not, go back to 2a.
      ii. If so, go to step 1

Note how the idea of reusing the portion of the program that applies game rules arises naturally. This idea is peculiar to programming languages, having no counterpart in prose (It's like being told at the end of a chapter to reread it!). This kind of *looping* behavior also occurs when we go back and allow the user to restart the program.

This kind of outline is a form of *pseudocode*: [†] A programming language-like expression of how the program operates. Note that at this point, the programming process is language-independent. Thus *informal pseudocode* allows us to determine the program's broad structure. We have not yet resolved the issue of how, or if, the array should be displayed: Should it be refreshed as soon as a generation is calculated, or should we wait until a final state is reached or a step limit is exceeded? Furthermore, if calculating each generation takes a fair amount of time, our candidate program organization will not allow the user to stop the program until a generation's calculations have been finished. Consequently, we may, depending on the speed of the computer, want to limit the size of the array. A more detailed issue is how to represent the array internally. These issues can be determined later; programmers frequently make notes at this stage about how the program would behave with this structure. Informal pseudocode should remain in the final program in the form of comments.

Writing a program's outline is not a meaningless exercise. How the program will behave is determined at that point. An alternative would be to ask the user how many generations should be calculated, then calculate all generations, and display the results as a movie, allowing the user to go backward, play in slow motion, freeze-frame, etc. Our outline will not allow such visual fun. Thus, programmers usually design several candidate program organizations, understand the consequences of each, and determine which best meets the specifications.

[†] The use of the word "code" is interesting here. It means program as both a noun and a verb: From the earliest days of programming, what the programmer produced was called *code*, and what he or she did was "code the algorithm." The origin of this word is somewhat mysterious. It may have arisen as an analogy to Morse code, which used a series of dots and dashes as an alternative to the alphabet. This code is tedious to read, but ideal for telegraphic transmission. A program is an alternate form of an algorithm better suited to computation.

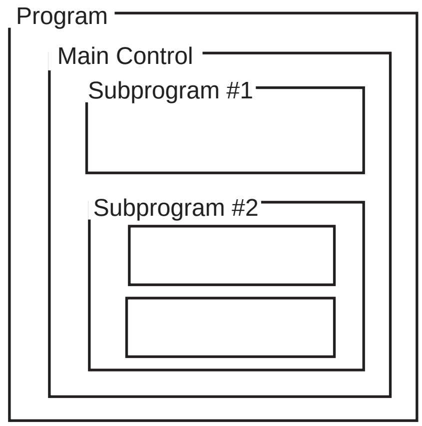


Figure 1.2: Modular program organization relies on self-contained routines where the passage of data (or messages) from one to the other is very well defined, and each routine's (or objects) role in the program becomes evident.

1.3 Modular Program Design

We now need to define what the routines are and how they are interwoven to archive the program's goals. (We will deepen this discussion to include objects and messages when we introduce object-oriented formulations in Sec. 1.7.) What granularity—how large should a routine be—comes with programming experience and depends somewhat on the language used to express it. A program typically begins with a main segment that controls or directs the solution of the problem by dividing it into sub-tasks (see Figure 1.2). Each of these may well be decomposed into other routines. This step-wise refinement continues as long as necessary, as long as it benefits program clarity and/or efficiency. This *modular program design* is the key feature of modern programming design practice. Furthermore, routines can be tested individually, and replaced or rewritten as needed. Before actually writing each routine, a job known in computer circles as the *implementation*, the program's organization can be studied: Will the whole satisfy design specifications? Will the program execute efficiently? As the implementation proceeds, each routine's *interface* is defined: How does it interact with its master—the routine that *called* it—and how are data exchanged between the two? In some most languages, this interface can be *prototyped*: The routine's interface—what it expects and what values it calculates—can be defined and the whole program merged together and compiled to check for consistency without performing *any* calculations. In small programs, where you can have these routine definitions easily fitting onto one page, this prototyping can almost be performed visually. In complex programs, where there may be hundreds or thousands of routines, such prototyping *really* pays off. Once the interfaces begin to form, we ask whether they make sense: Do they exchange information efficiently? Does each routine have the information it needs or should the program be reorganized so that data exchange can be accomplished more efficiently?

From another viewpoint, you should develop a programming style that "hedges your bets:" Programs should be written in such a way that allows their components to be used in a variety of contexts. Again, using a modular programming style, the fundamental components of the calculation should be expressed as a series of subroutines or functions, the interweaving of which is controlled by a main program that reads the input information and produces the output. A modular program can have its components extracted, and used in other programs (program re-use) or interfaced to environments. So-called monolithic programs, which tend not to use routines and express the calculation as a single, long-winded program, should not be written.

We emphasize that this modular design process proceeds *without* actually writing program statements. We use a programming-like language, known as *formal pseudocode*, to express in prose what routines call others and how. This prose might re-express a graphic representation of program organization, such as that shown in Figure 1.2. In addition, expressing the program's design in pseudocode eases the transition to program composition, the actual programming process. The components of formal pseudocode at this point are few:

```
!  This is a comment line in Fortran 90

program  main              ! a program called main
                           ! begin the main program
  print *,"Hello, world"   ! * means default format
end program main           ! end the main program
```

```
// This is a comment line in C++
#include <iostream.h>   // standard input output library

main ()                              // a program called main
                                     // begin the main program
  cout << "Hello, world" << endl ;  // endl means new line
  return 0;                          // needed by some compilers
                                     // end the main program
```

```
%  This is a comment line in MATLAB

function main ()              %  a program called main
                              %  begin the main program
  disp ('Hello, world');      %  display the string
                              %  end the main program
```

Figure 1.3: 'Hello World' Program and Comments in Three Languages

- *comments* that we allow to include the original outline and to describe computational details;
- *functions* that express each routine, whether it be computational or concerned with the user interface;
- *conditionals* that express changing the flow of a program; and
- *loops* that express iteration.

Comments. A comment begins with a comment character, which in our pseudocode we take to be the exclamation point `!`, and ends when the line ends. Comments can consume an entire line or the right portion of some line.

```
! This is a comment: you can read it, but the computer won't
statements
statement ! From the comment character to end of this line is a comment
statements
```

The statements cited in the above lines share the status of the sentence that characterizes most written languages. It is made up of components specific to the syntax of the programming language in use. For example, most programming books begin with a program that does nothing but print "Hello world" on the screen (or other output device). The pseudocode for this might have the following form:

```
! if necessary, include the device library

initiate my program, say main

      send the character string ''Hello world'' to the output device library

terminate my program
```

Figure 1.3 illustrates this in three common languages, beginning with F90. At this point one can now say that they are multi-lingual in computer languages. Here, too, we may note that, unlike the other two languages shown, in Fortran when we begin a specific type of software construct, we almost always explicitly declare where we are ending its scope. Here the construct pair was `program` and `end program`, but the same style holds true for `if` and `end if` pairs, for example. All languages have rules and syntax to terminate the scope of some construct, but when several types of different constructs occur in the same program segment, it may be unclear in which order they are terminating.

Functions. To express a program's organization through its component routines and routines, we use the notation of mathematical *functions*. Each program routine accepts inputs, expressed as arguments of a function, performs its calculations, and returns the computational results as functional values.

```
output_1 = routine (input_1,...,input_m)
```

or


```
call routine (input_1,..., input_m, output_1,..., output_n)
```

In Fortran, a routine evaluating a single output object, as in the first style, is called a *function* and, otherwise, it is called a *subroutine*. Other languages usually use the term function in both cases. Each routines's various inputs and results are represented by *variables*, which, in sharp contrast to mathematical variables, have text-like names that indicate what they contain. These names contain *no* spaces, but may contain several words. There are two conventions for variable names containing two or more words: either words are joined by the underbar character "_" (like `next_generation`) or each word begins with an uppercase letter (like `NextGeneration`). The results of a routines's computation are always indicated by a sequence of variables on the *left* side of the equals sign `=`. The use of an equals sign does not mean mathematical equality; it is a symbol in our pseudocode that means "assign a routines's results to the variables (in order) listed on the left."

Conditionals. To create something other than a sequential execution of routines, conditionals form a test on the values of one or more variables, and continue execution at one point or another depending on whether the test was true or false. That is usually done with the `if` statement. It either performs the instruction(s) that immediately follow (after the `then` keyword) if some condition is valid (like `x > 0`) or those that follow the `else` statement if the condition is not true.

```
if test then
  statement group A ! executed if true
else
  statement group B ! executed if false
end if
```

The test here can be very complicated, but is always based on values of variables. Parentheses should be used to clarify exactly what the test is. For example,

```
((x > 0) and (y = 2))
```

One special statement frequently found in `if` statements is `stop`: This command means to stop or abort the program, usually with a fatal error message.

Conditionals allow the program to execute non-sequentially (the *only* mode allowed by statements). Furthermore, program execution order can be data-dependent. In this way, how the program behaves—what output it produces and how it computes the output—depends on what data, or messages, it is given. *This means that exact statement execution order is determined by the data, and/or messages, and the programmer—not just the programmer.* It is this aspect of programming languages that distinguishes them from written or spoken languages. An analogy might be that chapters in a novel are read in the order specified by the reader's birthday; what that order might be *is* determined by the novelist through logical constructs. The tricky part is that in programming languages, each execution order *must* make sense and not lead to inconsistencies or, at worst, errors: The novel must make sense in all the ways the novelist allows. This data- and message-dependent execution order can be applied at *all* programming levels, from routine execution to statements. Returning to our analogy to the novel, chapter (routine) order and sentence (statement) order depend on the reader's birthday. Such complexity in prose has little utility, but does in programming. How else can a program be written that informs the user on what day of the week and under what phase of the moon she was born given the birth date?

Loops. Looping constructs in our formal pseudocode take the form of *do loops*, where the keyword `do` is paired with the key phrase `end do` to mean that the expressions and routine invocations contained therein are calculated in order (from top to bottom), then calculated again starting with the first, then again, then again, . . . , forever. The loop ceases only when we explicitly exit it with the `exit` command. The pseudocode loop shown below on the left has the execution history shown on the right.

```
do                                          y = routine_1(x)
  y = routine_1(x)                          z = routine_2(y)
  z = routine_2(y)                          x = routine_3(z) [let's say x=-1]
  x = routine_3(z)                          y = routine_1(x)
  if x > 0 then                             z = routine_2(y)
    exit                                    x = routine_3(z) [let's say x=1]
  end if                                    [program ends]
end do
```

Loop	Pseudocode
Indexed loop	`do index=b,i,e` *`statements`* `end do`
Pre-test loop	`while (test)` *`statements`* `end while`
Post-test loop	`do` *`statements`* `if test exit` `end do`

Table 1.1: Pseudocode loop constructs

Infinite loops occur when the Boolean expression always evaluates to true; these are usually not what the programmer intended and represent one type of program error—a "bug."† The constructs enclosed by the loop can be *anything*: statements, logical constructs, and other loops! Because of this variety, programs can exhibit extremely complex behaviors. How a program behaves depends *entirely* on the programmer and how their definition of the program flows based on user-supplied data and messages. The pseudocode loops are defined in Table 1.1.

1.4 Program Composition

Composing a program is the process of expressing or translating the program design into computer language(s) selected for the task. Whereas the program design can often be expressed as a broad outline, each routine's algorithm must be expressed in complete detail. This writing process elaborates the formal pseudocode and contains more explicit statements that more greatly resemble generic program statements.

Generic programming language elements fall into five basic categories: the four we had before—comments, loops, conditionals, and functions—and *statements*. We will expand the variety of comments, conditionals, loops, and functions/subroutines, which define routines and their interfaces. The new element is the statement, the workhorse of programming. It is the statement that actually performs a concrete computation. In addition to expanding the repertoire of programming constructs for formal pseudocode, we also introduce what these constructs are in MATLAB, Fortran, and C++. As we shall see, formal pseudocode parallels these languages; the translation from pseudocode to executable program is generally easy.

1.4.1 Comments

Comments need no further elaboration for pseudocode. However, programmers are encouraged to make heavy use of comments.

1.4.2 Statements

Calculation is expressed by *statements*, which share the structure (and the status) of the sentence that characterizes virtually all written language. Statements that are always executed one after the other as written. A statement in most languages has a simple, well-defined structure common to them all.

```
variable = expression
```

†This term was originated by Grace Hopper, one of the first programmers. In the early days of computers, they were partially built with mechanical devices known as relays. A relay is a mechanical switch that controls which way electric current flows: The realization of the logical construct in programming languages. One day, a previously working program stopped being so. Investigation revealed that an insect had crawled into the computer and had become lodged in a relay's contacts. She then coined the term "bug" to refer not only to such hardware failures, but to software ones as well since the user becomes upset no matter which occurs.

Statements are intended to bear a great resemblance to mathematical equations. This analogy with mathematics can appear confusing to the first-time programmer. For example, the statement `a = a+1`, which means "increment the variable `a` by one" makes perfect sense as a programming statement, but no sense as an algebraic equality since it seems to say that $0 = 1$. Once you become more fluent in programming languages, what is mathematics and what is programming become easily apparent. Statements are said to be *terminated* when a certain character is encountered by the interpreter or the compiler. In Fortran, the termination character is a carriage return or a semicolon (`;`). In C++, *all* statements must be terminated with a semicolon or a comma; carriage returns do *not* terminate statements. MATLAB statements may end with a semicolon '`;`' to suppress display of the calculated expression's value. Most statements in MATLAB programs end thusly.

Sometimes, statements become quite long, becoming unreadable. Two solutions to improve clarity can be used: decompose the expression into simpler expressions or use *continuation markers* to allow the statement to span more than one line of text. The first solution requires you to use intermediate variables, which only results in program clutter. Multiline statements can be broken at convenient arithmetic operators, and this approach is generally preferred. C++ has no continuation character; statements can span multiple text lines, and end only when the semicolon is encountered. In MATLAB, the continuation character sequence comprise three periods '`...`' placed at the end of each text line (before the carriage return or comment character). In Fortran, a statement is continued to the next line when an ampersand & is the last character on the line.

Variables. A *variable* is a named sequence of memory locations to which values can be assigned. As such, every variable has an address in memory, which most languages conceal from the programmer so as to present the programmer with a *storage model* independent of the architecture of the computer running the program. Program variables correspond roughly to mathematical variables that can be integer, real, or, complex-valued. Program variables can be more general than this, being able in some languages to have values equal to a user-defined data type or object which, in turn, contains sequences of other variables. Variables in all languages have *names*: a sequence of alphanumeric characters that cannot begin with a number. Thus, `a`, `A`, `a2`, and `a9b` are feasible variable names (i.e., the interpreter or compiler will not complain about these) while `3d` is not. Since programs are meant to be read by humans as well as interpreters and compilers, such names may not lead to program clarity *even if* they are carefully defined and documented. The compiler/interpreter does not care whether humans can read a program easily or not, but you should: *Use variable names that express what the variables represent.* For example, use `force` as a name rather than `f`; use `i`, `j`, and `k` for indices rather than `ii` or `i1`.

In most languages, variables have *type*: the kind of quantity stored in them. Frequently occurring data types are integer and floating point, for example. Integer variables would be chosen if the variable were only used as an array index; floating point if the variable might have a fractional part.

In addition to having a name, type, and address, each variable has a value of the proper type. The value should be assigned before the variable is used elsewhere. Compilers should indicate an error if a variable is used before it has been assigned a value. Some languages allow variables to have aliases which are usually referred to as "pointers" or "references". Most higher level languages also allow programmers to create "user defined" data types.

Assignment Operator. The symbol = in a statement means *assignment* of the expression into the variable provided on the left. This symbol does not mean algebraic equality; it means that once `expression` is computed, its value is stored in the `variable`. Thus, statements that make programming sense, like `a=a+1`, make no mathematical sense because '`=`' means different things in the two contexts. Fortran 90, and other languages, allow the user to extend the meaning of the assignment symbol (`=`) to other operations. Such advanced features are referred to as "operator overloading".

Expressions. Just as in mathematics, expressions in programming languages can have a complicated structure. Most encountered in engineering programs amount to a mathematical expression involving variables, numbers, and functions of variables and/or numbers. For example the following are all valid statements.

```
A = B
x = sin(2*z)
force = G*mass1*mass2/(r*r)
```

Thus, mathematical expressions obey the usual mathematical conventions, but with one added complexity: Vertical position cannot be used help express what the calculation is; program expressions have only one dimension. For example, the notation $\frac{a}{b}c$ clearly expresses to you how to perform the calculation. However, the one-dimensional equivalent, obtained by smashing this expression onto one line, becomes ambiguous: does a/bc mean divide a by b then multiply by c, or divide a by the product of b and c? This ambiguity is relieved in program expressions in two ways. The first, the human-oriented way, demands the use of parentheses—grouping constructs—to clarify what is being meant, as in $(a/b)c$. The language-oriented way makes use of *precedence rules*: What an expression means is inferred from a set of rules that specify what operations take effect first. In our example, because division is stronger than multiplication, a/bc means $(a/b)c$. Most people find that frequent reliance on precedence rules leads to programs that take a long time to decipher; the compiler/interpreter is "happy" either way.

Expressions make use of the common arithmetic and relational operators. They may also involve function evaluations; the `sin` function was called in the second expression given in the previous example. Programming expressions can be as complicated as the arithmetic or Boolean-algebra ones they emulate.

1.4.3 Flow Control

If a program consisted of a series of statements, statements would be executed one after the other, in the order they were written. Such is the structure of all prose, where the equivalent of a statement is the sentence. Programming languages differ markedly from prose in that statements can be meaningfully executed over and over, with details of each execution differing each time (the value of some variable might be changed), or some statements skipped, with statement ordering dependent on which statements were executed previously or upon external events (the user clicked the mouse). With this extra variability, programming languages can be more difficult for the human to trace program execution than the effort it takes to read a novel. In written languages, sentences can be incredibly complex, much more so than program statements; in programming, the sequencing of statements—*program flow*—can be more complex.

The basic flow control constructs present in virtually all programming languages are *loops* —repetitive execution of a series of statements—and *conditionals*—diversions around statements.

Loops. Historically, the loop has been a major tool in designing the flow control of a procedure and one would often code a loop segment without giving it a second thought. Today massively parallel computers are being widely used and one must learn to avoid coding explicit loops in order to take advantage of the power of such machines. Later we will review which intrinsic tools are included in F90 for use on parallel (and serial) computers to offer improved efficiency over explicit loops.

The loop allows the programmer to repeat a series of statements, with a parameter—the *loop variable*—taking on a different value for each repetition. The loop variable can be an integer or a floating-point number. Loops can be used to control iterative algorithms, such as the Newton-Raphson algorithm for finding solutions to nonlinear equations, to accumulate results for a sequential calculation, or to merely repeat a program phrase, such as awaiting for the next typed input. Loops are controlled by a `logical expression`, which when evaluated to `true` allows the loop another iteration and when false terminates the loop and commences program execution with the statement immediately following those statements enclosed within the loop.

There are three basic kinds of looping constructs, the choice of which is determined by the kind of iterative behavior most appropriate to the computation. The *indexed loop* occurs most frequently in programs. Here, one loop variable varies across a range of values. In pseudocode, the index's value begins at `b`, increments each time through the loop by `i`, and the loop ends when the index exceeds `e`. For example:

```
do j = b, e, i
```

or using the default increment of unity:

```
do j = b, e
```

As an example of an indexed loop, let's explore summing the series of numbers stored in the array `A`. *If* we knew the number of elements in the array when we write the program, the sum can be calculated explicitly without using a loop.

$$\texttt{sum} = A_1 + A_2 + A_3 + A_4$$

However, we have already said that our statements must be on a single line, so we need a way to represent the subscript attached to each number. We develop the convention that a subscript is placed inside parentheses like

```
sum = A(1) + A(2) + A(3) + A(4)
```

Such programs are very inflexible, and this *hard-wired* programming style is discouraged. For example, suppose in another problem the array contains 1,000 elements. With an indexed loop, a more flexible, easier to read program can be obtained. Here, the index assumes a succession of values, its value tested against the termination value *before* the enclosed statements are executed, with the loop terminating once this test fails to be true. The following generic indexed loop also sums array elements, but in a much more flexible, concise way.

```
sum = 0
for i = 1,n
  sum = sum + A(i)
end for
```

Here, the variable `n` does *not* need to be known when the program is written; this value can wait until the program executes, and can be established by the user or after data is read.

In F90 the extensive support for matrix expressions allows *implicit loops*. For example, consider the calculation of $\sum_{i=1}^{N} x_i y_i$. The language provides at least three ways of performing this calculation. Assuming the vectors `x` and `y` are column vectors,

1. ```
   sum_xy = 0
   N = size(x)
   do i = 1,N
      sum_xy = sum_xy + x(i)*y(i)
   end do
   ```

2. ```
   sum_xy = sum(x*y)
   ```

3. ```
   sum_xy = dot_product(x,y)
   ```

The first method is based on the basic loop construct, and yields the slowest running program of the three versions. In fact, avoiding the `do` statement by using implicit loops will almost always lead to faster running programs. The second, and third statements employ intrinsic functions and/or operators designed for arrays. In many circumstances, calculation efficiency and clarity of expression must be balanced. In practice, it is usually necessary to set aside memory to hold subscripted arrays, such as `x` and `y` above, before they can be referenced or used.

Conditionals. Conditionals test the veracity of logical expressions, and execute blocks of statements accordingly (see Table 1.2). The most basic operation occurs when we want to execute a series of statements when a logical expression, say `test`, evaluates to `true`. We call that a simple if conditional; the beginning and end of the statements to be executed when `test` evaluates to `true` are enclosed by special delimiters, which differ according to language. When only one statement is needed, C++ and Fortran allow that one statement to end the line that begins with the if conditional. When you want one group of statements to be executed when `test` is `true` and another set to be executed when `false`, you use the if-else construct. When you want to test a series of logical expressions that are not necessarily complementary, the nested-if construct allows for essentially arbitrarily complex structure to be defined. In such cases, the logical tests can interlock, thereby creating programs that are quite difficult to read. Here is where program comments become essential. For example, suppose you want to sum only the positive numbers less than or equal to 10 in a given sequence. Let's assume the entire sequence is stored in array `A`. In informal pseudocode, we might write

```
loop across A
  if A(i) > 0 and A(i) < = 10 add to sum
end of loop
```

More formally, this program fragment as a complete pseudocode would be

```
sum = 0
```
```

Conditional	Pseudocode
if	`if (test) statement`
if	`if test then` `  `*`statements`* `end if`
if-else	`if test then` `  `*`statements A`* `else` `  `*`statements B`* `end if`
nested if	`if test1 then` `  `*`statements A`* `  if test2 then` `    `*`statements B`* `  end if  % end of test2` `end if`

Table 1.2: Syntax of pseudocode conditionals

```
do i=1,n
  if (A(i) > 0) & (A(i) <= 10)
    sum = sum + A(i)
  end if
end do
```

Several points are illustrated by this pseudocode example. First of all, the statements that can be included with a loop can be arbitrary, comprised of simple statements, loops, and conditionals in any order. This same generality applies to statements within a conditional as well. Secondly, logical expressions can themselves be quite complicated. Finally, note how each level of statements in the program is indented, visually indicated the subordination of statements within higher level loops or conditionals. This stylistic practice lies at the heart of *structured programming*: explicit indication of each statement within the surrounding hierarchy. In modern programming, the structured approach has become the standard because it leads to greater clarity of expression, allowing others to understand the program more quickly and the programmer to find bugs more readily. Employing this style only requires the programmer to use the space key liberally when typing the program. Since sums are computed so often you might expect that a language would provide an intrinsic function to compute it. For F90 and MATLAB you would be correct.

1.4.4 Functions

Functions, which define sub-programs having a well-defined interface to other parts of the program, are an essential part of programming languages. For, if properly developed, these functions can be included in future programs, and they allow several programmers to work on complex programs. The function takes an ordered sequence of messages, objects, or variables as its *arguments*, and *returns* to the calling program a value (or set of values) that can be assigned to an object or variable. Familiar examples of a function are the mathematical ones: the `sin` function takes a real-valued argument, uses this value to calculate the trigonometric sine, and returns that value, which can be assigned to a variable.

```
y = sin(x)
```

Note that the argument need not be a variable: a number can be explicitly provided or an expression can be used. Thus, `sin(2.3)` and `sin(2*cos(x))` are all valid. Functions may require more than one argument. For example, the `atan2` function, which computes the arctangent function in such a way that the quadrant of the calculated angle is unambiguous, needs the `x` and `y` components of the triangle.

```
z = atan2(x, y)
```

Note that the order of the arguments—the `x` component must be the first—and the number of arguments—both `x` and `y` are needed—matter for all functions: The calling program's argument ordering

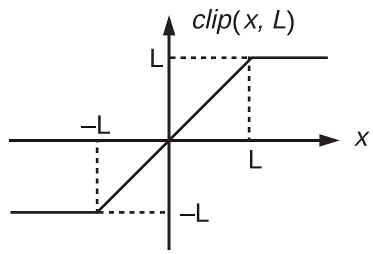


Figure 1.4: Input-output relationship for the function clip(x). So long as $|x| < L$, this function equals its argument; for larger values, the output equals the clipping constant L no matter how large the input might be.

and number must agree with those imposed by the function's definition. Said another way, the interface between the two must agree. Analogous to plugs and electric sockets in the home, a three prong plug won't fit into a two-hole socket, and, if you have a two-prong plug, you must plug it in the right way. A function is usually defined separately, outside the body of any program or other function. We call a program's extent its *scope*. In MATLAB, a program's scope is equivalent to what is in a file; in C and C++, scope is defined by brace pairs; and in Fortran, scope equals what occurs between function declaration and its corresponding `end` statement. Variables are also defined within a program's and a function's scope. What this means is that a variable named `x` defined within a function is available to all statements occurring within that function, and different functions can use the same variable name *without any conflict occurring*. What this means is that two functions `f1` and `f2` can each make use of a variable named `x`, and the value of `x` depends on which function is being referred to. In technical terms, the scope of every variable is limited to its defining function. At first, this situation may seem terribly confusing ("There are two variables both of which are named `x`?"); further thought brings the realization that this convention is what you want. Because each function is to be a routine—a program having a well-defined interface, execution of the function's internal statements must not depend on the program that uses it. This convention becomes especially important when different people write the programs or functions. Thus, such local variables—those defined locally within a function—do not conflict, and they are stored in different memory locations by the compiler or interpreter.

This limited scope convention can be countermanded when you explicitly declare variables to be *global*. Such variables are now potentially available to all functions, and each function cannot define a variable having the same name. For example, you may well want a variable pointedly named `pi` to be available to all functions; you can do so by declaring it to be a global variable. To demonstrate scope, consider the following simple example. Here, we want to clip the values stored in the array `x` and store the results in the array `y`.

Main Pseudocode Program

```
! Clip the elements of an array
limit = 3
do i=1,n
  y(i) = clip(x(i), limit)
end do
```

Function Pseudocode Definition

```
! function clip(x, edge)
! x - input variable
! edge - location of breakpoint
function clip(x, edge)
if abs(x) > edge then
   y = sign(x)*edge
else
   y = x
end if
end
```

The clipping function has the generic form show in Figure 1.4. Thus, values of the argument that are less than L in magnitude are not changed, while those exceeding this limit are set equal to the limiting value. In the program example, note that the name of the array in the calling program—`x`—is the same as the argument's name used in the definition of the function. Within the scope of a program or function, an array and a scalar variable cannot have the same name. In our case, because each variable's scope is limited to the function or program definition, no conflict occurs: Each is well defined and the meaning should be unambiguous. Also note that the second argument has a different name in the program that in the function. No matter how the arguments are defined, we say that they are *passed* to the function, with the function's variables set equal to values specified in the calling program. These interface rules allows the function to be used in other programs, which means that we can reuse functions whenever we like!

1.4.5 Modules

Another important programming concept is that of packaging a group of related routines and/or selective variables into a larger programming entity. In the Ada language they are called *packages*, while C++ and MATLAB call them *classes*. F90 has a generalization of this concept that it calls a *module*. As we will see later the F90 module includes the functionality of the C++ classes, as well as other uses such as defining global constants. Therefore, we will find the use of F90 modules critical to our object-oriented programming goals. In that context modules provide us with the means to take several routines related to a specific data type and to encapsulate them into a larger programming unit that has the potential to be reused for more than one application.

1.4.6 Dynamic Memory Management

From the very beginning, several decades ago, there was a clear need to be able to dynamically allocate and deallocate segments of memory for use by a program. The initial standards for Fortran did not allow for this. It was necessary to invoke machine language programs to accomplish that task or to write tools to directly manage arrays by defining "pseudo-pointers" to manually move things around in memory or to overwrite space that was no longer needed. It was very disappointing that the F77 standard failed to offer that ability, although several "non-standard" compilers offered such an option. Beginning with the F90 standard a full set of dynamic memory management abilities is now available within Fortran. Dynamic memory management is mainly needed for arrays and pointers. Both of these will be considered late, with a whole chapter devoted to arrays. Both of these entities can be declared as ALLOCATABLE and later one will ALLOCATE and then DEALLOCATE them. There are also new "automatic arrays" that have the necessary memory space supplied and then freed as needed.

Pointers are often used in "data structures", abstract data types, and objects. To check on the status of such features one can invoke the ALLOCATED intrinsic and use ASSOCIATED to check on the status of pointers and apply NULLIFY to pointers that need to be freed or initialized. Within F90 allocatable arrays cannot be used in the definitions of derived types, abstract data types, or objects. However, allocatable pointers to arrays can be used in such definitions. To assist in creating efficient executable codes, entities that might be pointed at by a pointer must have the TARGET attribute.

Numerous examples of dynamic memory management will be seen later. Persons that write compilers suggest that, in any language, it is wise to deallocate dynamic memory in the reverse order of its creation. The F90 language standard does not require that procedure but you see that advice followed in most of the examples.

1.5 Program evaluation and testing

Your fully commented program, written with the aid of an *editor*, must now come alive and be translated into another language that more closely matches computer instructions; it must be *executed* or *run*. Statements expressed in MATLAB, Fortran, or C++ may not directly correspond to computational instructions. However, the Fortran syntax was designed to more clearly match mathematical expressions. These languages are designed to allow humans to define computations easily and also allow easy translation. Writing programs in these languages provides some degree of *portability*: A program can be executed on very different computers without modification. So-called *assembly languages* allow more direct expression of program execution, but are very computer specific. Programmers that write in assembly language must worry about the exquisite details of computer organization, so much so that writing of what the computation is doing takes much longer. What they produce might run more rapidly that the same computation expressed in Fortran, for example, but no portability results and programs become incredibly hard to debug.

Programs become executable machine instructions in two basic ways. They are either *interpreted* or *compiled*. In the first case, an interpreter reads your program and translates it to executable instructions "on the fly." Because interpreters essentially examine programs on a line-by-line basis, they usually allow instructions accept typed user instructions as well as fully written programs. MATLAB is an example of an interpreter.† It can accept typed commands created as the user thinks of them (plot a graph, see that a parameter must have been typed incorrectly, change it, and replot, for example) or entire programs. Because interpreters examine programs locally (line-by-line), program execution tends to be slower than when a compiler is used.

Compilers are programs that take your program in its entirety and produce an executable version of it. Compiler output is known as an *executable* file that, in UNIX for example, can become a command essentially indistinguishable from others that are available. C++ is an example of a language that is frequently compiled rather than interpreted. Compilers will produce much more efficient (faster running) programs than interpreters, but if you find an error, you must edit and re-compile before you can attempt execution again. Because compilation takes time, this cycle can be time-consuming if the program is large.

Interpreters are themselves executable files written in compiled languages: MATLAB is written in C. Executable programs produced by compilers are stand-alone programs: *Everything*—user input and output, file reading, etc.—must be handled by the user's program. In an interpreter, you can supplement a program's execution by typed instructions. For example, in an interpreter you can type a simple command to make the variable `a` equal to 1; in a compiled program, you must include a program that asks for the value of `a`. Consequently, users frequently write programs in the context of an interpreter, understand how to make the program better by interacting with it, and then re-express it in a compiled language.

Both interpreters and compilers make extensive use of what are known as *library* commands or functions. A natural example of a library function is the `sin` function: Users typically do not want to program explicitly the computation of the trigonometric sine function. Instead, they want to be able to pull it "off the shelf" and use as need be. Library modules are just programs written in a computer language like you would write. Consequently, both interpreters and compilers allow user programs to become part of the library, which is usually written by many programmers over a long period of time. It is through modules available in a library that programming teams cooperate. Library modules tend to be more extensive and do more things in an interpreter. For example, MATLAB provides a program that produces pseudo-three-dimensional plots of functions. Such routines usually do not come with a compiler, but may be purchased separately from graphics programming specialists. For compiled languages, we refer to *linking* the library routines to the user's program (in interpreters, this happens as a matter of course). A linker is a program that takes modules produced by the compiler, be they yours or others, associates the modules, and produces the executable file we mentioned earlier. Most C++ compilers "hide" the linking step from you; you may think you are typing just the command to compile the program, but it is actually performing that step for you. When you are compiling a module not intended for stand-alone execution, a compiler option that you type can prevent the compiler from performing the linking step.

Debugging is the process of discovering and removing program errors. Two main types of errors occur in writing programs: what we would generally term "typos" and what are design errors. The first kind may be readily found (where is the function `sni`?) or more subtle (you type `aa` instead of `a` for a variable's name and `aa` also exists!). The second kind of error can be hard or subtle to find. The main components of this process are

1. Search the program module by eye as you do a "mental run through" of its task. This kind of error searching begins when you first think about program organization, and continues as you refine the program. Why write a program that is logically flawed?

2. If written in a compiled language, compile the program to find syntax errors or warnings about unused or undefined variables. If in an interpreted language, attempt preliminary execution to obtain similar error messages. Linking also can locate modules or libraries that are improperly referenced.

3. Running the executable file with typical data sets often causes the program to abort—a harsh word that expresses the situation where the program goes crazy and ceases to behave—and the system to supply an error message, such as division by zero. Error messages *may* help locate the programming error.

†This statement is only partially true. MATLAB does have some features of a compiler, like looking ahead to determine if interface errors exist with respect to functions called by the main program.

Easy errors to find are *syntactic* errors: You have violated the language's rules of what a well-formed program must be. Usually, the interpreter or compiler complain bitterly on encountering a syntax error. Compilers find these at compile time (when the program is compiled), interpreters at run time. Design errors are only revealed when we supply the program with data. The programmer should design test data that exercises each of the program's valid operations. Invalid user input (asking for the logarithm of a negative number, for example) should be caught by the program and warning messages sent to the user.

The previous description of generic programming languages indicates why finding bugs can be quite complicated. Programs can exhibit quite complex behaviors, and tracing incorrect behaviors can be correspondingly difficult. One often hears the (true) statement "Computers do what we say, not what we want." Users frequently want computers to be smart, fixing obvious design (mental) errors because they obviously conflict with what we want. However, this situation is much like what the novelist faces. Inexact meaning can confuse the reader; he or she does not have a direct pathway to the novelist's mind. As opposed to the novelist, extensive testing of your program can detect such errors and make your program approach perfection. Many operating systems supply interactive *debugger* programs that can trace the execution of a program in complete detail. They can display the values of any variable, stop at selected positions for evaluation, execute parts of the code in a statement-by-statement fashion, etc. These can be very helpful in finding difficult-to-locate bugs, but they still cannot read your mind.

Be that as it may, what can the programmer do when the program compiles (no syntactic errors), doesn't cause system error messages (no dividing by zero), but the results are ***not*** correct? The simplest approach is to include extra statements in your program, referred to as debugging statements, that display (somewhat verbosely) values of internal variables. For example, in a loop you would print the value of the loop index and all variables that the loop might be affecting. Because this output can be voluminous, the most fruitful approach is to debug smaller problems. With this debugging information, you can usually figure out the error, correct it, *and* change the comments accordingly. Without the latter, your program and your internal documentation are out-of-sync.

Once debugged, you could delete the debugging statements you added. A better approach is to just hide them. You can do this two ways: Comment them out or encase them in a conditional that is true when the program is in "debugging mode." The commenting approach completely removes the debugging statements from the program execution stream, and allows you to easily put them back if further program elaborations result in errors. The use of conditionals does put an overhead on computational efficiency, but usually a small one.

1.6 Program documentation

Comments inside a program are intended to help you and others understand program design and how it is organized. Frequently, comments describe what each variable means, how program execution is to proceed, and what each module's interface might be (what are the expected inputs and their formats, and what outputs are produced). Program comments occur in the midst of the program's source, and temporarily interrupts the highly restricted syntax of most programming languages. Comments are entirely ignored by the interpreter or compiler, and are allowed to enhance program clarity for humans.

Documentation includes program comments, but also includes external prose that describes what the program does, how the user interface controls program behavior, and how the display of results means. Making an executable program available to users does not help them understand how to use it. In UNIX, *all* provided commands are accompanied by what are referred to as *manual pages*: concise descriptions of what the program does, all user options, and descriptions of what error messages means. *Programs are useless without such documentation.* Many programs provide such documentation whenever the user types something that clearly indicates a lack of knowledge about how to use the program. This kind of documentation must also be supplemented by prose that a user can read. Professional programmers frequently write the documentation as the program is being designed. This simultaneous development of the program and documentation of how it is used often uncovers user interface design flaws.

1.7 Object Oriented Formulations

The above discussion of subprograms follows the older programming style where the emphasis is placed on the procedures that a subprogram is to apply to the supplied data. Thus, it is referred to as *procedural programming*. The alternate approach focuses on the data and its supporting functions, and is known as an *object oriented* approach and is the main emphasis of this work. It also generalizes the concept of data types and is usually heavily dependent on user defined data types and their extension to abstract data types. These concepts are sketched in Fig. 1.5.

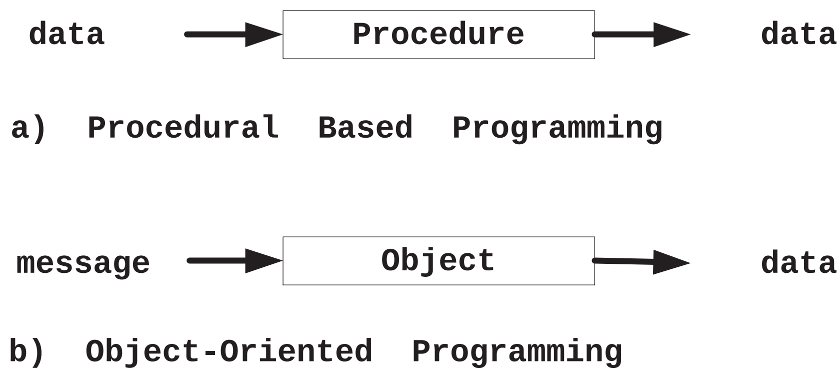


Figure 1.5: Two Approaches to Programming

The process or creating an "object-oriented" (OO) formulation involves at least three stages: Object-Oriented Analysis (OOA), Object-Oriented Design (OOD), and Object-Oriented Programming (OOP). Many books have been written on each of these three subjects. Formal graphical standards for representing the results of OOA and OOD have been established and are widely used in the literature. Here the main emphasis will be placed on OOP on the assumption that the two earlier stages have been completed. In an effort to give some level of completeness, summaries of OOA and OOD procedures are given in Tables 1–1 and 1–2, respectively. Having completed OOA and OOD studies one must select a language to actually implement the design. More than 100 objected-oriented languages are in existence and use today. They include "pure" OO languages like Crisp, Eiffel, Rexx, Simula, Smalltalk, etc. and "hybrid" OO languages like C++ , F90 , Object Pascal, etc. In which of them should you invest your time? To get some insight into answers to this question we should study the advice of some of the recognized leaders in the field. In his 1988 book on OO software construction B. Myers listed seven steps necessary to achieve object-orientedness in an implementation language. They are summarized in Table 1-3 and are all found to exist in F90 and F95 . Thus we proceed with F90 as our language of choice. The basic F90 procedures for OOP will be illustrated in some short examples in Chapter 3 after covering some preliminary material on abstract data types in Chapter 2. Additional OOP applications will also be covered in later chapters.

Table 1–1. OO Analysis Summary

Find objects and classes :

- Create an abstraction of the problem domain.
- Give attributes, behaviors, classes, and objects meaningful names.
- Identify structures pertinent to the system's complexity and responsibilities.
- Observe information needed to interact with the system, as well as information to be stored.
- Look for information re-use; are there multiple structures; can sub-systems be inherited?

Define the attributes :

- Select meaningful names.
- Describe the attribute and any constraints.
- What knowledge does it possess or communicate?
- Put it in the type or class that best describes it.
- Select accessibility as public or private.
- Identify the default, lower and upper bounds.
- Identify the different states it may hold.
- Note items that can either be stored or re-computed.

Define the behavior :

- Give the behaviors meaningful names.
- What questions should each be able to answer?
- What services should it provide?
- Which attribute components should it access?
- Define its accessibility (public or private).
- Define its interface prototype.
- Define any input/output interfaces.
- Identify a constructor with error checking to supplement the intrinsic constructor.
- Identify a default constructor.

Diagram the system :

- Employ an OO graphical representation such as the Coad/Yourdon method or its extension by Graham.

Table 1–2. OO Design Summary

- Improve and add to the OOA results during OOD.
- Divide the member functions into constructors, accessors, agents and servers.
- Design the human interaction components.
- Design the task management components.
- Design the data management components.
- Identify operators to be overloaded.
- Identify operators to be defined.
- Design the interface prototypes for member functions and for operators.
- Design code for re-use through “kind of” and “part of” hierarchies.
- Identify base classes from which other classes are derived.
- Establish the exception handling procedures for all possible errors.

Table 1–3. 7 Steps to Object-Orientedness (B. Myer, 1988)

1. Object-based modular structure :
   - Systems are modularized on the basis of their data structure (in F90).
2. Data Abstraction :
   - Objects should be described as implementations of abstract data types (in F90).
3. Automatic memory management :
   - Unused objects should be deallocated by the language system (most in F90, in F95).
4. Classes :
   - Every non-simple type is a module, and every high-level module is a type (in F90).
5. Inheritance :
   - A class may be defined as an extension or restriction of another (in F90).
6. Polymorphism and dynamic binding :
   - Entities are permitted to refer to objects of more than one class and operations can have different realizations in different classes (partially in F90/F95, expected in Fortran 2000).
7. Multiple and repeated inheritance :
   - Can declare a class as heir to more than one class, and more than once to the same class (in F90).

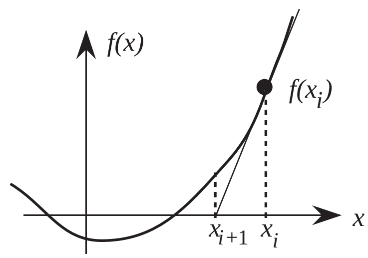
1.8 Exercises

1 Checking trigonometric identities

We know that the sine and cosine functions obey the trigonometric identity $\sin^2\theta + \cos^2\theta = 1$ no matter what value of θ is used. Write a pseudocode, or MATLAB , or F90 program that checks this identity. Let it consist of a loop that increments across N equally spaced angles between 0 and π, and calculates the quantity in question, printing the angle and the result. Test your program for several values of N. (Later we will write a second version of this program that does not contain *any* analysis loops, using instead MATLAB's, or F90's, ability to calculate functions of arrays.)

2 Newton-Raphson algorithm

A commonly used numerical method of solving the equation $f(x) = 0$ has its origins with the beginnings of calculus. Newton noted that the slope of a function tended to cross the x-axis near a function's position of zero value (called a *root*).



Because the function's slope at some point x_i equals its derivative $f'(x_i)$, the equation of the line passing through $f(x_i)$ is $f'(x_i)x + \big(f(x_i) - f'(x_i)x_i\big)$. Solving for the case when this expression equals the next trial root x_{i+1}.

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

The algorithm proceeds by continually applying this iterative equation until the error is "small." The definition of "small" is usually taken to mean that the absolute relative difference between successive iterates is less than some tolerance value ϵ. (Raphson extended these concepts to an array of functions.)

(a) In pseudocode, write a program that performs the Newton-Raphson algorithm. Assume that functions that evaluate the function and its derivative are available. What is the most convenient form of loop to use in your program?

(b) Translate your pseudocode into F90, or MATLAB, and apply your program to the simple function $f(x) = e^{2x} - 5x - 1$. Use the functional expressions directly in your program or make use of functions.

3 Game of Life pseudocode

Develop a pseudocode outline for the main parts of the "Game of Life" which was discussed earlier and shown in Fig. 1.3. Include pseudocode for a function to compute the next generation.

Chapter 2

Data Types

Any computer program is going to have to operate on the available data. The valid data types that are available will vary from one language to another. Here we will examine the intrinsic or built-in data types, user-defined data types or structures and, finally, introduce the concept of the abstract data type which is the basic foundation of object-oriented methods. We will also consider the precision associated with numerical data types. The Fortran data types are listed in Table 2–1. Such data can be used as constants, variables, pointers and targets.

Table 2–1. F90/95 Data Types and Pointer Attributes

```
                                Data Option
                        _____________________________
                        |                           |
                    Intrinsic                     Derived
                        |               [Components of intrinsic type and/or
                        |               previously declared derived types.]
                        |
 _______________________
 |            |         |
 Character    Logical   Numeric
                          |
                ______________________________
                |                            |
         Floating Point                   Integer
                |                   (Default Precision)
                |                    Selected-Int-Kind
                |
 _________________________________________________
 |                      |                       |
 Complex                Real                    Double Precision
 (Default Precision)    (Default Precision)         [Obsolete]
 Selected-Real-Kind's    Selected-Real-Kind
```

2.1 Intrinsic Types

The simplest data type is the `LOGICAL` type which has the Boolean values of either `.true.` or `.false.` and is used for relational operations. The other non-numeric data type is the `CHARACTER`. The sets of valid character values will be defined by the hardware system on which the compiler is installed. Character sets may be available in multiple languages, such as English and Japanese. There are international standards for computer character sets. The two most common ones are the English character sets defined in the ASCII and EBCDIC standards that have been adapted by the International Standards Organization (ISO). Both of these standards for defining single characters include the digits (0 to 9), the 26 upper case letters (A to Z), the 26 lower case letters (a to z), common mathematical symbols, and many non-printable codes known as control characters. We will see later that strings of characters are still referred to as being of the `CHARACTER` type, but they have a length that is greater than one. In other languages such a data type is often called a *string*. [While not part of the F95 standard, the ISO Committee created a user-defined type known as the `ISO_VARIABLE_LENGTH_STRING` which is available as a F95 source module.]

For numerical computations, numbers are represented as integers or decimal values known as *floating point numbers* or *floats*. The former is called an INTEGER type. The decimal values supported in Fortran are the REAL and COMPLEX types. The range and precision of these three types depends on the hardware being employed. At the present, 1999, most computers have 32 bit processors, but some offer 64 bit processors. This means that the precision of a calculated result from a single program could vary from one brand of computer to another. One would like to have a portable precision control so as to get the same answer from different hardware; whereas some languages, like C++, specify three ranges of precision (with specific bit widths). Fortran provides default precision types as well as two functions to allow the user to define the "kind" of precision desired.

Table 2–2. Numeric Types on 32 Bit Processors

Type	*Bit Width*	*Significant Digits*	*Common Range*
integer	16	10	–32,768 to 32,767
real	32	6	-10^{37} to 10^{37}
double precision†	64	15	-10^{307} to 10^{307}
complex	2@32	2@6	two reals

†obsolete in F90, see selected_real_kind

Still, it is good programming practice to employ a precision that is of the default, double, or quad precision level. Table 2–2 lists the default precisions for 32 bit processors. The first three entries correspond to types *int*, *float*, and *double*, respectively, of C++. Examples of F90 integer constants are

```
–32      0      4675123      24_short      24_long
```

while typical real constant examples are

```
–3.      0.123456      1.234567e+2      0.0      0.3_double
7.6543e+4_double       0.23567_quad    0.3d0
```

In both cases, we note that it is possible to impose a user-defined precision kind by appending an underscore (_) followed by the name of the integer variable that gives the precision kind number. For example, one could define

```
long = selected_int_kind(9)
```

to denote an integer in the range of -10^9 to 10^9, while

```
double = selected_real_kind(15,307)
```

defines a real with 15 significant digits with an exponent range of ± 307. Likewise, a higher precision real might be defined by the integer kind

```
quad = selected_real_kind(18,4932)
```

to denote 18 significant digits over the exponent range of ± 4932. If these kinds of precision are available on your processors, then the F90 types of "integer (long)," "real (double)," and "real (quad)" would correspond to the C++ precision types of "long int," "double," and "long double," respectively. If the processor cannot produce the requested precision, then it returns a negative number as the integer kind number. Thus, one should always check that the kind (i.e., the above integer values of long, double, or quad) is not negative, and report an exception if it is negative.

The old F77 intrinsic type of DOUBLE PRECISION has been declared obsolete, since it is now easy to set any level of precision available on a processor. Another way to always define a double precision real on any processor is to use the "kind" function such as

```
double = kind(1.0d0)
```

where the symbol 'd' is used to denote the I/O of a double precision real. For completeness it should be noted that it is possible on some processors to define different kinds of character types, such as "greek" or "ascii", but in that case, the kind value comes before the underscore and the character string such as: ascii_"a string".

```
[ 1]  Module Math_Constants     ! Define double precision math constants
[ 2]   implicit none
[ 3]   ! INTEGER, PARAMETER :: DP = SELECTED_REAL_KIND (15,307)
[ 4]     INTEGER, PARAMETER :: DP = KIND (1.d0) ! Alternate form
[ 5]  real(DP), parameter:: Deg_Per_Rad  = 57.295779513082320876798155_DP
[ 6]  real(DP), parameter:: Rad_Per_Deg  = 0.017453292519943295769237_DP
[ 7]
[ 8]  real(DP), parameter:: e_Value      =  2.71828182845904523560287_DP
[ 9]  real(DP), parameter:: e_Recip      =  0.3678794411714423215955238_DP
[10]  real(DP), parameter:: e_Squared    =  7.389056098930650227230427_DP
[11]  real(DP), parameter:: Log10_of_e  =  0.4342944819032518276511289_DP
[12]
[13]  real(DP), parameter:: Euler        =  0.5772156649015328606_DP
[14]  real(DP), parameter:: Euler_Log    = -0.5495393129816448223_DP
[15]  real(DP), parameter:: Gamma        =  0.577215664901532860606512_DP
[16]  real(DP), parameter:: Gamma_Log    = -0.549539312981644822337662_DP
[17]  real(DP), parameter:: Golden_Ratio =  1.618033988749894848_DP
[18]
[19]  real(DP), parameter:: Ln_2         =  0.6931471805599453094172321_DP
[20]  real(DP), parameter:: Ln_10        =  2.3025850929940456840179915_DP
[21]  real(DP), parameter:: Log10_of_2  =  0.3010299956639811952137389_DP
[22]
[23]  real(DP), parameter:: pi_Value     =  3.141592653589793238462643_DP
[24]  real(DP), parameter:: pi_Ln        =  1.144729885849400174143427_DP
[25]  real(DP), parameter:: pi_Log10     =  0.4971498726941338543512683_DP
[26]  real(DP), parameter:: pi_Over_2   =  1.570796326794896619231322_DP
[27]  real(DP), parameter:: pi_Over_3   =  1.047197551196597746154214_DP
[28]  real(DP), parameter:: pi_Over_4   =  0.7853981633974483096156608_DP
[29]  real(DP), parameter:: pi_Recip     =  0.3183098861837906715377675_DP
[30]  real(DP), parameter:: pi_Squared   =  9.869604401089358618834491_DP
[31]  real(DP), parameter:: pi_Sq_Root  =  1.772453850905516027298167_DP
[32]
[33]  real(DP), parameter:: Sq_Root_of_2 =  1.4142135623730950488_DP
[34]  real(DP), parameter:: Sq_Root_of_3 =  1.7320508075688772935_DP
[35]
[36]  End Module Math_Constants
[37]
[38]  Program Test
[39]    use Math_Constants                   ! Access all constants
[40]    real :: pi                            ! Define local data type
[41]    print *, 'pi_Value: ', pi_Value      ! Display a constant
[42]    pi = pi_Value; print *, 'pi = ', pi  ! Convert to lower precision
[43]  End Program Test                      ! Running gives:
[44]    ! pi_Value: 3.1415926535897931      ! pi = 3.14159274
```

Figure 2.1: Defining Global Double Precision Constants

To illustrate the concept of a defined precision intrinsic data type, consider a program segment to make available useful constants such as *pi* (3.1415. . .) or Avogadro's number $(6.02\ldots\times 10^{23})$. These are real constants that should not be changed during the use of the program. In F90, an item of that nature is known as a `PARAMETER`. In Fig. 2.1, a selected group of such constants have been declared to be of double precision and stored in a `MODULE` named `Math_Constants`. The parameters in that module can be made available to any program one writes by including the statement "`use math_constants`" at the beginning of the program segment. The figure actually ends with a short sample program that converts the tabulated value of *pi* (line 23) to a default precision real (line 42) and prints both.

2.2 User Defined Data Types

While the above intrinsic data types have been successfully employed to solve a vast number of programming requirements, it is logical to want to combine these types in some structured combination that represents the way we think of a particular physical object or business process. For example, assume we wish to think of a chemical element in terms of the combination of its standard symbol, atomic number and atomic mass. We could create such a data structure type and assign it a name, say `chemical_element`, so that we can refer to that type for other uses just like we might declare a real variable. In F90 we would define the structure with a `TYPE` construct as shown below (in lines 3–7):

```
[ 1]  program create_a_type
[ 2]  implicit none
[ 3]    type chemical_element              ! a user defined data type
[ 4]      character (len=2) :: symbol
[ 5]      integer           :: atomic_number
[ 6]      real              :: atomic_mass
```

```
[ 7]    end type
```

Having created the new data type, we would need ways to define its values and/or ways to refer to any of its components. The latter is accomplished by using the component selection symbol "%". Continuing the above program segment we could write:

```
[ 8]    type (chemical_element) :: argon, carbon, neon    ! elements
[ 9]    type (chemical_element) :: Periodic_Table(109)     ! an array
[10]    real                    :: mass                    ! a scalar
[11]
[12]    carbon%atomic_mass   = 12.010          ! set a component value
[13]    carbon%atomic_number = 6               ! set a component value
[14]    carbon%symbol        = "C"             ! set a component value
[15]
[16]    argon = chemical_element ("Ar", 18, 26.98) ! construct element
[17]
[18]    read *, neon                              ! get "Ne" 10 20.183
[19]
[20]    Periodic_Table( 5) = argon         ! insert element into array
[21]    Periodic_Table(17) = carbon        ! insert element into array
[22]    Periodic_Table(55) = neon          ! insert element into array
[23]
[24]    mass = Periodic_Table(5) % atomic_mass     ! extract component
[25]
[26]    print *, mass                       ! gives 26.9799995
[27]    print *, neon                       ! gives Ne 10 20.1830006
[28]    print *, Periodic_Table(17)         ! gives C  6  12.0100002
[29]  end program create_a_type
```

In the above program segment, we have introduced some new concepts:

- define argon, carbon and neon to be of the `chemical_element` type (line 7).
- define an array to contain 109 `chemical_element` types (line 8).
- used the selector symbol, %, to assign a value to each of the components of the carbon structure (line 15).
- used the intrinsic "structure constructor" to define the argon values (line 15). The intrinsic construct or initializer function must have the same name as the user-defined type. It must be supplied with all of the components, and they must occur in the order that they were defined in the `TYPE` block.
- read in all the neon components, in order (line 17). [The '*' means that the system is expected to automatically find the next character, integer and real, respectively, and to insert them into the components of `neon`.]
- inserted argon, carbon and neon into their specific locations in the periodic table array (lines 19–21).
- extracted the `atomic_mass` of argon from the corresponding element in the `periodic_element` array (line 23).
- print the real variable, `mass` (line 25). [The '*' means to use a default number of digits.]
- printed all components of neon (line 26). [Using a default number of digits.]
- printed all the components of carbon by citing its reference in the periodic table array (line 27). [Note that the printed real value differs from the value assigned in line 12. This is due to the way reals are represented in a computer, and will be considered elsewhere in the text.]

A defined type can also be used to define other data structures. This is but one small example of the concept of code re-use. If we were developing a code that involved the history of chemistry, we might use the above type to create a type called *history* as shown below.

```
type (chemical_element)   :: oxygen

type history                      ! a second type using the first
  character (len=31)       :: element_name
  integer                  :: year_found
  type (chemical_element)  :: chemistry
```

```
end type history
type (history) :: Joseph_Priestley                  ! Discoverer
oxygen = chemical_element ("O", 76, 190.2)   ! construct element
Joseph_Priestley = history ("Oxygen", 1774, oxygen)  ! construct
print *, Joseph_Priestley ! gives Oxygen 1774 O 76 1.9020000E+02
```

Shortly we will learn about other important aspects of user-defined types, such as how to define operators that use them as operands.

2.3 Abstract Data Types

Clearly, data alone is of little value. We must also have the means to input and output the data, subprograms to manipulate and query the data, and the ability to define operators for commonly used procedures. The coupling or encapsulation of the data with a select group of functions that defines everything that can be done with the data type introduces the concept of an abstract data type (ADT). An ADT goes a step further in that it usually hides from the user the details of how functions accomplish their tasks. Only knowledge of input and output interfaces to the functions are described in detail. Even the components of the data types are kept private.

The word *abstract* in the term *abstract data type* is used to: 1) indicate that we are interested only in the essential features of the data type, 2) to indicate that the features are defined in a manner that is independent of any specific programming language, and 3) to indicate that the instances of the ADT are being defined by their behavior, and that the actual implementation is secondary. An ADT is an abstraction that describes a set of items in terms of a hidden or encapsulated data structure and a set of operations on that data structure.

Previously we created user-defined entity types such as the `chemical_element`. The primary difference between entity types and ADTs is that all ADTs include methods for operating on the type. While entity types are defined by a name and a list of attributes, an ADT is described by its name, attributes, encapsulated methods, and possibly encapsulated rules.

Object-oriented programming is primarily a data abstraction technique. The purpose of abstraction and data hiding in programming is to separate behavior from implementation. For abstraction to work, the implementation must be encapsulated so that no other programming module can depend on its implementation details. Such encapsulation guarantees that modules can be implemented and revised independently. Hiding of the attributes and some or all of the methods of an ADT is also important in the process. In F90 the `PRIVATE` statement is used to hide an attribute or a method; otherwise, both will default to `PUBLIC`. Public methods can be used outside the program module that defines an ADT. We refer to the set of public methods or operations belonging to an ADT as the public interface of the type.

The user-defined data type, as given above, in F90 is not an ADT even though each is created with three intrinsic methods to construct a value, read a value, or print a value. Those methods cannot modify a type; they can only instantiate the type by assigning it a value and display that value. (Unlike F90, in C or C++ a user-defined type, or “struct”, does not have an intrinsic constructor method, or input/output methods.) Generally ADTs will have methods that modify or query a type’s state or behavior.

From the above discussion we see that the intrinsic data types in any language (such as complex, integer and real in F90) are actually ADTs. The system has hidden methods (operators) to assign them values and to manipulate them. For example, we know that we can multiply any one of the numerical types by any other numerical type.

We do not know how the system does the multiplication, and we don’t care. All computer languages provide functions to manipulate the intrinsic data types. For example, in F90 a square root function, named *sqrt*, is provided to compute the square root of a real or complex number. From basic mathematics you probably know that two distinctly different algorithms must be used and the choice depends on the type of the supplied argument. Thus, we call the *sqrt* function a generic function since its single name, *sqrt*, is used to select related functions in a manner hidden from the user. In F90 you can not take the square root of an integer; you must convert it to a real value and you receive back a real answer. The

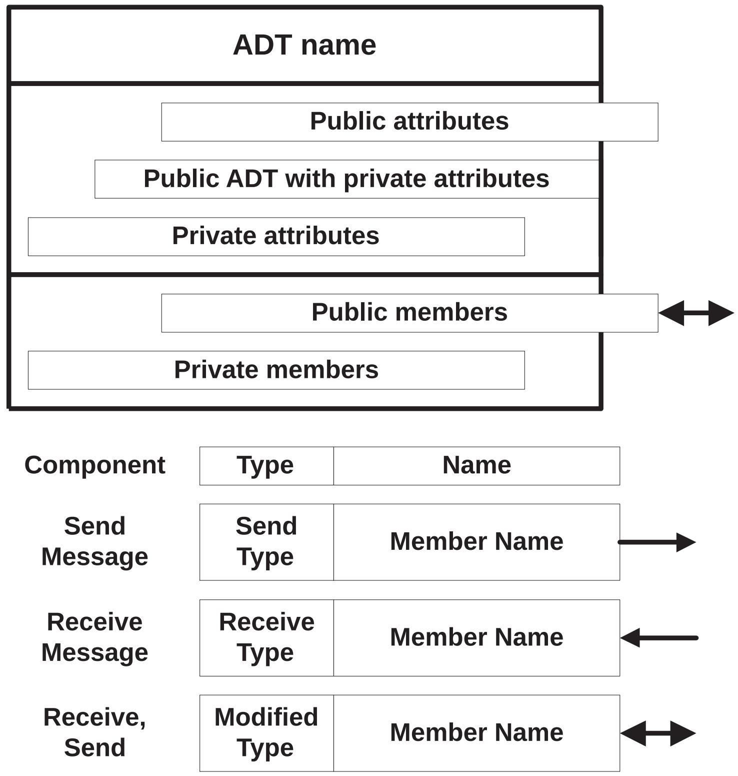


Figure 2.2: Graphical Representation of ADTs

above discussions of the methods (routines) that are coupled to a data type and describe what you can and can not do with the data type should give the programmer good insight into what must be done to plan and implement the functions needed to yield a relatively complete ADT.

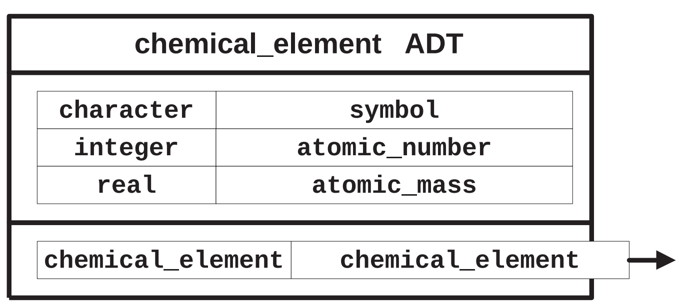


Figure 2.3: Representation of the Public Chemical_Element ADT

It is common to have a graphical representation of the ADTs and there are several different graphical formats suggested in the literature. We will use the form shown in Fig. 2.4 where a rectangular box begins with the ADT name and is followed by two partitions of that box that represent the lists of attribute data and associated member routines. Items that are available to the outside world are in sub-boxes that cross over the right border of the ADT box. They are the parts of the public interface to the ADT. Likewise those items that are strictly internal, or private, are contained fully within their respective partitions of the ADT box. There is a common special case where the name of the data type itself is available for external use, but its individual attribute components are not. In that case the right edge of the private attributes lists lie on the right edge of the ADT box. In addition, we will often segment the smallest box for an item to give its type (or the most important type for members) and the name of the item. Public member boxes are also supplemented with an arrow to indicate which take in information (<--), or send out information (-->). Such a graphical representation of the previous `chemical_element` ADT, with all its items public, is shown in Fig. 2.4.

The sequence of numbers known as Fibonacci numbers is the set that begins with one and two and where the next number in the set is the sum of the two previous numbers (1, 2, 3, 5, 8, 13, ...). A primarily private ADT to print a list of Fibonacci numbers up to some limit is represented graphically in Fig. 2.5.

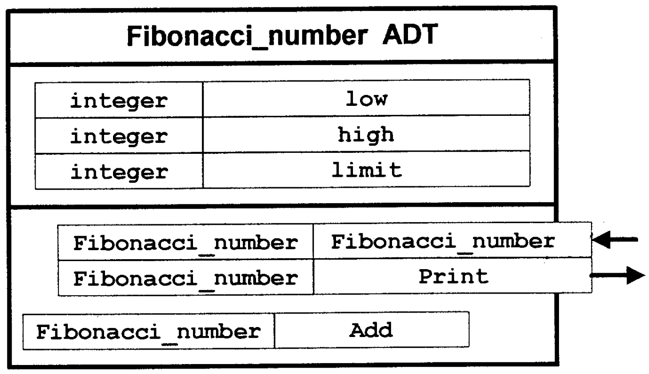


Figure 2.4: Representation of a Fibonacci_Number ADT

2.4 Classes

A class is basically the extension of an ADT by providing additional member routines to serve as *constructors*. Usually those additional members should include a *default constructor* which has no arguments. Its purpose is to assure that the class is created with acceptable default values assigned to all its data attributes. If the data attributes involve the storage of large amounts of data (memory) then one usually also provides a *destructor* member to free up the associated memory when it is no longer needed. F95 has an automatic deallocation feature which is not present in F90 and thus we will often formally deallocate memory associated with data attributes of classes.

As a short example we will consider an extension of the above Fibonacci_Number ADT. The ADT for Fibonacci numbers simply keeps up with three numbers (low, high, and limit). Its intrinsic initializer has the (default) name Fibonacci. We generalize that ADT to a class by adding a constructor named new_Fibonacci_number. The constructor accepts a single number that indicates how many values in the infinite list we wish to see. It is also a default constructor because if we omit the one optional argument it will list a minimum number of terms set in the constructor. The graphical representation of the Fibonacci_Number class extends Fig. 2.4 for its ADT by at least adding one public constructor, called new_Fibonacci_number, as shown in Fig. 2.5. Technically, it is generally accepted that a constructor should only be able to construct a specific object once. This differs from the intrinsic initializer which could be invoked multiple times to assign different values to a single user-defined type. Thus, an additional logical attribute has been added to the previous ADT to allow the constructor, new_Fibonacci_number, to verify that it is being invoked only once for each instance of the class. The coding for this simple class is illustrated in Fig. 2.6. There the access restrictions are given on lines 4, 5, and 7 while the attributes are declared on line 8 and the member functions are given in lines 13-33. The validation program is in lines 36–42, with the results shown as comments at the end (lines 44–48).

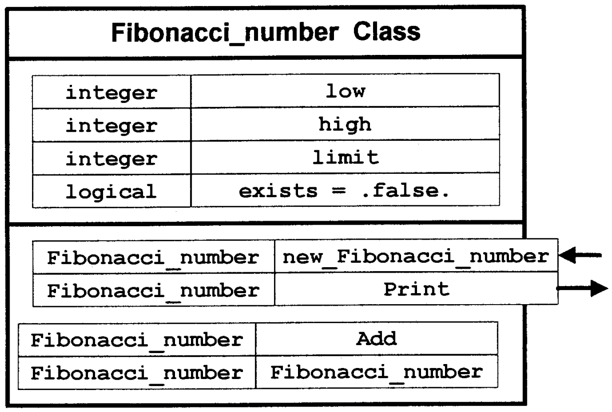


Figure 2.5: Representation of a Fibonacci_Number Class

```
! Fortran 90 OOP to print list of Fibonacci Numbers
Module class_Fibonacci_Number           ! file: Fibonacci_Number.f90
 implicit none
  public  :: Print                      ! member access
  private :: Add                        ! member access
  type Fibonacci_Number                ! attributes
    private
    integer :: low, high, limit         ! state variables & access
  end type Fibonacci_Number

Contains                                ! member functionality

  function new_Fibonacci_Number (max)  result (num) ! constructor
  implicit none
    integer, optional       :: max
    type (Fibonacci_Number) :: num
      num = Fibonacci_Number (0, 1, 0)                       ! intrinsic
      if ( present(max) ) num = Fibonacci_Number (0, 1, max) ! intrinsic
      num%exists = .true.
  end function new_Fibonacci_Number

  function Add (this) result (sum)
  implicit none
    type (Fibonacci_Number), intent(in) :: this      ! cannot modify
    integer                            :: sum
      sum = this%low + this%high ; end function add  ! add components

  subroutine Print (num)
  implicit none
    type (Fibonacci_Number), intent(inout) :: num    ! will modify
    integer                               :: j, sum ! loops
      if ( num%limit < 0 ) return                    ! no data to print
      print *, 'M  Fibonacci(M)'                     ! header
      do j = 1, num%limit                            ! loop over range
        sum = Add(num)     ; print *, j, sum         ! sum and print
        num%low = num%high ; num%high = sum          ! update
      end do ; end subroutine Print
End Module class_Fibonacci_Number

program Fibonacci                      !** The main Fibonacci program
implicit none
  use class_Fibonacci_Number        ! inherit variables and members
  integer, parameter       :: end = 8    ! unchangeable
  type (Fibonacci_Number) :: num
    num = new_Fibonacci_Number(end)     ! manual constructor
    call Print (num)                    ! create and print list
end program Fibonacci                   ! Running gives:

!  M  Fibonacci(M)    ; !  M  Fibonacci(M)
!  1 1                ; !  5 8
!  2 2                ; !  6 13
!  3 3                ; !  7 21
!  4 5                ; !  8 34
```

Figure 2.6: A Simple Fibonacci Class

2.5 Exercises

1. Create a module of global constants of common a) physical constants, b) common units conversion factors.

2. Teams in a Sports League compete in matches that result in a tie or a winning and loosing team. When the result is not a tie the status of the teams is updated. The winner is declared better that the looser and better than any team that was previously bettered by the loser. Specify this process by ADTs for the League, Team, and Match. Include a logical member function `is_better_than` which expresses whether a team is better than another.

Chapter 3

Object Oriented Programming Concepts

3.1 Introduction

The use of Object Oriented (OO) design and Object Oriented Programming (OOP) are becoming increasingly popular. Thus, it is useful to have an introductory understanding of OOP and some of the programming features of OO languages. You can develop OO software in any high level language, like C or Pascal. However, newer languages such as Ada, C++, and F90 have enhanced features that make OOP much more natural, practical, and maintainable. C++ appeared before F90 and currently, is probably the most popular OOP language, yet F90 was clearly designed to have almost all of the abilities of C++. However, rather than study the new standards many authors simply refer to the two decades old F77 standard and declare that Fortran can not be used for OOP. Here we will overcome that misinformed point of view.

Modern OO languages provide the programmer with three capabilities that improve and simplify the design of such programs: *encapsulation*, *inheritance*, and *polymorphism* (or generic functionality). Related topics involve *objects*, *classes*, and *data hiding*. An *object* combines various classical data types into a set that defines a new variable type, or structure. A *class* unifies the new entity types and supporting data that represents its state with routines (functions and subroutines) that access and/or modify those data. Every object created from a class, by providing the necessary data, is called an *instance* of the class. In older languages like C and F77, the data and functions are separate entities. An OO language provides a way to couple or encapsulate the data and its functions into a unified entity. This is a more natural way to model real-world entities which have both data and functionality. The encapsulation is done with a "module" block in F90, and with a "class" block in C++. This encapsulation also includes a mechanism whereby some or all of the data and supporting routines can be hidden from the user. The accessibility of the specifications and routines of a class is usually controlled by optional "public" and "private" qualifiers. *Data hiding* allows one the means to protect information in one part of a program from access, and especially from being changed in other parts of the program. In C++ the default is that data and functions are "private" unless declared "public," while F90 makes the opposite choice for its default protection mode. In a F90 "module" it is the "contains" statement that, among other things, couples the data, specifications, and operators before it to the functions and subroutines that follow it.

Class hierarchies can be visualized when we realize that we can employ one or more previously defined classes (of data and functionality) to organize additional classes. Functionality programmed into the earlier classes may not need to be re-coded to be usable in the later classes. This mechanism is called *inheritance*. For example, if we have defined an `Employee_class`, then a `Manager_class` would inherit all of the data and functionality of an employee. We would then only be required to add only the totally new data and functions needed for a manager. We may also need a mechanism to re-define specific `Employee_class` functions that differ for a `Manager_class`. By using the concept of a class hierarchy, less programming effort is required to create the final enhanced program. In F90 the earlier class is brought into the later class hierarchy by the "use" statement followed by the name of the "module" statement block that defined the class.

Polymorphism allows different classes of objects that share some common functionality to be used in code that requires only that common functionality. In other words, routines having the same generic name are interpreted differently depending on the class of the objects presented as arguments to the routines. This is useful in class hierarchies where a small number of meaningful function names can be used to manipulate different, but related object classes. The above concepts are those essential to object oriented design and OOP. In the later sections we will demonstrate by example additional F90 implementations of these concepts.

3.2 Encapsulation, Inheritance, and Polymorphism

We often need to use existing classes to define new classes. The two ways to do this are called *composition* and *inheritance*. We will use both methods in a series of examples. Consider a geometry program that uses two different classes: `class_Circle` and `class_Rectangle`, as represented graphically in Figs. 3.1 and 3.2. and as partially implemented in F90 as shown in Fig. 3.3. Each class shown has the data types and specifications to define the object and the functionality to compute their respective areas (lines 3–22). The operator % is employed to select specific components of a defined type. Within the geometry (main) program a single routine, `compute_area`, is invoked (lines 38 and 44) to return the area for *any* of the defined geometry classes. That is, a generic function name is used for all classes of its arguments and it, in turn, branches to the corresponding functionality supplied with the argument class. To accomplish this branching the geometry program first brings in the functionality of the desired classes via a "use" statement for each class module (lines 25 and 26). Those "modules" are coupled to the generic function by an "interface" block which has the generic function name `compute_area` (lines 28, 29). There is included a "module procedure" list which gives one class routine name for each of the classes of argument(s) that the generic function is designed to accept. The ability of a function to respond differently when supplied with arguments that are objects of different types is called *polymorphism*. In this example we have employed different names, `rectangular_area` and `circle_area`, in their respective class modules, but that is not necessary. The "use" statement allows one to rename the class routines and/or to bring in only selected members of the functionality.

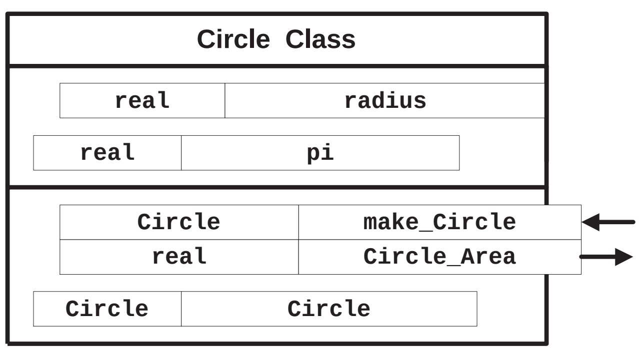


Figure 3.1: Representation of a Circle Class

Another terminology used in OOP is that of *constructors* and *destructors* for objects. An intrinsic constructor is a system function that is automatically invoked when an object is declared with all of its possible components in the defined order (see lines 37 and 43). In C++, and F90 the intrinsic constructor has the same name as the "type" of the object. One is illustrated in the statement

```
four_sides = Rectangle (2.1,4.3)
```

where previously we declared

```
type (Rectangle) :: four_sides
```

which, in turn, was coupled to the `class_Rectangle` which had two components, base and height, defined in that order, respectively. The intrinsic constructor in the example statement sets component

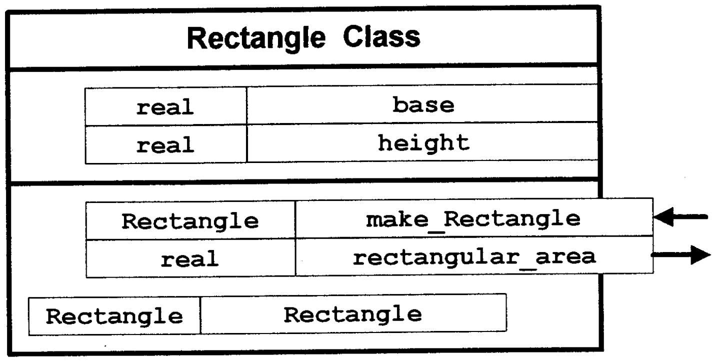


Figure 3.2: Representation of a Rectangle Class

```
!   Areas of shapes of different classes, using different
!           function names in each class
module class_Rectangle    ! define the first object class
implicit none
  type Rectangle
    real :: base, height ; end  type Rectangle
contains !  Computation of area for rectangles.
  function rectangle_area ( r ) result ( area )
    type ( Rectangle ), intent(in) :: r
    real                         :: area
      area = r%base * r%height ; end function rectangle_area
end module class_Rectangle

module class_Circle    ! define the second object class
  real :: pi = 3.1415926535897931d0 ! a circle constant
  type Circle
    real :: radius ; end  type Circle
contains !      Computation of area for circles.
  function circle_area ( c ) result ( area )
    type ( Circle ), intent(in) :: c
    real                        :: area
      area = pi * c%radius**2 ; end function circle_area
end module class_Circle

program geometry  ! for both types in a single function
 use class_Circle
 implicit none
 use class_Rectangle
!     Interface to generic routine to compute area for any type
 interface compute_area
   module procedure rectangle_area, circle_area ; end interface

!     Declare a set geometric objects.
 type ( Rectangle ) :: four_sides
 type ( Circle    ) :: two_sides       ! inside, outside
 real               :: area = 0.0       ! the result

!     Initialize a rectangle and compute its area.
   four_sides = Rectangle ( 2.1, 4.3 )    ! implicit constructor
   area = compute_area ( four_sides )    ! generic function
   write ( 6,100 ) four_sides, area       ! implicit components list
   100 format ("Area of ",f3.1," by ",f3.1," rectangle is ",f5.2)

!     Initialize a circle and compute its area.
   two_sides = Circle ( 5.4 )             ! implicit constructor
   area = compute_area ( two_sides )     ! generic function
   write ( 6,200 ) two_sides, area
   200 format ("Area of circle with ",f3.1," radius is ",f9.5 )
end program geometry                    ! Running gives:
! Area of 2.1 by 4.3 rectangle is  9.03
! Area of circle with 5.4 radius is  91.60885
```

Figure 3.3: Multiple Geometric Shape Classes

`base = 2.1` and component `height = 4.3` for that instance, `four_sides`, of the type `Rectangle`. This intrinsic construction is possible because all the expected components of the type were supplied. If all the components are not supplied, then the object cannot be constructed unless the functionality of the

```
[ 1]   function  make_Rectangle (bottom, side) result (name)
[ 2]  !          Constructor for a Rectangle type
[ 3]  implicit none
[ 4]     real, optional, intent(in) :: bottom, side
[ 5]     type (Rectangle)           :: name
[ 6]      name = Rectangle (1.,1.)      ! default to unit square
[ 7]      if ( present(bottom) ) then   ! default to square
[ 8]        name = Rectangle (bottom, bottom) ; end if
[ 9]      if ( present(side) ) name = Rectangle (bottom, side) ! intrinsic
[10]   end function  make_Rectangle
[11]   . . .
[12]   type ( Rectangle ) :: four_sides, square, unit_sq
[13]  !     Test manual constructors
[14]    four_sides = make_Rectangle (2.1,4.3)  ! manual constructor, 1
[15]    area = compute_area ( four_sides)      ! generic function
[16]    write ( 6,100 ) four_sides, area
[17]  !     Make a square
[18]    square = make_Rectangle (2.1)          ! manual constructor, 2
[19]    area = compute_area ( square)          ! generic function
[20]    write ( 6,100 ) square, area
[21]  !     "Default constructor", here a unit square
[22]    unit_sq = make_Rectangle ()            ! manual constructor, 3
[23]    area = compute_area (unit_sq)          ! generic function
[24]    write ( 6,100 ) unit_sq, area
[25]    . . .
[26]  ! Running gives:
[27]  ! Area of 2.1 by 4.3 rectangle is  9.03
[28]  ! Area of 2.1 by 2.1 rectangle is  4.41
[29]  ! Area of 1.0 by 1.0 rectangle is  1.00
```

Figure 3.4: A Manual Constructor for Rectangles

class is expanded by the programmer to accept a different number of arguments.

Assume that we want a special member of the `Rectangle` class, a square, to be constructed if the height is omitted. That is, we would use `height = base` in that case. Or, we may want to construct a unit square if both are omitted so that the constructor defaults to `base = height = 1`. Such a manual constructor, named `make_Rectangle`, is illustrated in Fig. 3.4 (see lines 5, 6). It illustrates some additional features of F90. Note that the last two arguments were declared to have the additional type attributes of "optional" (line 3), and that an associated logical function "present" is utilized (lines 6 and 8) to determine if the calling program supplied the argument in question. That figure also shows the results of the area computations for the corresponding variables "square" and "unit_sq" defined if the manual constructor is called with one or no optional arguments (line 5), respectively.

In the next section we will illustrate the concept of data hiding by using the `private` attribute. The reader is warned that the intrinsic constructor can not be employed if any of its arguments have been hidden. In that case a manual constructor must be provided to deal with any hidden components. Since data hiding is so common it is probably best to plan on prividing a manual constructor.

3.2.1 Example Date, Person, and Student Classes

Before moving to some mathematical examples we will introduce the concept of data hiding and combine a series of classes to illustrate composition and inheritance[†]. First, consider a simple class to define dates and to print them in a pretty fashion, as shown in Figs. 3.5 and 3.6. While other modules will have access to the Date class they will not be given access to the number of components it contains (3), nor their names (month, day, year), nor their types (integers) because they are declared "private" in the defining module (lines 5 and 6). The compiler will not allow external access to data and/or routines declared as private. The module, `class_Date`, is presented as a source "include" file in Fig. 3.6, and in the future will be reference by the file name `class_Date.f90`. Since we have chosen to hide all the user defined components we must decide what functionality we will provide to the users, who may have only executable access. The supporting documentation would have to name the public routines and describe their arguments and return results. The default intrinsic constructor would be available only to those that know full details about the components of the data type, and if those components are "public."

[†]These examples mimic those given in Chapter 11 and 8 of the J.R. Hubbard book "Programming with C++," McGraw-Hill, 1994, and usually use the same data for verification.

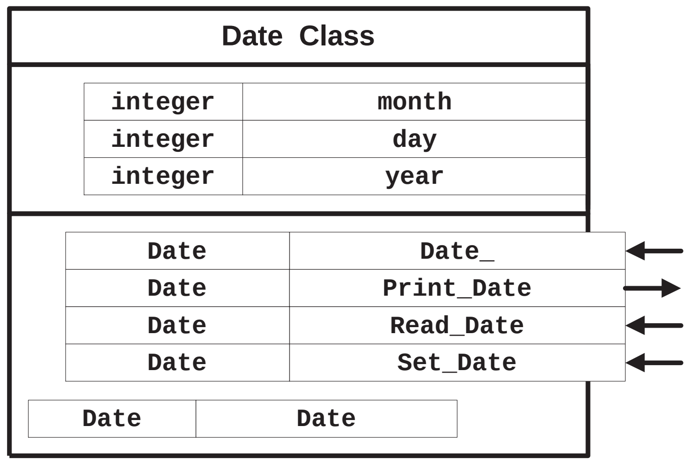


Figure 3.5: Graphical Representation of a Date Class

The intrinsic constructor, `Date` (lines 14 and 34), requires all the components be supplied, but it does no error or consistency checks. My practice is to also define a "public constructor" whose name is the same as the intrinsic constructor except for an appended underscore, that is, `Date_`. Its sole purpose is to do data checking and invoke the intrinsic constructor, `Date`. If the function `Date_` (line 10) is declared "public" it can be used outside the module `class_Date` to invoke the intrinsic constructor, even if the components of the data type being constructed are all "private." In this example we have provided another manual constructor to set a date, `set_Date` (line 31), with a variable number of optional arguments. Also supplied are two subroutines to read and print dates, `read_Date` (line 27) and `print_Date` (line 16), respectively.

A sample main program that employs this class is given in Fig. 3.7, which contains sample outputs as comments. This program uses the default constructor as well as all three programs in the public class functionality. Note that the definition of the class was copied in via an "include" (line 1) statement and activated with the "use" statement (line 4).

Now we will employ the `class_Date` within a `class_Person` which will use it to set the date of birth (DOB) and date of death (DOD) in addition to the other `Person` components of name, nationality, and sex. As shown in Fig. 3.8, we have made all the type components "private," but make all the supporting functionality public, as represented graphically in Fig. 3.8. The functionality shown provides a manual constructor, `make_Person`, routines to set the DOB or DOD, and those for the printing of most components. The source code for the new `Person` class is given in Fig. 3.9. Note that the manual constructor (line 12) utilizes "optional" arguments and initializes all components in case they are not supplied to the constructor. The `Date_` public function from the `class_Date` is "inherited" to initialize the DOB and DOD (lines 18, 57, and 62). That function member from the previous module was activated with the combination of the "include" and "use" statements. Of course, the include could have been omitted if the compile statement included the path name to that source. A sample main program for testing the `class_Person` is in Fig. 3.10 along with comments containing its output. It utilizes the constructors `Date_` (line 7), `Person_` (line10), and `make_Person` (line 24).

Next, we want to use the previous two classes to define a `class_Student` which adds something else special to the general `class_Person`. The student person will have additional "private" components for an identification number, the expected date of matriculation (DOM), the total course credit hours earned (credits), and the overall grade point average (GPA), as represented in Fig. 3.11. The source lines for the type definition and selected public functionality are given in Fig. 3.12. There the constructors are `make_Student` (line 19) and `Student_` (line 47). A testing main program with sample output is illustrated in Fig. 3.13. Since there are various ways to utilize the various constructors three alternate methods have been included as comments to indicate some of the programmers options. The first two `include` statements (lines 1, 2) are actually redundant because the third `include` automatically brings in those first two classes.

```
module class_Date        ! filename: class_Date.f90
implicit none
 public  :: Date ! and everything not "private"

 type Date
   private
   integer :: month, day, year ; end type Date

contains ! encapsulated functionality

 function Date_ (m, d, y) result (x) ! public constructor
   integer, intent(in) :: m, d, y    ! month, day, year
   type (Date)         :: x          ! from intrinsic constructor
     if ( m < 1 .or. d < 1 ) stop 'Invalid components, Date_'
       x = Date (m, d, y) ; end function Date_

subroutine  print_Date (x)    ! check and pretty print a date
  type (Date), intent(in)     :: x
  character (len=*),parameter :: month_Name(12) = &
    (/ "January  ", "February ", "March    ", "April    ",&
       "May      ", "June     ", "July     ", "August   ",&
       "September", "October  ", "November ", "December "/)
    if ( x%month < 1 .or. x%month > 12 ) print *, "Invalid month"
    if ( x%day   < 1 .or. x%day   > 31 ) print *, "Invalid day  "
    print *, trim(month_Name(x%month)),' ', x%day, ", ", x%year;
end subroutine  print_Date

 subroutine  read_Date (x)       ! read month, day, and year
   type (Date), intent(out) :: x  ! into intrinsic constructor
     read *, x ; end subroutine  read_Date

 function set_Date (m, d, y) result (x)    ! manual constructor
   integer, optional, intent(in) :: m, d, y ! month, day, year
   type (Date)                   :: x
     x = Date (1,1,1997)          ! default, (or use current date)
     if ( present(m) ) x%month = m ; if ( present(d) ) x%day   = d
     if ( present(y) ) x%year  = y ; end function set_Date

end module class_Date
```

Figure 3.6: Defining a Date Class

```
include 'class_Date.f90'   ! see previous figure
program  main
 use class_Date
 implicit none
   type (Date) :: today, peace

   ! peace = Date (11,11,1918) ! NOT allowed for private components
     peace = Date_ (11,11,1918)             ! public constructor
     print *, "World War I ended on "  ; call print_Date (peace)
     peace = set_Date (8, 14, 1945)         ! optional constructor
     print *, "World War II ended on " ; call print_Date (peace)
     print *, "Enter today as integer month, day, and year: "
     call read_Date(today)                  ! create today's date

     print *, "The date is ";  call print_Date (today)
end program  main                        ! Running produces:
! World War I ended on November 11, 1918
! World War II ended on August 14, 1945
! Enter today as integer month, day, and year: 7 10 1997
! The date is July 10, 1997
```

Figure 3.7: Testing a Date Class

3.3 Object Oriented Numerical Calculations

OOP is often used for numerical computation, especially when the standard storage mode for arrays is not practical or efficient. Often one will find specialized storage modes like linked lists, or tree structures used for dynamic data structures. Here we should note that many matrix operators are intrinsic to F90, so one is more likely to define a `class_sparse_matrix` than a `class_matrix`. However, either class would allow us to encapsulate several matrix functions and subroutines into a module that could be reused easily in other software. Here, we will illustrate OOP applied to rational numbers and introduce

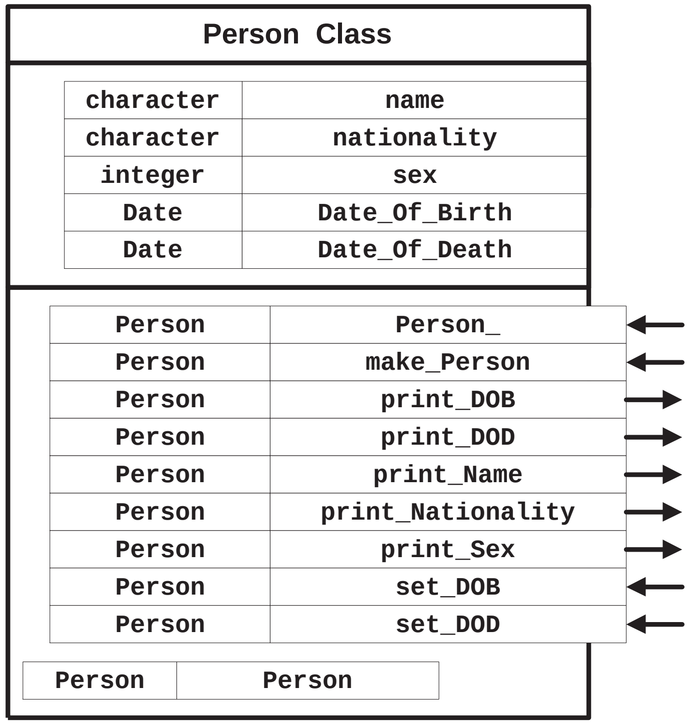


Figure 3.8: Graphical Representation of a Person Class

the important topic of operator overloading. Additional numerical applications of OOP will be illustrated in later chapters.

3.3.1 A Rational Number Class and Operator Overloading

To illustrate an OOP approach to simple numerical operations we will introduce a fairly complete rational number class, called `class_Rational` which is represented graphically in Fig. 3.14. The defining F90 module is given in Fig. 3.15. The type components have been made private (line 5), but not the type itself, so we can illustrate the intrinsic constructor (lines 38 and 102), but extra functionality has been provided to allow users to get either of the two components (lines 52 and 57). The provided routines shown in that figure are:

```
add_Rational    convert        copy_Rational     delete_Rational
equal_integer   gcd            get_Denominator   get_Numerator
invert          is_equal_to    list              make_Rational
mult_Rational   Rational_      reduce
```

Procedures with only one return argument are usually implemented as functions instead of subroutines.

Note that we would form a new rational number, z, as the product of two other rational numbers, x and y, by invoking the `mult_Rational` function (line 90),

```
z = mult_Rational (x, y)
```

which returns z as its result. A natural tendency at this point would be to simply write this as $z = x * y$. However, before we could do that we would have to have to tell the operator, "*", how to act when provided with this new data type. This is known as *overloading* an intrinsic operator. We had the foresight to do this when we set up the module by declaring which of the "module procedures" were equivalent to this operator symbol. Thus, from the "interface operator (*)" statement block (line 14) the system now knows that the left and right operands of the "*" symbol correspond to the first and second arguments in the function `mult_Rational`. Here it is not necessary to overload the assignment operator, "=", when both of its operands are of the same intrinsic or defined type. However, to convert


```
module class_Person        ! filename: class_Person.f90
use class_Date
implicit none
  public  :: Person
    type Person
      private
      character (len=20) :: name
      character (len=20) :: nationality
      integer            :: sex
      type (Date)        :: dob, dod    ! birth, death
    end type Person
contains
  function make_Person (nam, nation, s, b, d) result (who)
  !       Optional Constructor for a Person type
    character (len=*), optional, intent(in) :: nam, nation
    integer,           optional, intent(in) :: s     ! sex
    type (Date),       optional, intent(in) :: b, d  ! birth, death
    type (Person)                           :: who
      who = Person (" ","USA",1,Date_(1,1,0),Date_(1,1,0)) ! defaults
      if ( present(nam)    ) who % name        = nam
      if ( present(nation) ) who % nationality = nation
      if ( present(s)      ) who % sex         = s
      if ( present(b)      ) who % dob         = b
      if ( present(d)      ) who % dod         = d ; end function

  function Person_ (nam, nation, s, b, d) result (who)
  !       Public Constructor for a Person type
    character (len=*), intent(in) :: nam, nation
    integer,           intent(in) :: s     ! sex
    type (Date),       intent(in) :: b, d  ! birth, death
    type (Person)                 :: who
      who = Person (nam, nation, s, b, d) ; end function Person_

  subroutine print_DOB (who)
    type (Person), intent(in) :: who
      call  print_Date (who % dob) ; end subroutine  print_DOB

  subroutine print_DOD (who)
    type (Person), intent(in) :: who
      call print_Date (who % dod) ; end subroutine  print_DOD

  subroutine print_Name (who)
    type (Person), intent(in) :: who
      print *, who % name ; end subroutine print_Name

  subroutine print_Nationality (who)
    type (Person), intent(in) :: who
      print *, who % nationality ; end subroutine  print_Nationality

  subroutine print_Sex (who)
    type (Person), intent(in) :: who
      if ( who % sex == 1 ) then ; print *, "male"
      else ; print *, "female" ; end if ; end subroutine print_Sex

  subroutine set_DOB (who, m, d, y)
    type (Person), intent(inout) :: who
    integer, intent(in)          :: m, d, y ! month, day, year
      who % dob = Date_ (m, d, y) ;  end subroutine set_DOB

  subroutine set_DOD(who, m, d, y)
    type (Person), intent(inout) :: who
    integer, intent(in)          :: m, d, y ! month, day, year
      who % dod = Date_ (m, d, y) ;  end subroutine set_DOD
end module class_Person
```

Figure 3.9: Definition of a Typical Person Class

an integer to a rational we could, and have, defined an overloaded assignment operator procedure (line 10). Here we have provided the procedure, `equal_Integer`, which is automatically invoked when we write: `type(Rational)y; y = 4`. That would be simpler than invoking the constructor called `make_rational`. Before moving on note that the system does not yet know how to multiply an integer times a rational number, or visa versa. To do that one would have to add more functionality, such as a function, say `int_mult_rn`, and add it to the "module procedure" list associated with the "*" operator. A typical main program which exercises most of the rational number functionality is given in Fig. 3.16, along with typical numerical output. It tests the constructors `Rational_` (line 8), `make_Rational`

```
include 'class_Date.f90'
include 'class_Person.f90'                      ! see previous figure
program main
 use class_Date ; use class_Person            ! inherit class members
 implicit none
   type (Person) :: author, creator
   type (Date)   :: b, d                        ! birth, death
     b = Date_(4,13,1743) ; d = Date_(7, 4,1826) ! OPTIONAL
   !                      Method 1
   ! author =  Person ("Thomas Jefferson", "USA", 1, b, d) ! NOT if private
     author = Person_  ("Thomas Jefferson", "USA", 1, b, d) ! constructor
     print *, "The author of the Declaration of Independence was ";
     call  print_Name (author);
     print *, ". He was born on "; call print_DOB (author);
     print *, " and died on ";     call print_DOD (author); print *, ".";
   !                      Method 2
     author = make_Person ("Thomas Jefferson", "USA") ! alternate
     call  set_DOB (author, 4, 13, 1743)              ! add DOB
     call  set_DOD (author, 7,  4, 1826)              ! add DOD
     print *, "The author of the Declaration of Independence was ";
     call  print_Name (author)
     print *, ". He was born on "; call print_DOB (author);
     print *, " and died on ";     call print_DOD (author); print *, ".";
   !                      Another Person
     creator = make_Person ("John Backus", "USA")     ! alternate
     print *, "The creator of Fortran was "; call print_Name (creator);
     print *, " who was born in ";    call print_Nationality (creator);
     print *, ".";
end program main                                    ! Running gives:
! The author of the Declaration of Independence was Thomas Jefferson.
! He was born on April 13, 1743 and died on July 4, 1826.
! The author of the Declaration of Independence was Thomas Jefferson.
! He was born on April 13, 1743 and died on July 4, 1826.
! The creator of Fortran was John Backus who was born in the USA.
```

Figure 3.10: Testing the Date and Person Classes

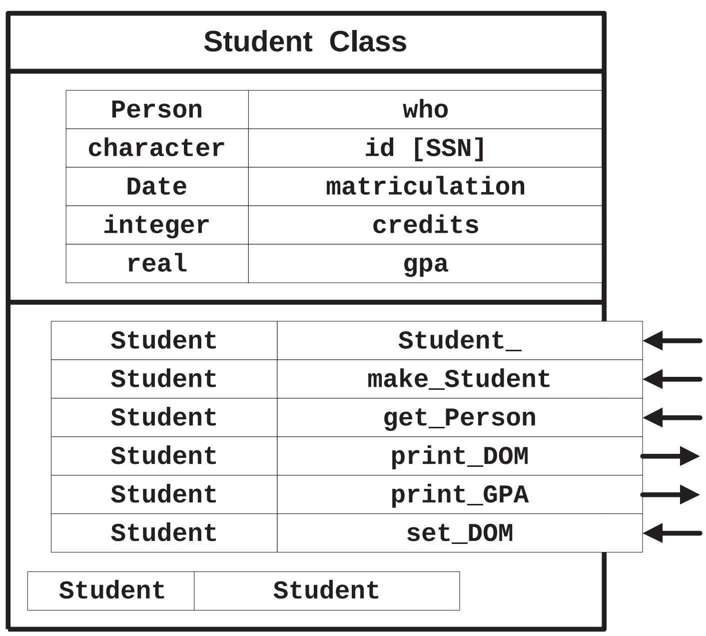


Figure 3.11: Graphical Representation of a Student Class

(lines 14, 18, 25), and a simple destructor `delete_Rational` (line 38). The intrinsic constructor (line 6) could have been used only if all the attributes were public, and that is considered an undesirable practice in OOP. The simple destructor actually just sets the "deleted" number to have a set of default components. Later we will see that constructors and destructors often must dynamically `allocate` and `deallocate`, respectively, memory associated with a specific instance of some object.

```
module class_Student            ! filename class_Student.f90
use class_Person                ! inherits class_Date
implicit none
 public :: Student, set_DOM, print_DOM
   type Student
     private
     type (Person)     :: who    ! name and sex
     character (len=9) :: id     ! ssn digits
     type (Date)       :: dom    ! matriculation
     integer           :: credits
     real              :: gpa    ! grade point average
   end type Student
contains  ! coupled functionality

  function get_person (s) result (p)
    type (Student), intent(in) :: s
    type (Person)              :: p      ! name and sex
      p = s % who ; end function get_person

 function make_Student (w, n, d, c, g) result (x) ! constructor
 !        Optional Constructor for a Student type
   type (Person),                intent(in) :: w ! who
   character (len=*), optional, intent(in) :: n ! ssn
   type (Date),       optional, intent(in) :: d ! matriculation
   integer,           optional, intent(in) :: c ! credits
   real,              optional, intent(in) :: g ! grade point ave
   type (Student)                           :: x ! new student
     x = Student_(w, " ", Date_(1,1,1), 0, 0.)   ! defaults
     if ( present(n) ) x % id      = n           ! optional values
     if ( present(d) ) x % dom     = d
     if ( present(c) ) x % credits = c
     if ( present(g) ) x % gpa     = g ; end function make_Student

  subroutine print_DOM (who)
    type (Student), intent(in) :: who
      call print_Date(who%dom) ; end subroutine print_DOM

  subroutine print_GPA (x)
    type (Student), intent(in) :: x
      print *, "My name is "; call print_Name (x % who)
      print *, ", and my G.P.A. is ", x % gpa, "." ; end subroutine

  subroutine set_DOM (who, m, d, y)
    type (Student), intent(inout) :: who
    integer,        intent(in)    :: m, d, y
      who % dom = Date_( m, d, y) ; end subroutine set_DOM

  function Student_ (w, n, d, c, g) result (x)
  !        Public Constructor for a Student type
    type (Person),     intent(in) :: w ! who
    character (len=*), intent(in) :: n ! ssn
    type (Date),       intent(in) :: d ! matriculation
    integer,           intent(in) :: c ! credits
    real,              intent(in) :: g ! grade point ave
    type (Student)                :: x ! new student
      x = Student (w, n, d, c, g) ; end function Student_
end module class_Student
```

Figure 3.12: Defining a Typical Student Class

When considering which operators to overload for a newly defined object one should consider those that are used in `sorting` operations, such as the greater-than, $>$, and less-than, $<$, operators. They are often useful because of the need to sort various types of objects. If those symbols have been correctly overloaded then a generic object sorting routine might be used, or require few changes.

3.4 Discussion

The previous sections have only briefly touched on some important OOP concepts. More details will be covered later after a general overview of the features of the Fortran language. There are more than one hundred OOP languages. Persons involved in software development need to be aware that F90 can meet almost all of their needs for a OOP language. At the same time it includes the F77 standard as a subset and thus allows efficient use of the many millions of Fortran functions and subroutines developed in the past. The newer F95 standard is designed to make efficient use of super computers and massively parallel


```
include 'class_Date.f90'
include 'class_Person.f90'
include 'class_Student.f90' ! see previous figure
program main                ! create or correct a student
 use class_Student          ! inherits class_Person, class_Date also
 implicit none
  type (Person) :: p  ; type (Student) :: x
!               Method 1
    p = make_Person ("Ann Jones","",0)  ! optional person constructor
    call set_DOB (p, 5, 13, 1977)       ! add birth to person data
    x = Student_(p, "219360061", Date_(8,29,1955), 9, 3.1) ! public
    call print_Name (p)                                ! list name
    print *, "Born         :"; call print_DOB (p)      ! list dob
    print *, "Sex          :"; call print_Sex (p)      ! list sex
    print *, "Matriculated:"; call print_DOM (x)       ! list dom
    call print_GPA (x)                                 ! list gpa
 !               Method 2
    x = make_Student (p, "219360061")    ! optional student constructor
    call set_DOM (x, 8, 29, 1995)        ! correct matriculation
    call print_Name (p)                                ! list name
    print *, "was born on :"; call print_DOB (p)      ! list dob
    print *, "Matriculated:"; call print_DOM (x)       ! list dom
 !               Method 3
    x = make_Student (make_Person("Ann Jones"), "219360061") ! optional
    p = get_Person (x)                   ! get defaulted person data
    call set_DOM (x, 8, 29, 1995)        ! add matriculation
    call set_DOB (p, 5, 13, 1977)        ! add birth
    call print_Name (p)                                ! list name
    print *, "Matriculated:"; call print_DOM (x)       ! list dom
    print *, "was born on :"; call print_DOB (p)      ! list dob
end program main                                     ! Running gives:
! Ann Jones
! Born         : May 13, 1977
! Sex          : female
! Matriculated: August 29, 1955
! My name is Ann Jones, and my G.P.A. is 3.0999999.
! Ann Jones was born on: May 13, 1977 , Matriculated: August 29, 1995
! Ann Jones Matriculated: August 29, 1995 , was born on: May 13, 1977
```

Figure 3.13: Testing the Student, Person, and Date Classes

machines. It includes most of the High Performance Fortran features that are in wide use. Thus, efficient use of OOP on parallel machines is available through F90 and F95.

None of the OOP languages have all the features one might desire. For example, the useful concept of a "template" which is standard in C++ is not in the F90 standard. Yet the author has found that a few dozen lines of F90 code will define a preprocessor that allows templates to be defined in F90 and expanded in line at compile time. The real challenge in OOP is the actual OOA and OOD that must be completed before programming can begin, regardless of the language employed. For example, several authors have described widely different approaches for defining classes to be used in constructing OO finite element systems. Additional example applications of OOP in F90 will be given in the following chapters.

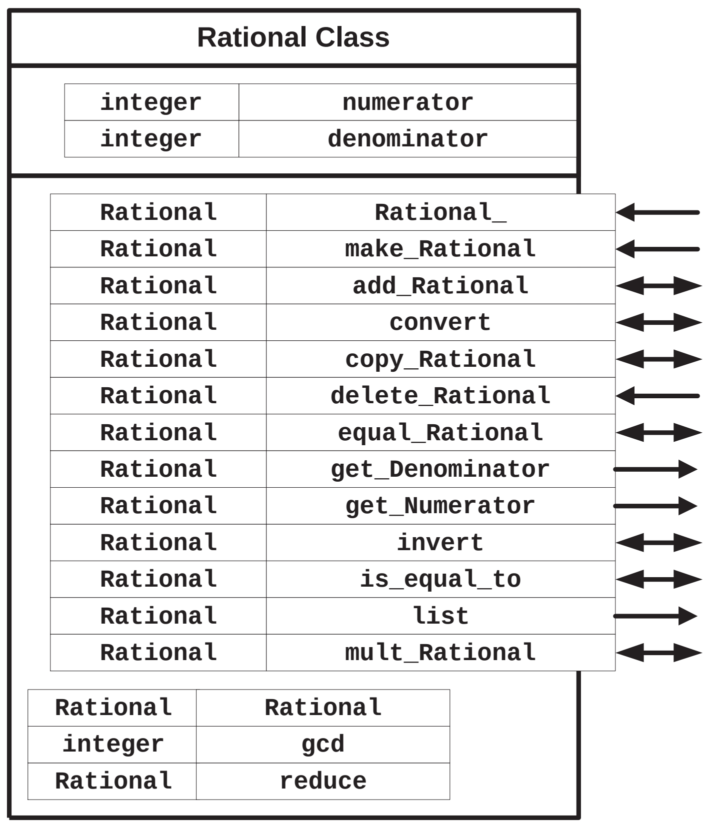


Figure 3.14: Representation of a Rational Number Class

```
module class_Rational                ! filename: class_Rational.f90
implicit none
 ! public, everything but following private routines
 private :: gcd, reduce
   type Rational
     private ! numerator and denominator
     integer :: num, den ; end type Rational

          ! overloaded operators interfaces
   interface assignment (=)
     module procedure equal_Integer ; end interface
   interface operator (+)          ! add unary versions & (-) later
     module procedure add_Rational ; end interface
   interface operator (*)          ! add integer_mult_Rational, etc
     module procedure mult_Rational ; end interface
   interface operator (==)
     module procedure is_equal_to ; end interface
contains                      ! inherited operational functionality
 function add_Rational (a, b) result (c)       ! to overload +
   type (Rational), intent(in) :: a, b          ! left + right
   type (Rational)             :: c
     c % num = a % num*b % den + a % den*b % num
     c % den = a % den*b % den
     call reduce (c) ; end function add_Rational

 function convert (name) result (value) ! rational to real
   type (Rational), intent(in) :: name
   real                        :: value  ! decimal form
     value = float(name % num)/name % den ; end function convert

 function copy_Rational (name) result (new)
   type (Rational), intent(in) :: name
   type (Rational)             :: new
     new % num = name % num
     new % den = name % den ; end function copy_Rational

 subroutine delete_Rational (name)     ! deallocate allocated items
   type (Rational), intent(inout) :: name      ! simply zero it here
     name = Rational (0, 1) ; end subroutine delete_Rational

 subroutine equal_Integer (new, I) ! overload =, with integer
   type (Rational), intent(out) :: new  ! left  side of operator
   integer,         intent(in)  :: I    ! right side of operator
     new % num = I ; new % den = 1 ; end subroutine equal_Integer

 recursive function gcd (j, k) result (g) ! Greatest Common Divisor
   integer, intent(in) :: j, k ! numerator, denominator
   integer             :: g
     if ( k == 0 ) then ; g = j
     else ; g = gcd ( k, modulo(j,k) )           ! recursive call
     end if ; end function gcd

 function  get_Denominator (name) result (n)   ! an access function
   type (Rational), intent(in) :: name
   integer                     :: n             ! denominator
     n = name % den ; end function  get_Denominator
```

(Fig. 3.15, A Fairly Complete Rational Number Class (continued))

```
 function  get_Numerator (name) result (n)     ! an access function
   type (Rational), intent(in) :: name
   integer                     :: n            ! numerator
     n = name % num ; end function  get_Numerator

 subroutine  invert (name)         ! rational to rational inversion
   type (Rational), intent(inout) :: name
   integer                        :: temp
     temp       = name % num
     name % num = name % den
     name % den = temp ; end subroutine invert

  function is_equal_to (a_given, b_given) result (t_f)
   type (Rational), intent(in) :: a_given, b_given  ! left == right
   type (Rational)             :: a, b              ! reduced copies
   logical                     :: t_f
     a = copy_Rational (a_given) ; b = copy_Rational (b_given)
     call reduce(a) ; call reduce(b)        ! reduced to lowest terms
     t_f = (a%num == b%num) .and. (a%den == b%den) ; end function

  subroutine list(name)                 ! as a pretty print fraction
   type (Rational), intent(in) :: name
     print *, name % num, "/", name % den ; end subroutine list

  function make_Rational (numerator, denominator) result (name)
  !        Optional Constructor for a rational type
   integer, optional, intent(in) :: numerator, denominator
   type (Rational)               :: name
     name = Rational(0, 1)                           ! set defaults
     if ( present(numerator)  ) name % num = numerator
     if ( present(denominator)) name % den = denominator
     if ( name % den == 0     ) name % den = 1        ! now simplify
     call reduce (name) ; end function make_Rational

 function  mult_Rational (a, b) result (c)         ! to overload *
   type (Rational), intent(in) :: a, b
   type (Rational)             :: c
     c % num = a % num * b % num
     c % den = a % den * b % den
     call reduce (c) ; end function mult_Rational

 function Rational_ (numerator, denominator) result (name)
 !        Public Constructor for a rational type
   integer, optional, intent(in) :: numerator, denominator
   type (Rational)               :: name
     if ( denominator == 0 ) then ; name = Rational (numerator, 1)
     else ; name = Rational (numerator, denominator) ; end if
 end function Rational_

 subroutine reduce (name)               ! to simplest rational form
   type (Rational), intent(inout) :: name
   integer                        :: g     ! greatest common divisor
     g          = gcd (name % num, name % den)
     name % num = name % num/g
     name % den = name % den/g ; end subroutine reduce
end module class_Rational
```

Figure 3.15: A Fairly Complete Rational Number Class

```
include 'class_Rational.f90'
program main
use class_Rational
implicit none
  type (Rational) :: x, y, z
  ! ------- only if Rational is NOT private ----------
  ! x = Rational(22,7)    ! intrinsic constructor if public components

    x = Rational_(22,7)   ! public constructor if private components
    write (*,'("public    x  = ")',advance='no'); call list(x)
    write (*,'("converted x  = ", g9.4)') convert(x)
    call invert(x)
    write (*,'("inverted 1/x = ")',advance='no');  call list(x)

    x = make_Rational ()               ! default constructor
    write (*,'("made null x  = ")',advance='no'); call list(x)
    y = 4                              ! rational = integer overload
    write (*,'("integer y    = ")',advance='no'); call list(y)
    z = make_Rational (22,7)           ! manual constructor
    write (*,'("made full z  = ")',advance='no'); call list(z)
  !                 Test Accessors
    write (*,'("top of z     = ", g4.0)') get_numerator(z)
    write (*,'("bottom of z  = ", g4.0)') get_denominator(z)
  !                 Misc. Function Tests
    write (*,'("making x = 100/360, ")',advance='no')
    x = make_Rational (100,360)
    write (*,'("reduced x = ")',advance='no'); call list(x)
    write (*,'("copying x to y gives ")',advance='no')
    y = copy_Rational (x)
    write (*,'("a new y = ")',advance='no'); call list(y)
  !                Test Overloaded Operators
    write (*,'("z * x gives ")',advance='no'); call list(z*x) ! times
    write (*,'("z + x gives ")',advance='no'); call list(z+x) ! add
    y = z                                     ! overloaded assignment
    write (*,'("y = z gives y as ")',advance='no'); call list(y)
    write (*,'("logic y == x gives ")',advance='no'); print *, y==x
    write (*,'("logic y == z gives ")',advance='no'); print *, y==z
  !                 Destruct
    call delete_Rational (y)    ! actually only null it here
    write (*,'("deleting y gives y = ")',advance='no'); call list(y)
end program main                                     ! Running gives:
!  public    x  =  22 / 7       !  converted x  = 3.143
!  inverted 1/x =  7 / 22       !  made null x  =  0 / 1
!  integer y    =  4 / 1        !  made full z  =  22 / 7
!  top of z     =   22          !  bottom of z  =    7
!  making x = 100/360, reduced x =  5 / 18
!  copying x to y gives a new y =  5 / 18
!  z * x gives  55 / 63         !  z + x gives  431 / 126
!  y = z gives y as  22 / 7     !  logic y == x gives  F
!  logic y == z gives  T        !  deleting y gives y =  0 / 1
```

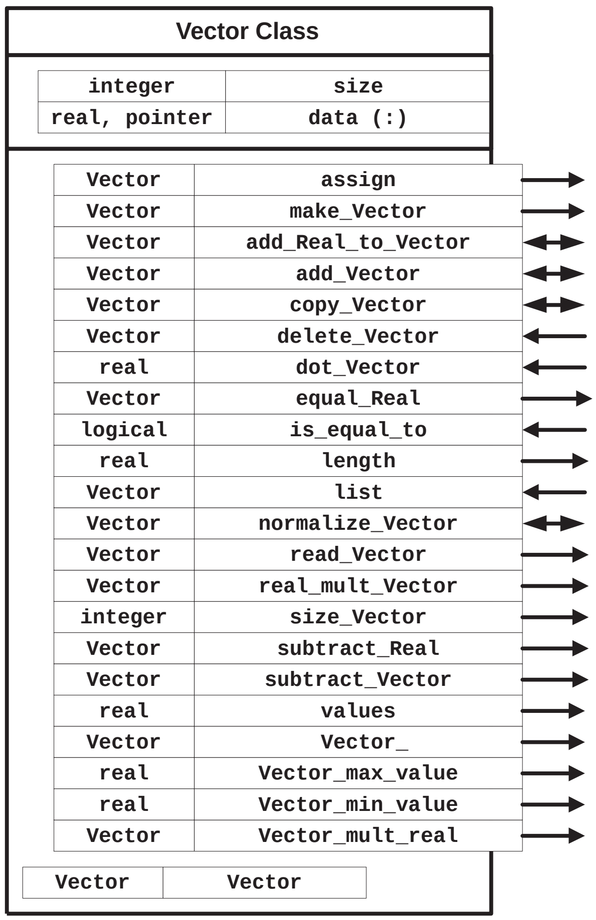
Figure 3.16: Testing the Rational Number Class

3.5 Exercises

1. Use the `class_Circle` to create a `class_Sphere` that computes the volume of a sphere. Have a method that accepts an argument of a `Circle`. Use the `radius` of the `Circle` via a new member `get_Circle_radius` to be added to the `class_Circle`.

2. Use the `class_Circle` and `class_Rectangle` to create a `class_Cylinder` that computes the volume of a right circular cylinder. Have a method that accepts arguments of a `Circle` and a `height`, and a second method that accepts arguments of a `Rectangle` and a `radius`. In the latter member use the `height` of the `Rectangle` via a new member `get_Rectangle_height` to be added to the `class_Rectangle`.

3. Create a vector class to treat vectors with an arbitrary number of real coefficients. Assume that the `class_Vector` is defined as follows:



Overload the common operators of (+) with `add_Vector` and `add_Real_to_Vector`, (–) with `subtract_Vector` and `subtract_Real`, (*) with `dot_Vector`, `real_mult_Vector` and `Vector_mult_real`, (=) with `equal_Real` to set all coefficients to a single real number, and (==) with routine `is_equal_to`.

Include two constructors *assign* and `make_Vector`. Let *assign* convert a real array into an instance of a Vector. Provide a destructor, means to read and write a Vector, normalize a Vector, and determine its extreme values.

4. Modify the above Vector class to extend it to a `Sparse_Vector_Class` where the vast majority of the coefficients are zero. Store and operate only on the non-zero entries.

Sparse_Vector Class

integer	non_zeros
integer, pointer	rows (:)
real, pointer	values (:)

Sparse_Vector	make_Sparse_Vector
Sparse_Vector	add_Real_to_Sparse_Vector
Sparse_Vector	add_Sparse_Vector
Sparse_Vector	delete_Sparse_Vector
real	dot_Vector
Sparse_Vector	el_by_el_Mult
Sparse_Vector	equal_Vector
real	get_element
logical	is_equal_to
integer	largest_index
real	length
real	norm
Sparse_Vector	normalize_Vector
Sparse_Vector	pretty
Sparse_Vector	read_Vector
Sparse_Vector	real_mult_Sparse
integer	rows_of
Sparse_Vector	set_element
Sparse_Vector	show
Sparse_Vector	show_r_v
integer	size_of
Sparse_Vector	Sparse_mult_real
Sparse_vector	sub_Sparse_Vector
Sparse_Vector	sum_Sparse_Vector
real	Vector_max_value
real	Vector_min_value
Sparse_Vector	Vector_to_Sparse
Sparse_Vector	zero_Sparse

Sparse_Vector	Sparse_Vector

Chapter 4

Features of Programming Languages

The preceding chapter described the programming process as starting with a clearly specified task, expressing it mathematically as a set of algorithms, translating the algorithms in pseudocode, and finally, translating the pseudocode into a "real" programming language. The final stages of this prescription work because most (if not all) computational languages have remarkable similarities: They have statements, the sequencing of which are controlled by various loop and conditional constructs, and functions that foster program modularization. We indicated how similar MATLAB, C++, and Fortran are at this level, but these languages differ the more they are detailed. It is the purpose of this chapter to describe those details, and bring you from a superficial acquaintance with a computational language to fluency. Today, the practicing engineer needs more than one programming language or environment. Once achieving familiarity with one, you will find that learning other languages is easy.

When selecting a programming tool for engineering calculations, one is often faced with two different levels of need. One level is where you need to quickly solve a small problem once, such as a homework assignment, and computational efficiency is not important. You may not care if your code takes ten seconds or one hundred seconds to execute; you want convenience. At that level it may make sense to use an engineering environment like MATLAB, or Mathematica. At the other extreme you may be involved in doing a wide area weather prediction where a one-day run time, instead of a ten-day run time, defines a useful versus a non-useful product. You might be developing a hospital laboratory system for reporting test results to an emergency room physician where an answer in ten seconds versus an answer in ten minutes can literally mean the difference between life or death for a patient. For programming at this level one wants an efficient language. Since such projects can involve programming teams in different countries, you want your language to be based on an international standard. Then you would choose to program a language such as C++ or F90. Since most students have experienced only the first need level, they tend to overvalue the first approach and devalue the second. This chapter will illustrate that the skills needed for either approach are similar.

The structure of this chapter follows our usual progression to learning a language: What are *variables*, how can variables be combined into *expressions*, what constructs are available to control program *flow*, and how are *functions* defined so that we can employ modularity. The basics are described in Chapter 1; we assume you are familiar with the language basics described there. Initially, this chapter will parallel the program composition section of Chapter 1 as applied in the C++, F90, and MATLAB languages, and then it will bring in more advanced topics.

The features of F90 that are to be discussed here have been combined in a series of tables and placed in Appendix B. It is expected that we will want to refer to those tables as we read this section as well as later when we program. At times, references to C++ and MATLAB have been given to show the similarities between most languages and to provide an aid for when having to interface in reading codes in those languages.

4.1 Comments

In MATLAB and Fortran, a single character — '`%`' in MATLAB, '`!`' in F90 — located anywhere in a line of text means that the *remainder* of the text on that line comprises the comment. In C, an entirely different

Language	Syntax	Location
MATLAB	`% comment (to end of line)`	anywhere
C++	`// comment (to end of line)`	anywhere
F90	`!  comment (to end of line)`	anywhere
F77	`* comment (to end of line)`	column 1

Table 4.1: Comment syntax

structure for comments occurs. Comments begin with the two-character sequence '`/*`' and end with the *next* occurrence of the two-character sequence '`*/`'. In C, comments can occur anywhere in a program; they can consume a portion of a line, temporarily interrupting a statement, or they can span multiple lines of text. C++ allows the use of the C comment syntax, but has added a more popular two-character sequence '`//`' to proceed a comment to the end of a line. Table 4.1 gives a summary of these comments syntax. It is also in the "Fortran 90 Overview" for quick reference. Samples of comment statements are shown in Fig. 1.3, which gives the corresponding versions of the classic "hello world" program included in most introductory programming texts.

4.2 Statements and Expressions

Before introducing statements and expressions, a word about documenting what you program. We encourage the heavy usage of comments. The three languages of concern here all allow comment lines and comments appended to the end of statements. Their form is given above in Fig. 1.3 and Table 4.1.

The above languages currently allow variable names to contain up to 31 characters and allow the use of the underscore, '`_`', to aid in clarity by serving as a virtual space character, as in `my_name`. Another useful convention is to use uppercase first letters for words comprising part of a variable's name: `MyName`. Fortran and MATLAB allow a program line to contain up to 132 characters, while C++ has no limit on line length. Since the old F77 standard was physically limited to holes punched in a card, it allowed only a line length of 72 characters, a maximum name length of six characters, and did not allow the use of the underscore in a name. In this text, we will usually keep line lengths to less than 65 characters in order to make the programs more readable.

A statement in these three languages has a structure common to them all:

```
variable = expression
```

The built-in, or intrinsic, data types allowed for variables are summarized in Table 4.2. Additional user defined types will be considered later. The expressions usually involves the use of arithmetic operators and/or relational operators which are given in Tables 4.3 and 4.4, respectively. The order in which the language applies these operators is called their precedence, and they are shown in Table 4.5. They are also in the "Fortran 90 Overview" for quick reference.

In moving from MATLAB to high level languages one finds that it is necessary to define the type of each variable. Fortran has a default naming convention for its variables and it allows an easy overriding of that built in "implicit" convention. Since most engineering and mathematical publications used the letters from "i" through "n" as subscripts, summation ranges, loop counters, etc. Fortran first was released with implicit variable typing such that all variables whose name begin with the letters "i" through "n", inclusive, defaulted to integers, unless declared otherwise. All other variables default to be real, unless declared otherwise. In other words, you can think of the default code as if it contained the statements:

```
IMPLICIT INTEGER (I-N)       ! F77 and F90 Default
IMPLICIT REAL    (A-H, O-Z) ! F77 and F90 Default
```

The effect is automatic even if the statements are omitted. Explicit type declarations override any given `IMPLICIT` types. For example, if the code had the above implicit defaults one could also explicitly identify the exceptions to those default rules, such as the statements:

```
INTEGER :: Temp_row
```

Storage	MATLAB[a]	C++	F90	F77
byte		`char`	`character::`	`character`
integer		`int`	`integer::`	`integer`
single precision		`float`	`real::`	`real`
double precision		`double`	`real*8::`	`double precision`
complex		[b]	`complex::`	`complex`
Boolean		`bool`	`logical::`	`logical`
argument			`parameter::`	`parameter`
pointer		`*`	`pointer::`	
structure		`struct`	`type::`	

[a]MATLAB4 requires no variable type declaration; the only two distinct types in MATLAB are strings and reals (which include complex). Booleans are just 0s and 1s treated as reals. MATLAB5 allows the user to select more types.
[b]There is no specific data type for a complex variable in C++; they must be created by the programmer.

Table 4.2: Intrinsic data types of variables

Description	MATLAB[a]	C++	Fortran[b]
addition	`+`	`+`	`+`
subtraction[c]	`-`	`-`	`-`
multiplication	`*` and `.*`	`*`	`*`
division	`/` and `./`	`/`	`/`
exponentiation	`^` and `.^`	pow[d]	`**`
remainder		`%`	
increment		`++`	
decrement		`--`	
parentheses (expression grouping)	`()`	`()`	`()`

[a]When doing arithmetic operations on matrices in MATLAB, a period ('`.`') must be put before the operator if scalar arithmetic is desired. Otherwise, MATLAB assumes matrix operations; figure out the difference between '`*`' and '`.*`'. Note that since matrix and scalar addition coincide, no '`.+`' operator exists (same holds for subtraction).
[b]Fortran 90 allows the user to change operators and to define new operator symbols.
[c]In all languages the minus sign is used for negation (i.e., changing sign).
[d]In C++ the exponentiation is calculated by function *pow* (x, y).

Table 4.3: Arithmetic operators

```
REAL :: Interest = 0.04  ! declare and initialize
CHARACTER (Len=8) :: Months_of_year(12)
```

We will also see that the programmer can define new data types and explicitly declare their type as well.

The F90 standard discourages the use of any `IMPLICIT` variables such as

```
IMPLICIT COMPLEX (X-Z)           ! Complex variables
IMPLICIT DOUBLE PRECISION (A-H) ! Double Precision reals
```

and encourages the use of

```
IMPLICIT NONE
```

which forces the programmer to specifically declare the type of each and every variable used, and is referred to as *strong typing*. However, you need to know that such default variable types exist because they are used in many millions of lines of older Fortran code and at some point you will need to use or change such an existing program.

<table>
<tr><th>Description</th><th>MATLAB</th><th>C++</th><th>F90</th><th>F77</th></tr>
<tr><td>Equal to</td><td>==</td><td>==</td><td>==</td><td>.EQ.</td></tr>
<tr><td>Not equal to</td><td>~=</td><td>!=</td><td>/=</td><td>.NE.</td></tr>
<tr><td>Less than</td><td><</td><td><</td><td><</td><td>.LT.</td></tr>
<tr><td>Less or equal</td><td><=</td><td><=</td><td><=</td><td>.LE.</td></tr>
<tr><td>Greater than</td><td>></td><td>></td><td>></td><td>.GT.</td></tr>
<tr><td>Greater or equal</td><td>>=</td><td>>=</td><td>>=</td><td>.GE.</td></tr>
<tr><td>Logical NOT</td><td>~</td><td>!</td><td>.NOT.</td><td>.NOT.</td></tr>
<tr><td>Logical AND</td><td>&</td><td>&&</td><td>.AND.</td><td>.AND.</td></tr>
<tr><td>Logical inclusive OR</td><td>!</td><td>||</td><td>.OR.</td><td>.OR.</td></tr>
<tr><td>Logical exclusive OR</td><td>xor</td><td></td><td>.XOR.</td><td>.XOR.</td></tr>
<tr><td>Logical equivalent</td><td>==</td><td>==</td><td>.EQV.</td><td>.EQV.</td></tr>
<tr><td>Logical not equivalent</td><td>~=</td><td>!=</td><td>.NEQV.</td><td>.NEQV.</td></tr>
</table>

Table 4.4: Relational operators (arithmetic and logical)

<table>
<tr><th>MATLAB Operators</th><th>C++ Operators</th><th>F90 Operators[a]</th><th>F77 Operators</th></tr>
<tr><td>()</td><td>() [] -> .</td><td>()</td><td>()</td></tr>
<tr><td>+ -</td><td>! ++ -- +
- * & (type)
sizeof</td><td>**</td><td>**</td></tr>
<tr><td>* /</td><td>* / %</td><td>* /</td><td>* /</td></tr>
<tr><td>+ -[b]</td><td>+ -[b]</td><td>+ -[b]</td><td>+ -[b]</td></tr>
<tr><td>< <= > >=</td><td><< >></td><td>//</td><td>//</td></tr>
<tr><td>== ~=</td><td>< <= > =></td><td>== /= < <= >
>=</td><td>.EQ. .NE.
.LT. .LE.
.GT. .GE.</td></tr>
<tr><td>~</td><td>== !=</td><td>.NOT.</td><td>.NOT.</td></tr>
<tr><td>&</td><td>&&</td><td>.AND.</td><td>.AND.</td></tr>
<tr><td>|</td><td>||</td><td>.OR.</td><td>.OR.</td></tr>
<tr><td>=</td><td>|</td><td>.EQV. .NEQV.</td><td>.EQV. .NEQV.</td></tr>
<tr><td></td><td>?:</td><td></td><td></td></tr>
<tr><td></td><td>= += -= *= /=
%= &= ^= |=
<<= >>=</td><td></td><td></td></tr>
<tr><td></td><td>,</td><td></td><td></td></tr>
</table>

[a]User-defined unary (binary) operators have the highest (lowest) precedence in F90.
[b]These are binary operators representing addition and subtraction. Unary operators + and - have higher precedence.

Table 4.5: Precedence pecking order

```
[ 1]  program main
[ 2]  !  Examples of simple arithmetic in F90
[ 3]  implicit none
[ 4]    integer :: Integer_Var_1, Integer_Var_2      ! user inputs
[ 5]    integer :: Mult_Result, Div_Result, Add_Result
[ 6]    integer :: Sub_Result, Mod_Result
[ 7]    real    :: Pow_Result, Sqrt_Result
[ 8]
[ 9]     print *, 'Enter two integers:'
[10]     read  *, Integer_Var_1, Integer_Var_2
[11]
[12]     Add_Result = Integer_Var_1 + Integer_Var_2
[13]     print *, Integer_Var_1,' + ', Integer_Var_2,' = ', Add_
[14]
[15]     Sub_Result = Integer_Var_1 - Integer_Var_2
[16]     print *, Integer_Var_1,' - ', Integer_Var_2,' = ', Sub_
[17]
[18]     Mult_Result = Integer_Var_1 * Integer_Var_2
[19]     print *, Integer_Var_1,' * ', Integer_Var_2,' = ', Mult_
[20]
[21]     Div_Result = Integer_Var_1 / Integer_Var_2
[22]     print *, Integer_Var_1,' / ', Integer_Var_2,' = ', Div_
[23]
[24]     Mod_Result = mod (Integer_Var_1, Integer_Var_2) ! remai
[25]     print *, Integer_Var_1,' mod ', Integer_Var_2,' = ', Mod_
[26]
[27]     Pow_Result = Integer_Var_1 ** Integer_Var_2   ! raise t
[28]     print *, Integer_Var_1,' ^ ', Integer_Var_2,' = ', Pow_
[29]
[30]     Sqrt_Result = sqrt( real(Integer_Var_1))
[31]     print *,'Square root of ', Integer_Var_1,' = ', Sqrt_Result
[32]
[33]  end program main         !  Running produces:
[34]    ! Enter two integers:
[35]    ! 25  +  4  =  29
[36]    ! 25  -  4  =  21
[37]    ! 25  *  4  =  100
[38]    ! 25  /  4  =  6, note integer
[39]    ! 25  mod  4  =  1
[40]    ! 25  ^  4  =  3.9062500E+05
[41]    ! Square root of  25  =  5.0000000
```

Figure 4.1: Typical Math and Functions in F90

An example program that employs the typical math operators in F90 is shown in Fig. 4.1. It presents examples of addition (line 11), subtraction (line 14), multiplication (line 17), division (line 20), as well as the use of the remainder or modulo function (line 23), exponentiation (line 26), and square root operators (line 29). In addition it shows a way of inputing data from the default input device (line 9). The results are appended as comments (lines 33-40). Observe that a program must include one and only one segment that begins with the word `program` (line 1) and ends with the line `end program` (line 32). If a name is assigned to the program then it must be appended to both of these lines. Often the name of `main` is used, as here, but it is not required as it is in C++ . A C++ formulation of this example is included for comparison in the appendix as are several other examples from this chapter.

A special expression available in MATLAB and F90 uses the colon operator `(:)` to indicate forming a vector (row matrix) of numbers according to an arithmetic progression. In MATLAB, the expression `b:i:e` means the vector $[b\,(b+i)\,(b+2i)\,\cdots\,(b+Ni)]$, where $(b+Ni)$ is the largest number less than or equal to (greater than or equal to if i is negative) the value of the variable `e`. Thus, `b` means "beginning value", `i` means the increment, and `e` the end value. The expression `b:e` means that the increment equals one. You can use this construct to excise a portion of a vector or matrix. For example, `x(2:5)` equals the vector comprised by the second through fifth elements of `x`, and `A(3:5,i:j)` creates a matrix from the third, fourth, and fifth rows, i^{th} through j^{th} columns of the matrix `A`. F90 uses the convention of `b:e:i` and has the same defaults when `:i` is omitted. This operator, also known as the *subscript triplet*, is described in Table 4.6.

Of course, expressions often involve the use of functions. A tabulation of the built-in functions in our languages is given in Table 4.7 and the F90 overview, as are all the remaining tables of this chapter. The arguments of functions and subprograms have some important properties that vary with the language used. Primarily, we are interested in how actual arguments are passed to the dummy arguments in the subprogram. This data passing happens by either of two fundamentally different ways: by reference, or

`B` = Beginning, `E` = Ending, `I` = Increment

Syntax	F90	MATLAB
Default	`B:E:I`	`B:I:E`
$\geq$ `B`	`B:`	`B:`
$\leq$ `E`	`:E`	`:E`
Full range	`:`	`:`

Use	F90	MATLAB
Array subscript ranges	yes	yes
Character positions in a string	yes	yes
Loop control	no	yes
Array element generation	no	yes

Table 4.6: Colon Operator Syntax and its Applications.

Description	MATLAB	C++	F90	F77
exponential	`exp(x)`	`exp(x)`	`exp(x)`	`exp(x)`
natural log	`log(x)`	`log(x)`	`log(x)`	`log(x)`
base 10 log	`log10(x)`	`log10(x)`	`log10(x)`	`log10(x)`
square root	`sqrt(x)`	`sqrt(x)`	`sqrt(x)`	`sqrt(x)`
raise to power (x^r)	`x.^r`	`pow(x,r)`	`x**r`	`x**r`
absolute value	`abs(x)`	`fabs(x)`	`abs(x)`	`abs(x)`
smallest integer>x	`ceil(x)`	`ceil(x)`	`ceiling(x)`	
largest integer<x	`floor(x)`	`floor(x)`	`floor(x)`	
division remainder	`rem(x,y)`	`fmod(x,y)`	`mod(x,y)`[a]	`mod(x,y)`
modulo			`modulo(x,y)`[a]	
complex conjugate	`conj(z)`		`conjg(z)`	`conjg(z)`
imaginary part	`imag(z)`		`imag(z)`	`aimag(z)`
drop fraction	`fix(x)`		`aint(x)`	`aint(x)`
round number	`round(x)`		`nint(x)`	`nint(x)`
cosine	`cos(x)`	`cos(x)`	`cos(x)`	`cos(x)`
sine	`sin(x)`	`sin(x)`	`sin(x)`	`sin(x)`
tangent	`tan(x)`	`tan(x)`	`tan(x)`	`tan(x)`
arc cosine	`acos(x)`	`acos(x)`	`acos(x)`	`acos(x)`
arc sine	`asin(x)`	`asin(x)`	`asin(x)`	`asin(x)`
arc tangent	`atan(x)`	`atan(x)`	`atan(x)`	`atan(x)`
arc tangent[b]	`atan2(x,y)`	`atan2(x,y)`	`atan2(x,y)`	`atan2(x,y)`
hyperbolic cosine	`cosh(x)`	`cosh(x)`	`cosh(x)`	`cosh(x)`
hyperbolic sine	`sinh(x)`	`sinh(x)`	`sinh(x)`	`sinh(x)`
hyperbolic tangent	`tanh(x)`	`tanh(x)`	`tanh(x)`	`tanh(x)`
hyperbolic arc cosine	`acosh(x)`			
hyperbolic arc sine	`asinh(x)`			
hyperbolic arctan	`atanh(x)`			

[a]Differ for $x < 0$.

[b]`atan2(x,y)` is used to calculate the arc tangent of x/y in the range $[-\pi, +\pi]$. The one-argument function `atan(x)` computes the arc tangent of x in the range $[-\pi/2, +\pi/2]$.

Table 4.7: Mathematical functions

by value. One should understand the difference between these two mechanisms.

"Passing by reference" means that the address in memory of the actual argument is passed to the subprogram instead of the value stored at that address. The corresponding dummy argument in the subprogram has the same address. That is, both arguments refer to the same memory location so any change to that argument within the subprogram is passed back to the calling code. A variable is passed by reference to a subroutine whenever it is expected that it should be changed by the subprogram. A related term is "dereferencing". When you dereference a memory address, you are telling the computer to get the information located at the address. Typically, one indirectly gives the address by citing the

Description	**C++**	**F90**	**F77**	**MATLAB**
Conditionally execute statements	`if` `{ }`	`if` `end if`	`if` `end if`	`if` `end`
Loop a specific number of times	`for k=1:n` `{ }`	`do k=1,n` `end do`	`do # k=1,n` `# continue`	`for k=1:n` `end`
Loop an indefinite number of times	`while` `{ }`	`do while` `end do`	— —	`while` `end`
Terminate and exit loop	`break`	`exit`	`go to`	`break`
Skip a cycle of loop	`continue`	`cycle`	`go to`	—
Display message and abort	`error()`	`stop`	`stop`	`error`
Return to invoking function	`return`	`return`	`return`	`return`
Conditional array action	—	`where`	—	`if`
Conditional alternate statements	`else` `else if`	`else` `elseif`	`else` `elseif`	`else` `elseif`
Conditional array alternatives	— —	`elsewhere` —	— —	`else` `elseif`
Conditional case selections	`switch { }`	`select case` `end select`	`if` `end if`	`if` `end`

Table 4.8: Flow Control Statements.

name of a pointer variable or a reference variable.

"Passing by value" means that the value of the actual argument stored at its address in memory is copied and the copy is passed to the dummy argument in the subprogram. Thus any change to the argument within the subprogram is **not** passed back to the calling code. The two passing methods do not clearly show the intended use of the argument within the subprogram. Is it to be passed in for use only, passed in for changing and returned, or is it to be created in the subprogram and passed out for use in the calling code? For additional safety and clarity modern languages provide some way to allow the programmer to optionally specify such intent explicitly.

Both C++ and MATLAB use the pass by value method as their default mode. This means the value associated with the argument name, say `arg_name`, is copied and passed to the function. That copying could be very inefficient if the argument is a huge array. To denote that you want to have the C++ argument passed by reference you must precede the argument name with an ampersand (&), e.g. `&arg_name`, in the calling code. Then within the subprogram the corresponding dummy variable must be dereferenced by preceding the name with an asterisk (*), e.g. `*arg_name`. Conversely, Fortran uses the passing by reference method as its default mode. On the rare occasions when one wants to pass by value simply surround the argument name with parentheses, e.g. (`arg_name`), in the calling code. In either case it is recommended that you cite each argument with the optional "intent" statement within the subprogram. Examples of the two passing options are covered in Sec. 4.5.

4.3 Flow Control

The basic flow control constructs present in our selected engineering languages are *loops*—repetitive execution of a block of statements—and *conditionals*—diversions around blocks of statements. A typical set of flow control statement types are summarized in Table 4.8. Most of these will be illustrated in detail in the following sections.

4.3.1 Explicit Loops

The following discussion will introduce the important concept of loops. These are required in most programs. However, the reader is warned that today the writing of explicit loops are generally *not* the most efficient way to execute a loop operation in Fortran90 and MATLAB. Of course, older languages like F77 and C do require them, so that the time spent here not only covers the explicit loop concepts but aids one in reading older languages. Our pseudocode for the common loops is :

Loop	MATLAB	C++	Fortran
Indexed loop	`for index=matrix` *`statements`* `end`	`for (init;test;inc)` `{` *`statements`* `}`	`do index=b,e,i` *`statements`* `end do`
Pre-test loop	`while test` *`statements`* `end`	`while (test) {` *`statements`* `}`	`do while (test)` *`statements`* `end do`
Post-test loop		`do {` *`statements`* `} while (test)`	`do` *`statements`* `if (test) exit` `end do`

Table 4.9: Basic loop constructs

Loop	Pseudocode
Indexed loop	`for index=b,i,e` *`statements`* `end for`
Pre-test loop	`while (test)` *`statements`* `end while`
Post-test loop	`do` *`statements`* `if test exit` `end do`

In engineering programming one often needs to repeatedly perform a group of operations. Most computer languages have a statement to execute this powerful and widely-used feature. In Fortran this is the `DO` statement, while in C++ and MATLAB it is the `FOR` statement. This one statement provides for the initialization, incrementing and testing of the loop variable, plus repeated execution of a group of statements contained within the loop. In Fortran77, the loop always cites a label number that indicates the extent of the statements enclosed in the loop. This is allowed in F90, but not recommended, and is considered obsolete. Instead, the `END DO` indicates the extent of the loop, and the number label is omitted in both places. F90 does allow one to give a name to a loop. Then the structure is denoted as `NAME:DO` followed by `END DO NAME`. Examples of the syntax for these statements for the languages of interest are given in Table 4.9.

A simple example of combining loops and array indexing is illustrated in Figs. 4.2 and 4.3. Note in Fig. 4.2 that the final value of a loop counter (called *Integer_Var* here) upon exiting the loop (line 10) can be language or compiler dependent despite the fact that they are same here. In Fig. 4.3, we introduce for the first time a variable with a single subscript (line 5) and containing five numbers (integers) to be manually initialized (lines 8-10) and then to be listed in a loop (lines 12-15) over all their values. Note that C++ stores the first entry in an array at position zero (see appendix listing), MATLAB uses position one, and F90 defaults to position one.

C++ and Fortran 90 allow a special option to create loops that run "forever." These could be used, for example, to read an unknown amount of data until terminated, in a non-fatal way, by the input statement. In C++, one omits the three loop controls, such as

```
for (;;) {// forever loop
    loop_block
    } // end forever loop
```

while in F90, one simply omits the loop control and gives only the DO command:

```
do ! forever
```

```
program  main
!  Examples of a simple loop in F90
implicit none
   integer  Integer_Var

     do Integer_Var = 0,4,1
         print *, 'The loop variable is:', Integer_Var
     end do ! over Integer_Var

     print *, 'The final loop variable is:', Integer_Var

end program main                  !  Running produces:
!  The loop variable is: 0
!  The loop variable is: 1
!  The loop variable is: 2
!  The loop variable is: 3
!  The loop variable is: 4
!  The final loop variable is: 5 <- NOTE
```

Figure 4.2: Typical Looping Concepts in F90

```
program  main
!  Examples of simple array indexing in F90
implicit none
  integer, parameter :: max = 5
  integer  Integer_Array(max) ! =(/ 10 20 30 40 50 /), or set below
  integer  loopcount

    Integer_Array(1) = 10   ! F90 index starts at 1, usually
    Integer_Array(2) = 20 ; Integer_Array(3) = 30
    Integer_Array(4) = 40 ; Integer_Array(5) = 50

    do loopcount = 1, max                          ! & means continued
        print *, 'The loop counter is: ', loopcount, &
         ' with an array value of: ',Integer_Array(loopcount)
    end do ! over loopcount

    print *, 'The final loop counter is: ', loopcount

end program main
!  Running produces:
! The loop counter is: 1 with an array value of: 10
! The loop counter is: 2 with an array value of: 20
! The loop counter is: 3 with an array value of: 30
! The loop counter is: 4 with an array value of: 40
! The loop counter is: 5 with an array value of: 50
! The final loop counter is: 6
```

Figure 4.3: Simple Array Indexing in F90

```
     loop_block
  end do ! forever
```

Most of the time, an infinite loop is used as a *loop_while_true* or a *loop_until_true* construct. These will be considered shortly.

4.3.2 Implied Loops

Fortran and MATLAB have shorthand methods for constructing "implied loops." Both languages offer the colon operator to imply an incremental range of integer values. Its syntax and types of applications are given in Table 4.6 (page 56). The allowed usages of the operator differ slightly between the two languages. Note that this means that the loop controls are slightly different in that the `do` control employs commas instead of colons. For example, two equivalent loops are

Fortran	MATLAB
`do k=B,E,I` `  A(k) = k**2` `end do`	`for k=B:I:E` `  A(k) = k^2` `end`

Fortran offers an additional formal implied `do` loop that replaces the `do` and `end do` with a closed pair of parentheses in the syntax:

```
(object, k = B,E,I)
```

where again the increment, `I`, defaults to unity if not supplied. The above implied `do` is equivalent to the formal loop

```
do k=B,E,I
  define object
end do
```

However, the object defined in the implied loop can only be utilized for four specific Fortran operations: *1)* `read` actions, *2)* `print` and `write` actions, *3)* `data` variables (not value) definitions, and *4)* defining array elements. For example,

```
print *, (4*k-1, k=1,10,3) ! 3, 15, 27, 39
read *, (A(j,:), j=1,rows) ! read A by rows, sequentially
```

The implied `do` loops can be nested to any level like the standard `do` statement. One simply makes the inner loop the object of the outer loop, so that

```
((object_j_k, j=min, max), k=k1,k2,inc)
```

implies the nested loop

```
do k=k1,k2,inc
  do j=min, max
    use object_j_k
  end do ! over j
end do ! over k
```

For example,

```
print *, (((A(k)*B(j)+3), j=1,5), k=1,max)
! read array by rows in each plane
read *, (((A(i,j,k), j=1,cols), i=1,rows), k=1,max)
```

Actually, there is even a simpler default form of implied `do`s for reading and writing arrays. That default is to access arrays by columns. That is, process the leftmost subscript first. Thus, for an array with three subscripts,

```
read *, A   ⟺   read *, (((A(i,j,k), i=1,rows), j=1,cols), k=1,planes)
```

Both languages allow the implied loops to be employed to create an array vector simply by placing the implied loop inside the standard array delimit symbols. For example, we may want an array to equally distribute $N + 1$ points over the distance from zero to D.

F90: `X = (/(k,k=0,N)/)* D/(N+1)`
MATLAB: `X = [0:N] * D / (N+1),`

which illustrates that MATLAB allows the use of the colon operator to define arrays, but F90 does not.

In addition to locating elements in an array by the regular incrementing of loop variables, both Fortran90 and MATLAB support even more specific selections of elements: by random location via vector subscripts, or by value via logical masks such as `where` and `if` in F90 and MATLAB, respectively.

4.3.3 Conditionals

Logic tests are frequently needed to control the execution of a block of statements. The most basic operation occurs when we want to do something when a logic test gives a true answer. We call that a simple `IF` statement. When the test is true, the program executes the block of statements following the `IF`. Often only one statement is needed, so C++ and Fortran allow that one statement to end the line that begins with the `IF` logic. Frequently we will *nest* another `IF` within the statements from a higher level `IF`. The common language syntax forms for the simple `IF` are given below in Table 4.10, along with the examples of where a second true group is nested inside the first as shown in Table 4.11.

The next simplest case is where we need to do one thing when the answer is true, and a different thing when the logic test is false. Then the syntax changes simply to an `IF` {*true group*} `ELSE` {*false group*} mode of execution. The typical `IF-ELSE` syntaxes of the various languages are given in Table 4.12. Of course, the above statement groups can contain other `IF` or `IF-ELSE` statements nested within them. They can also contain any valid statements, including `DO` or `FOR` loops.

The most complicated logic tests occur when the number of cases for the answer go beyond the two (true-false) of the `IF-ELSE` control structure. These multiple case decisions can be handled with the `IF-ELSEIF-ELSE` control structures whose syntax is given in Table 4.13. They involve a sequence of logic

MATLAB	Fortran	C++
`if l_expression` *true group* `end`	`IF (l_expression) THEN` *true group* `END IF`	`if (l_expression)` { *true group;* }
	`IF (l_expression)` *true statement*	`if (l_expression)` *true statement;*

Table 4.10: `IF` Constructs. The quantity `l_expression` means a logical expression having a value that is either `TRUE` of `FALSE`. The term *`true statement`* or *`true group`* means that the statement or group of statements, respectively, are executed if the conditional in the `if` statement evaluates to `TRUE`.

MATLAB	Fortran	C++
`if l_expression1` *true group A* `if l_expression2` *true group B* `end` *true group C* `end` *statement group D*	`IF (l_expression1) THEN` *true group A* `IF (l_expression2) THEN` *true group B* `END IF` *true group C* `END IF` *statement group D*	`if (l_expression1)` { `true group A` `if (l_expression2)` { *true group B* } *true group C* } *statement group D*

Table 4.11: Nested `IF` Constructs.

MATLAB	Fortran	C++
`if l_expression` *true group A* `else` *false group B* `end`	`IF (l_expression) THEN` *true group A* `ELSE` *false group B* `END IF`	`if (l_expression)` { *true group A* } `else` { *false group B* }

Table 4.12: Logical `IF-ELSE` Constructs.

tests, each of which is followed by a group of statements that are to be executed if, and only if, the test answer is true. There can be any number of such tests. They are terminated with an `ELSE` group of default statements to be executed if *none* of the logic tests are true. Actually, the `ELSE` action is optional. For program clarity or debugging, it should be included even if it only prints a warning message or contains a comment statement. Typical “if” and “if-else” coding is given in Figs. 4.4, 4.5, and 4.6. Figure 4.4 simply uses the three logical comparisons of “greater than” (line 9), “less than” (line 12), or “equal to” (line 15), respectively. Figure 4.5 goes a step further by combining two tests with a logical “and” test (line 9), and includes a second else branch (line 11) to handle the case where the `if` is false. While the input to these programs were numbers (line 7), the third example program in Fig. 4.6 accepts logical input (lines 6,8) that represents either true or false values and carries out Boolean operations to negate an input (via `NOT` in line 9), or to compare two inputs (with an `AND` in line 11, or `OR` in line 17, etc.) to produce a third logical value.

Since following the logic of many `IF-ELSEIF-ELSE` statements can be very confusing both the C++ and Fortran languages allow a `CASE` selection or “switching” operation based on the value (numerical or character) of some expression. For any allowed specified `CASE` value, a group of statements is executed. If the value does not match any of the specified allowed `CASE` values, then a default group of statements are executed. These are illustrated in Table 4.14.

<table>
<tr><th>MATLAB</th><th>Fortran</th><th>C++</th></tr>
<tr>
<td>if l_expression1
  true group A
elseif l_expression2
  true group B
elseif l_expression3
  true group C
else
  default group D
end</td>
<td>IF (l_expression1) THEN
  true group A
ELSE IF (l_expression2) THEN
  true group B
ELSE IF (l_expression3) THEN
  true group C
ELSE
  default group D
END IF</td>
<td>if (l_expression1)
  {
  true group A
  }
else if (l_expression2)
  {
  true group B
  }
else if (l_expression3)
  {
  true group C
  }
else
  {
  default group D
  }</td>
</tr>
</table>

Table 4.13: Logical `IF-ELSE-IF` Constructs.

```
program main
! Examples of relational "if" operator in F90
implicit none
   integer :: Integer_Var_1, Integer_Var_2      ! user inputs

     print *, 'Enter two integers:'
     read  *, Integer_Var_1, Integer_Var_2

     if ( Integer_Var_1 > Integer_Var_2 ) &
       print *, Integer_Var_1,' is greater than ', Integer_Var_2

     if ( Integer_Var_1 < Integer_Var_2 ) &
       print *, Integer_Var_1,' is less than ', Integer_Var_2

     if ( Integer_Var_1 == Integer_Var_2 ) &
       print *, Integer_Var_1,' is equal to ', Integer_Var_2

end program main

!  Running with 25 and 4 produces:
! Enter two integers:
! 25  is greater than 4
```

Figure 4.4: Typical Relational Operators in F90

```
program main
!  Illustrate a simple if-else logic in F90
implicit none
   integer Integer_Var

     print *,'Enter an integer: '
     read  *, Integer_Var

     if ( Integer_Var > 5 .and. Integer_Var < 10 ) then
        print *, Integer_Var, ' is greater than 5 and less than 10'
     else
        print *, Integer_Var, ' is not greater than 5 and less than 10'
     end if ! range of input

end program main
!
! Running with 3 gives: 3  is not greater than 5 and less than 10
! Running with 8 gives: 8  is greater than 5 and less than 10
```

Figure 4.5: Typical If-Else Uses in F90

Fortran90 offers an additional optional feature called *construct names* that can be employed with the above `IF` and `SELECT CASE` constructs to improve the readability of the program. The optional name, followed by a colon, precedes the key words `IF` and `SELECT CASE`. To be consistent, the name should also follow the key words `END IF` or `END SELECT` which always close the constructs. The construct name option also is available for loops where it offers an additional pair of control actions that will be explained later. Examples of these optional F90 features are given in Table 4.15.

While C++ and MATLAB do not formally offer this option, the same enhancement of readability can

```
program main
!  Examples of Logical operators in F90
implicit none
  logical :: Logic_Var_1, Logic_Var_2
    print *,'Print logical value of A (T or F):'
    read  *, Logic_Var_1
    print *,'Print logical value of B (T or F):'
    read  *, Logic_Var_2
    print *,'NOT A is ', (.NOT. Logic_Var_1)

    if ( Logic_Var_1 .AND. Logic_Var_2 ) then
      print *, 'A ANDed with B is true'
    else
      print *, 'A ANDed with B is false'
    end if ! for AND

    if ( Logic_Var_1 .OR. Logic_Var_2 ) then
      print *, 'A ORed with B is true'
    else
      print *, 'A ORed with B is false'
    end if ! for OR

    if ( Logic_Var_1 .EQV. Logic_Var_2 ) then
      print *, 'A EQiValent with B is true'
    else
      print *, 'A EQiValent with B is false'
    end if ! for EQV

    if ( Logic_Var_1 .NEQV. Logic_Var_2 ) then
      print *, 'A Not EQiValent with B is true'
    else
      print *, 'A Not EQiValent with B is false'
    end if ! for NEQV

end program main
! Running with T and F produces:
! Print logical value of A (T or F): T
! Print logical value of B (T or F): F
! NOT A is F
! A ANDed with B is false
! A ORed with B is true
! A EQiValent with B is false
! A Not EQiValent with B is true
```

Figure 4.6: Typical Logical Operators in F90

F90	C++
SELECT CASE (expression) CASE (value 1) *group 1* CASE (value 2) *group 2* : : CASE (value n) *group n* CASE DEFAULT *default group* END SELECT	switch (expression) { case value 1 : *group 1* break; case value 2 : *group 2* break; : : case value n : *group n* break; default: *default group* break; }

Table 4.14: Case Selection Constructs.

be achieved by using the trailing comment feature to append a name or description at the beginning and end of these logic construct blocks.

Both C++ and Fortran allow statement labels and provide controls to branch to specific labels. Today you are generally advised **not** to use a `GO TO` and its associated label! However, they are common in many F77 codes. There are a few cases where a `GO TO` is still considered acceptable. For example, the pseudo-`WHILE` construct of F77 requires a `GO TO`.

F90 Named `IF`	F90Named `SELECT`
`name: IF (logical_1) THEN` *true group A* `ELSE IF (logical_2) THEN` *true group B* `ELSE` *default group C* `ENDIF name`	`name: SELECT CASE (expression)` `CASE (value 1)` *group 1* `CASE (value 2)` *group 2* `CASE DEFAULT` *default group* `END SELECT name`

Table 4.15: F90 Optional Logic Block Names.

Fortran	C++
`DO 1 ...` `DO 2 ...` `...` `IF (disaster) THEN` `GO TO 3` `END IF` `...` `2  END DO` `1 END DO` `3` *next statement*	`for (...) {` `for (...) {` `...` `if (disaster)` `go to error` `...` `}` `}` `error:`

Table 4.16: `GO TO` Break-out of Nested Loops. This situation can be an exception to the general recommendation to avoid `GO TO` statements.

F77	F90	C++
`DO 1 I = 1,N` `...` `IF (skip condition) THEN` `GO TO 1` `ELSE` *false group* `END IF` `1 continue`	`DO I = 1,N` `...` `IF (skip condition) THEN` `CYCLE ! to next I` `ELSE` *false group* `END IF` `END DO`	`for (i=1; i<n; i++)` `{` `if (skip condition)` `continue; // to next` `else if` *false group* `end` `}`

Table 4.17: Skip a Single Loop Cycle.

```
initialize test
IF (l_expression) THEN
    true statement group
    modify logical value
    GO TO #
END IF
```

The `GO TO` can also be effectively utilized in both Fortran and C++ to break out of several nested loops. This is illustrated in Table 4.16. The "break-out" construct can be used in the situation when, as a part of a subroutine, you wanted the program exit the loop and also exit the subroutine, returning control to the calling program. To do that, one would simply replace the `GO TO` statement with the `RETURN` statement. In F90, one should also append the comment "! to calling program" to assist in making the subroutine more readable.

You may find it necessary to want to skip a cycle in loop execution and/or exit from a single loop. Both Fortran and C++ provide these control options without requiring the use of a `GO TO`. To skip a loop cycle, Fortran90 and C++ use the statements `CYCLE` and `continue`, respectively, and `EXIT` and `break` to abort a loop. These constructs are shown in Tables 4.17 and 4.18. Other forms of the `GO TO` in F77 were declared obsolete in F90, and should not be used. The Fortran abort examples could also use the `RETURN` option described above in the rare cases when it proves to be more desirable or efficient.

As mentioned earlier, F90 allows the programmer to use "named" `DO` constructs. In addition to im-

F77	F90	C++
`DO 1 I = 1,N` `  IF (exit condition) THEN` `    GO TO 2` `  ELSE` `    false group` `  END IF` `1 CONTINUE` `2 next statement`	`DO I = 1,N` `  IF (exit condition) THEN` `    EXIT ! this do` `  ELSE` `    false group` `  END IF` `END DO` `next statement`	`for (i=1; i<n; i++)` `  {` `  if (exit condition)` `    break;// out of loop` `  else if` `    false group` `  end` `  }` `next statement`

Table 4.18: Abort a Single Loop.

```
main: DO ! forever
  test: DO k=1,k_max
    third: DO m=m_max,m_min,-1
      IF (test condition) THEN
        CYCLE test ! loop on k
      END IF
    END DO third ! loop on m
    fourth: DO n=n_min,n_max,2
      IF (main condition) THEN
        EXIT main ! forever loop
    END DO fourth ! on n
  END DO test ! over k
END DO main
next statement
```

Table 4.19: F90 `DO`s Named for Control.

proving readability, this feature also offers additional control over nested loops because we can associate the `CYCLE` and `EXIT` commands with a specific loop (Table 4.19). Without the optional name, the `CYCLE` and `EXIT` commands act only on the inner-most loop in which they lie. We will see later that Fortran90 allows another type of loop called `WHERE` that is designed to operate on arrays.

4.3.3.1 Looping While True or Until True

It is very common to need to perform a loop so long as a condition is true, or to run the loop until a condition becomes `true`. The two are very similar and both represent loops that would run forever unless specifically terminated. We will refer to these two approaches as `WHILE` loops and `UNTIL` loops. The `WHILE` logic test is made first in order to determine if the loop will be entered. Clearly, this means that if the logic test is `false` the first time it is tested, then the statement blocks controlled by the `WHILE` are never executed. If the `WHILE` loop is entered, something in the loop must eventually change the value of a variable in the logic test or the loop would run forever. Once a change causes the `WHILE` logic test to be `false` control is transferred to the first statement following the `WHILE` structure. By way of comparison, an `UNTIL` loop is always entered at least once. Upon entering the loop, a beginning statement group is executed. Then the logic test is evaluated. If the test result is `true`, the loop is exited and control is passed to the next statement after the group. If the test is `false`, then an optional second statement group is executed before the loop returns to the beginning statement group. The pseudo-code for these two similar structures are given as follows:

while true	until true
`logic_variable = true` `begin:` `if (logic_variable) then % true` `  true_group` `  re-evaluate logic_variable` `go to begin` `else  % false` `  exit loop` `end if`	`logic_variable = false` `begin:` `statements` `if (logic_variable) then` `  exit the loop` `else % false` `  false_group` `  re-evaluate logic_variable` `go to begin` `end if`

Since these constructs are commonly needed, several programming languages offer some support for them. For example, Pascal has a `REPEAT UNTIL` command and C++ has the `DO-WHILE` pair for the until-true construct. For the more common while-true loops, C++ and MATLAB offer a `WHILE` command, and Fortran 90 includes the `DO WHILE`. F77, however, only has the obsolete `IF-GO TO` pairs as illustrated in a previous example. Many current programmers consider the `WHILE` construct obsolete because it is less clear than a `DO-EXIT` pair or a "for-break" pair. Indeed, the F90 standard has declared the `DO WHILE` as obsolete and eligible for future deletion from the language. We can see how the loop-abort feature of C++ and F90 includes both the `WHILE` and `UNTIL` concepts. For example, the F90 construct

```
initialize logical_variable
DO WHILE (logical_variable) ! is true
  true_group
  re-evaluate logical_variable
END DO ! while true
      ⋮
```

is entirely equivalent to the aborted endless loop

```
initialize logical_variable
DO ! forever while true
  IF (.NOT. logical_variable) EXIT ! as false
  true_group
  re-evaluate logical_variable
END DO ! while true
      ⋮
```

Likewise, a minor change includes the UNTIL construct.

```
DO ! forever until true
  beginning statements and initialization
  IF (logical_expression) EXIT ! as true
    false group
    re-evaluate logical_variable
END DO ! until true
```

When approached in the C++ language, we have the `WHILE` loop.

```
initialize logical_variable
while (logical_variable)
  { // is true
  true_group
  re-evaluate logical_variable
  } // end while true
```

Recalling the standard `for` syntax,

```
for (expr_1; expr_2; expr_3)
  {
  true_group
  } // end for
```

could be viewed as equivalent to the above `WHILE` in `for` form.

```
expr_1;
while (expr_2)
  { // is true
  true_group
  expr_3;
  } // end while true
```

If one omits all three `for` expressions, then it becomes an "infinite loop" or a "do forever" which can represent a `WHILE` or `UNTIL` construct by proper placement of the `break` command. Furthermore, C has the `do-while` construct that is equivalent to Pascal's `REPEAT-UNTIL`.

```
do // forever until true
  statements
  evaluate logical_variable
while (logical_variable) // is true
```

The syntax for the classical `WHILE` statements in C++, Fortran and MATLAB are given in Table 4.20. Fortran90 has declared the `DO WHILE` as obsolete, and recommends the `DO-EXIT` pair instead! Using infinite loops with clearly aborted stages is a less error-prone approach to programming.

MATLAB	C++
initialize test while l_expression true group change test end	*initialize test* while (l_expression) { *true group* *change test* }

F77	F90
initialize test # continue IF (l_expression) THEN *true group* *change test* go to # END IF	initialize test do while (l_expression) *true group* *change test* end do

Table 4.20: Looping While a Condition is True.

Function Type	MATLAB[a]	C++	Fortran
program	*statements* [y1...yn]=f(a1,...,am) [end of file]	main(argc,char **argv) { *statements* y = f(a1,I,am); }	program main type y type a1,...,type am *statements* y = f(a1,...,am) call s(a1,...,am) end program
subroutine		void f (type a1,...,type am) { *statements* }	subroutine s(a1,...,am) type a1,...,type am *statements* end
function	function [r1...rn] =f(a1,...,am) *statements*	type f (type a1,...,type am) { *statements* }	function f(a1,...,am) type f type a1,...,type am *statements* end

[a]Every function or program in MATLAB must be in separate files.

Table 4.21: Function definitions. In each case, the function being defined is named `f` and is called with `m` arguments `a1,...,am`.

4.4 Subprograms

The concept of modular programming requires the use of numerous subprograms or procedures to execute independent segments of the calculations or operations. Typically, these procedures fall into classes such as functions, subroutines, and modules. We will consider examples of the procedures for each of our target languages. These are shown in Table 4.21.

Recall that Table 8.6 compared several intrinsic functions that are common to both F90 and MATLAB. For completeness, all of the Fortran90 functions are listed both alphabetically and by subject in Appendix B. Similar listings for MATLAB can be found in the MATLAB *Primer*.

4.4.1 Functions and Subroutines

Historically, a function was a subprogram that employed one or more input arguments and returned a single result value. For example, a square root or logarithm function would accept a single input value and return a single result. All of the languages of interest allow the user to define such a function, and they

One-Input, One-Result Procedures	
MATLAB	`function out = name (in)`
F90	`function name (in) ! name = out`
	`function name (in) result (out)`
C++	`name (in, out)`*

Multiple-Input, Multiple-Result Procedures	
MATLAB	`function [inout, out2] = name (in1, in2, inout)`
F90	`subroutine name (in1, in2, inout, out2)`*
C++	`name(in1, in2, inout, out2)`*

* Other arrangements acceptable

Table 4.22: Arguments and return values of subprograms.

all provide numerous intrinsic or built-in functions of this type. As you might expect, such a procedure is called a *function* in C++, Fortran and MATLAB. As an example of such a procedure, consider the calculation of the mean value of a sequence of numbers defined as

$$\text{mean} = \frac{1}{n}\sum_{k=1}^{n} x_k \ .$$

In Fortran90, a subprogram to return the mean (average) could be

```
function mean(x)
! mean = sum of vector x, divided by its size
  real ::  mean, x(:)
    mean = sum(x)/size(x)
end function mean
```

Note that our function has employed two other intrinsic functions: `size` to determine the number of elements in the array `x`, and `sum` to carry out the summation of all elements in `x`. Originally in Fortran, the result value was required to be assigned to the name of the function. That is still a valid option in F90, but today it is considered better practice to specify a result value name to be returned by the function. The `mean` function is a MATLAB intrinsic and can be used directly.

To illustrate the use of a result value, consider the related “median” value in F90.

```
function mid_value(x) result(median)
! return the middle value of vector x
  real :: median, x(:)
    median = x(size(x)/2) ! what if size = 1 ??
end function mid_value
```

To apply these two functions to an array, say `y`, we would simply write `y_ave = mean(y)`, and `y_mid = mid_value(y)`, respectively. While Fortran allows a “function” to return only a single object, both C++ and MATLAB use that subprogram name to return any number of result objects. Fortran employs the name “subroutine” for such a procedure. Such procedures are allowed to have multiple inputs and multiple outputs (including none). The syntax of the first line of these two subprogram classes are shown in Table 4.22. Note that a typical subprogram may have no arguments, multiple input arguments (`in1, in2, inout`), multiple result arguments (`inout, out2`), and arguments that are used for both input and result usage (`inout`). These example names have been selected to reflect the fact that a programmer usually intends for arguments to be used for input only, or for result values only, or for input, modification, and output. It is considered good programming practice to declare such intentions to aid the compiler in detecting unintended uses. F90 provides the `INTENT` statement for this purpose, but does not require its use.

Having outlined the concepts of subprograms, we will review some presented earlier and then give some new examples. Figure 1.3 presented a clipping function which was earlier expressed in pseudocode. A corresponding Fortran implementation of such a clipping function is given in Fig. 4.7. Note that it is very similar to the pseudocode version.

```
  program main
!     clip the elements of an array
   implicit none
    real, parameter    :: limit = 3
    integer, parameter :: n = 5
    real               :: y(n), x(n)
!    Define x values that will be clipped
      x = (/ (-8. + 3.*k, k = 1,n) /)  ! an implied loop
      do i = 1, n
        y(i) = clip (x(i), limit)
      end do
      print *, x
      print *, y

  contains  ! methods

  function clip (x, L) result (c)
!   c = clip(x, L) - clip the variable x, output
!   x = scalar variable,                  input
!   L = limit of the clipper,             input
!
    real, intent(in) :: x, L   ! variable types
    real             :: c      ! variable types
    intent (in) x, L           ! argument uses
      if  ( abs(x) <= L ) then   ! abs of x less than or equal L
        c = x;                   ! then use x
      else                       ! absolute of x greater than L ?
        c = sign(L,x)            ! sign of x times L
      end if ! of value of x
    end function ! clip
  end program main
!
! produces:
! -5.0000000  -2.0000000   1.0000000   4.0000000   7.0000000
! -3.0000000  -2.0000000   1.0000000   3.0000000   3.0000000
```

Figure 4.7: Clipping a Set of Array Values in F90

For the purpose of illustration an alternate F90 version of the Game of Life, shown earlier in Chapter 1 as pseudocode, is given in the assignment solutions section. Clearly we have not introduced all the features utilized in these example codes so the reader should continue to refer back to them as your programming understanding grows.

A simple program that illustrates program composition is `maximum.f90`, which asks the user to specify several integers from which the program finds the largest. It is given in Fig. 4.8. Note how the main program accepts the user input (lines 15,20), with the `maxint` function (line 22) finding the maximum (lines 25-34). Perhaps modularity would have been better served by expressing the input portion by a separate function. Of course, this routine is not really needed since F90 provides intrinsic functions to find maximum and minimum values (`maxval, minval`) and their locations in any array (`maxloc, minloc`). A similar C++ program composition is shown for comparison in the appendix.

```
program maximum ! of a set of integers (see intrinsic maxval)
 implicit none
  interface ! declare function interface protype
    function maxint (input, input_length) result(max)
    integer, intent(in) :: input_length, input(:)
    integer             :: max
    end function ! maxint
  end interface

  integer, parameter :: ARRAYLENGTH=100
  integer            :: integers(ARRAYLENGTH);
  integer            :: i, n;

  ! Read in the number of integers
     print *,'Find maximum; type n: '; read *, n
     if ( n > ARRAYLENGTH .or. n < 0 ) &
         stop 'Value you typed is too large or negative.'

     do i = 1, n           ! Read in the user's integers
        print *, 'Integer ', i, '?'; read  *, integers(i)
     end do ! over n values
     print *, 'Maximum: ', maxint (integers, n)
end program maximum

function maxint (input, input_length) result(max)
! Find the maximum of an array of integers
  integer, intent(in) :: input_length, input(:)
  integer             :: i, max

    max = input(1);   ! initialize
     do i = 1, input_length ! note could be only 1
       if ( input(i) > max ) max = input(i);
     end do ! over values
end function maxint                ! produces this result:
! Find maximum; type n:  4
! Integer  1?  9
! Integer  2?  6
! Integer  3?  4
! Integer  4?  -99
! Maximum:  9
```

Figure 4.8: Search for Largest Value in F90

Global Variable Declaration	
MATLAB	`global` list of variables
F77	`common` /set_name/ list of variables
F90	`module` set_name `save` `type` (type_tag) :: list of variables `end module` set_name
C++	`extern` list of variables

Access to Global Variables	
MATLAB	`global` list of variables
F77	`common` /set_name/ list of variables
F90	`use` set_name, `only` subset of variables `use` set_name2 list of variables
C++	`extern` list of variables

Table 4.23: Defining and referring to global variables.

4.4.2 Global Variables

We have seen that variables used inside a procedure can be thought of as dummy variable names that exist only in the procedure, unless they are members of the argument list. Even if they are arguments to the procedure, they can still have names different from the names employed in the calling program. This approach can have disadvantages. For example, it might lead to a long list of arguments, say 20 lines, in a complicated procedure. For this and other reasons, we sometimes desire to have variables that are accessible by any and all procedures at any time. These are called *global variables* regardless of their type.

Generally, we explicitly declare them to be global and provide some means by which they can be accessed, and thus modified, by selected procedures. When a selected procedure needs, or benefits from, access to a global variable, one may wish to control which subset of global variables are accessible by the procedure. The typical initial identification of global variables and the ways to access them are shown in Table 4.23, respectively.

An advanced aspect of the concept of global variables are the topics of inheritance and object-oriented programming. Fortran90, and other languages like C++, offer these advanced concepts. In F90, inheritance is available to a `module` and/or a main `program` and their "internal sub-programs" defined as those procedures following a `contains` statement, but occurring before an `end module` or the `end program` statement. Everything that appears before the `contains` statement is available to, and can be changed by, the internal sub-programs. Those inherited variables are more than local in nature, but not quite global; thus, they may be thought of as *territorial* variables. The structure of these internal sub-programs with inheritance is shown in Fig. 4.9

Perhaps the most commonly used global variables are those necessary to calculate the amount of central processor unit (cpu) time, in seconds, that a particular code segment used during its execution. All systems provide utilities for that purpose but some are more friendly than others. MATLAB provides a pair of functions, called `tic` and `toc`, that act together to provide the desired information. To illustrate the use of global variables we will develop a F90 module called `tic_toc` to hold the necessary variables along with the routines `tic` and `toc`. It is illustrated in Fig. 4.10 where the module constants (lines 2-6) are set (lines 17, 26) and computed (line 28) in the two `internal` functions.

```
module or program  name_inherit
     Optional territorial variable, type specification, and calls
     contains

            subroutine  Internal_1
            territorial specifications and calls
            contains

                  subroutine  Internal_2
                  local computations
                  end subroutine  Internal_2

                  subroutine  Internal_3
                  local computations
                  end subroutine  Internal_3

            end subroutine  Internal_1

end  name_inherit
```

Figure 4.9: F90 Internal Subprogram Structure.

```
module tic_toc
! Define global constants for timing increments
 implicit none
   integer  :: start  ! current value of system clock
   integer  :: rate   ! system clock counts/sec
   integer  :: finish ! ending value of system clock
   real     :: sec    ! increment in sec, (finish-start)/rate
  ! Useage:   use tic_toc      ! global constant access
  !           call tic         ! start clock
  !           . . .            ! use some cpu time
  !           cputime = toc () ! for increment
contains ! access to start, rate, finish, sec
  subroutine  tic
! ---------------------------------------------------
! Model the matlab tic function, for use with toc
! ---------------------------------------------------
    implicit none
      call system_clock ( start, rate ) ! Get start value and rate
  end subroutine tic

  function  toc ( ) result(sec)
! ---------------------------------------------------
! Model the matlab toc function, for use with tic
! ---------------------------------------------------
    implicit none
    real    :: sec
      call system_clock ( finish )         ! Stop the execution timer
      sec = 0.0
      if ( finish >= start ) sec = float(finish - start) / float(rate)
  end function toc
end module tic_toc
```

Figure 4.10: A Module for Computing CPU Times

Action	C++	F90
Bitwise AND	`&`	`iand`
Bitwise exclusive OR	`^`	`ieor`
Bitwise exclusive OR	`|`	`ior`
Circular bit shift		`ishftc`
Clear bit		`ibclr`
Combination of bits		`mvbits`
Extract bit		`ibits`
Logical complement	`~`	`not`
Number of bits in integer	`sizeof`	`bit_size`
Set bit		`ibset`
Shift bit left	`<<`	`ishft`
Shift bit right	`>>`	`ishft`
Test on or off		`btest`
Transfer bits to integer		`transfer`

Table 4.24: Bit Function Intrinsics.

4.4.3 Bit Functions

We have discussed the fact that the digital computer is based on the use of individual bits. The subject of bit manipulation is one that we do not wish to pursue here. However, advanced applications do sometimes require these abilities, and the most common uses have been declared in the so-called *military standards* USDOD-MIL-STD-1753, and made part of the Fortran90 standard. Several of these features are also a part of C++. Table 4.24 gives a list of those functions.

4.4.4 Exception Controls

An exception handler is a block of code that is invoked to process specific error conditions. Standard exception control keywords in a language are usually associated with the allocation of resources, such as files or memory space, or input/output operations. For many applications we simply want to catch an unexpected result and output a message so that the programmer can correct the situation. In that case we may not care if the exception aborts the execution. However, if one is using a commerical execute only program then it is very distubing to have a code abort. We would at least expect the code to respond to a fatal error by closing down the program in some gentle fashion that saves what was completed before the error and maybe even offer us a restart option. Here we provide only the minimum form of an exceptions module that can be used by other modules to pass warnings of fatal messages to the user. It includes an integer flag that can be utilized to rank the severity of possible messages. It is shown in Fig. 4.11. Below we will summarize the F90 optional error flags that should always be checked and are likely to lead to a call to the exception handler.

Dynamic Memory: The `ALLOCATE` and `DEALLOCATE` statements both use the optional flag `STAT=` to return an integer flag that can be tested to invoke an exception handler. The integer value is zero after a successful (de)allocation, and a positive value otherwise. If `STAT=` is absent, an unsuccessful result stops execution.

File Open/Close: The `OPEN`, `CLOSE`, and `ENDFILE` statements allow the use of the optional keyword `IOSTAT=` to return an integer flag which is zero if the statement executes successfully, and a positive value otherwise. They also allow the older standard exception keyword `ERR=` to be assigned a positive integer constant label number of the statement to which control is passed if an error occurs. An exception handler could be called by that statement.

File Input/Output: The `READ`, `WRITE`, `BACKSPACE`, and `REWIND` statements allow the `IOSTAT=` keyword to return a negative integer if an end-of-record (EOR) or end-of-file (EOF) is encountered, a zero if there is no error, and a positive integer if an error occurs (such as reading a character during an

```
module exceptions
 implicit none
  integer, parameter :: INFO = 1, WARN = 2, FATAL = 3
  integer            :: error_count = 0
  integer            :: max_level   = 0
contains

 subroutine exception (program, message, flag)
   character(len=*)     :: program
   character(len=*)     :: message
   integer,    optional :: flag

     error_count = error_count + 1

     print *, 'Exception Status Thrown'
     print *, '  Program :', program
     print *, '  Message :', message
     if ( present(flag) ) then
       print *, '  Level   :', flag
       if ( flag > max_level ) max_level = flag
     end if ! flag given
 end subroutine exception

 subroutine exception_status ()
   print *
   print *, "Exception Summary:"
   print *, "  Exception count = ", error_count
   print *, "  Highest level   = ", max_level
 end subroutine exception_status
end module exceptions
```

Figure 4.11: A Minimal Exception Handling Module

integer input). They also allow the `ERR=` error label branching described above for the file open/close operations.

In addition, the `READ` statement also retains the old standard keyword `END=` to identify a label number to which control transfers when an end-of-file (EOF) is detected.

Status Inquiry: Whether in `UNIT` mode or `FILE` mode, the `INQUIRE` statement for file operations allows the `IOSTAT=` and `ERR=` keywords like the `OPEN` statement. In addition, either mode supports two logical keywords: `EXISTS=` to determine if the `UNIT` (or `FILE`) exists, and `OPENED=` to determine if a (the) file is connected to this (an) unit.

Optional Arguments: The `PRESENT` function returns a logical value to indicate whether or not an optional argument was provided in the invocation of the procedure in which the function appears.

Pointers and Targets: The `ASSOCIATED` function returns a logical value to indicate whether a pointer is associated with a specific target, or with any target.

4.5 Interface Prototype

Compiler languages are more efficient than interpreted languages. If the compiler is going to correctly generate calls to functions, or subprograms, it needs to know certain things about the arguments and returned values. The number of arguments, their type, their rank, their order, etc. must be the same. This collection of information is called the "interface" to the function, or subprogram. In most of our example codes the functions and subprograms have been included in a single file. In practice they are usually stored in separate external files, and often written by others. Thus, the program that is going to use these external files must be given a "prototype" description of them. In other words, a segment of prototype, or interface, code is a definition that is used by the compiler to determine what parameters are required by the subprogram as it is called by your program. The interface prototype code for any subprogram can usually be created by simply copying the first few lines of the subprogram (and maybe the last one) and placing them in an interface directory.

To successfully compile a subprogram modern computer science methods sometimes require the programmer to specifically declare the interface to be used in invoking a subprogram, even if that subprogram is included in the same file. This information is called a "prototype" in C and C++, and an "interface" in F90. If the subprogram already exists, one can easily create the needed interface details by making a copy of the program and deleting from the copy all information except that which describes the arguments and subprogram type. If the program does not exist, you write the interface first to define what will be expected of the subprogram regardless of who writes it. It is considered good programming style to include explicit interfaces, or prototype code, even if they are not required.

If in doubt about the need for an explicit interface see if the compiler gives an error because it is not present. In F90 the common reasons for needing an explicit interface are: *1)* Passing an array that has only its rank declared. For example, `A(:,:), B(:)`. These are known as "assumed-shape" arrays; *2)* Using a function to return a result that is: *a)* an array of unknown size, or *b)* a pointer, or *c)* a character string with a dynamically determined length. Advanced features like optional argument lists, user defined operators, generic subprogram names (to allow differing argument types) also require explicit operators.

In C++ before calling an external function, it must be declared with a prototype of its parameters. The general form for a function is

```
function_type function_name ( argument_type_list);
```

where the `argument_type_list` is the comma separated list of pairs of type and name for each argument of the function. These names are effectively treated as comments, and may be different from the names in the calling program, or even omitted. The use of a prototype was shown in Fig. 4.8 and is used again in Fig. 4.12 which also illustrates passing arguments by reference or by value.

An interface block for external subprograms was not required by F77 (thereby leading to hard to find errors), but is strongly recommended if F90 and is explicitly required in several situations. The general form for a F90 interface is

```
 interface interface_name
     function_interface_body
     subroutine_interface_body
     module_procedure_interface_body
 end interface interface_name
```

where a typical function_interface_body would be

```
function_type function_name (argument_name_list) result ( name )
  implicit none
  argument_type, intent_class :: name_list
end function function_name
```

where the argument_name_list is the comma separated list of names. Of course, the function_type refers to the result argument name. These names may be different from the names in the calling program. A typical subroutine_interface_body would be

```
subroutine subroutine_name (argument_name_list)
  implicit none
   argument_type, intent_class :: name_list
end subroutine subroutine_name
```

where the argument_name_list is the comma separated list of names. The topic of a module procedure is covered elsewhere. The use of a interface block was shown in Fig. 4.8 and used in two new codes, shown in Fig. 4.12, and the corresponding C++ code in the appendix, which also illustrate passing arguments by reference (line 23) and by value (line 19) in both F90 and C++. The important, and often confusing, topic of passing by reference or value was discussed in Sec. 4.2 and is related to other topics to be considered later, such as the use of "pointers" in C++ and F90, and the "intent" attribute of F90 arguments. Passing by reference is default in F90 while passing by value is default in C++ .

4.6 Characters and Strings

All of our example languages offer convenient ways to manipulate and compare strings of characters. The characters are defined by one of the international standards such as ASCII, which is usually used on UNIX, or the EBCDIC set. These contain both printable and non-printable (control) characters. On a UNIX system, the full set can be seen with the command `man ascii`. In the 256-character ASCII set, the upper case letters begin at character number 65, 'A', and the corresponding lower case values are

```
program main
implicit none
!  declare the interface prototypes
interface
  subroutine  Change (Refer)
    integer :: Refer; end subroutine Change
  subroutine No_Change (Value)
    integer :: Value; end subroutine No_Change
end interface

! illustrate passing by reference and by value in F90

  integer :: Input_Val, Dummy_Val

    print *, "Enter an integer: "
    read *, Input_Val; print *, "Input value was ", Input_Val

  ! pass by value
    call No_Change ( (Input_Val) )  !  Use but do not change
    print *, "After No_Change it is ", Input_Val

  ! pass by reference
    call Change ( Input_Val )       !  Use and change
    print *, "After Change it is ", Input_Val
end program

  subroutine  Change (Refer)
  ! changes Refer in calling code IF passed by reference
    integer :: Refer
      Refer = 100;
      print *, "Inside Change it is set to ", Refer
  end subroutine Change

  subroutine No_Change (Value)
  ! does not change Value in calling code IF passed by value
    integer :: Value
      Value  = 100;
      print *, "Inside No_Change it is set to ", Value
  end subroutine No_Change

! Running gives:
! Enter an integer: 12
! Input value was  12
! Inside No_Change it is set to  100
! After No_Change it is  12
! Inside Change it is set to  100
! After Change it is  100
```

Figure 4.12: Passing Arguments by Reference and by Value in F90

32 positions higher (character 97 is 'a'). These printable characters begin at character 32, as shown in Table 4.25 for the ASCII standard. The first 33 characters are "non-printing" special control characters. For example, `NUL` = null, `EOT` = end of transmission, `BEL` = bell, `BS` = backspace, and `HT` = horizontal tab. To enter a control character, one must simultaneously hold down the `CONTROL` key and hit the letter that is 64 positions higher in the list. That is, an end of transmission `EOT` is typed as `CONTROL-D`. The code `SP` denotes the space character, and we will use the underscore "_" to represent a blank in strings.

We can employ the standard relational operators (e.g., less than) to compare strings and would find that ′bad′ < ′dog′ < ′same′ == ′same__′, that ′word′ > ′WORD′, and that ′four′ < ′one′ < ′two′ while ′1′ < ′2′ < ′4′. Note that the above equality occurred because trailing blanks are not considered in relational operations, *but* leading blanks are considered: ′same′ ≠ ′__same′. The F90 function `adjustL` removes leading blanks and appends them to the right end. Thus, it adjusts the string to the left, so that ′same′ == `adjustL`(′__same′). This and other F90 intrinsic character functions are summarized in Table 4.26.

All blanks are considered when determining the length of a character string. In F90 the intrinsic function `LEN` provides these data so that `LEN`(′same′) = 4, `LEN`(′__same′) = 6, and `LEN`(′same__′) = 7. There is another intrinsic function, `LEN_TRIM`, that provides the string length ignoring trailing blanks. By way of comparison: `LEN_TRIM`(′same′) = 4, `LEN_TRIM`(′__same′) = 6, and `LEN_TRIM`(′same__′) = 4. Each character in a string or any internal substrings may be referenced by the colon operator. Given a character variable we can define a substring, say `sub` as

```
sub = variable(K:L) for 0 < K,L <= LEN(variable)
    = null          for K > L
```

0	NUL	1	SOH	2	STX	3	ETX	4	EOT	5	ENQ	6	ACK	7	BEL
8	BS	9	HT	10	NL	11	VT	12	NP	13	CR	14	SO	15	SI
16	DLE	17	DC1	18	DC2	19	DC3	20	DC4	21	NAK	22	SYN	23	ETB
24	CAN	25	EM	26	SUB	27	ESC	28	FS	29	GS	30	RS	31	US
32	SP	33	!	34	"	35	#	36	$	37	%	38	&	39	’
40	(	41	)	42	*	43	+	44	,	45	-	46	.	47	/
48	0	49	1	50	2	51	3	52	4	53	5	54	6	55	7
56	8	57	9	58	:	59	;	60	<	61	=	62	>	63	?
64	@	65	A	66	B	67	C	68	D	69	E	70	F	71	G
72	H	73	I	74	J	75	K	76	L	77	M	78	N	79	O
80	P	81	Q	82	R	83	S	84	T	85	U	86	V	87	W
88	X	89	Y	90	Z	91	[	92	\	93	]	94	ˆ	95	_
96	‘	97	a	98	b	99	c	100	d	101	e	102	f	103	g
104	h	105	i	106	j	107	k	108	l	109	m	110	n	111	o
112	p	113	q	114	r	115	s	116	t	117	u	118	v	119	w
120	x	121	y	122	z	123	{	124	|	125	}	126	˜	127	DEL

Table 4.25: The ACSII Character Set

`ACHAR (I)`	Character number I in ASCII collating set
`ADJUSTL (STRING)`	Adjust left
`ADJUSTR (STRING)`	Adjust right
`CHAR (I) *`	Character I in processor collating set
`IACHAR (C)`	Position of C in ASCII collating set
`ICHAR (C)`	Position of C in processor collating set
`INDEX (STRING, SUBSTRING)`[a]	Starting position of a substring
`LEN (STRING)`	Length of a character entity
`LEN_TRIM (STRING)`	Length without trailing blanks
`LGE (STRING_A, STRING_B)`	Lexically greater than or equal
`LGT (STRING_A, STRING_B)`	Lexically greater than
`LLE (STRING_A, STRING_B)`	Lexically less than or equal
`LLT (STRING_A, STRING_B)`	Lexically less than
`REPEAT (STRING, NCOPIES)`	Repeated concatenation
`SCAN (STRING, SET)`[a]	Scan a string for a character in a set
`TRIM (STRING)`	Remove trailing blank characters
`VERIFY (STRING, SET)`[a]	Verify the set of characters in a string
`STRING_A//STRING_B`	Concatenate two strings

[a]Optional arguments not shown.

Table 4.26: F90 Character Functions

```
          = error          for K or L  >  LEN(variable).
```

For example, given the string ’howl’, then we can define `bird = string(2:4) = ’owl’`, and `prep = string(1:3) = ’how’`.

The F90 and F77 operator used to concatenate strings into larger strings is “`//`”. Continuing the last example, we see that the concatenation `string(1:3)//’_’//string(2:4)//’?’` is `’how_owl?’`, while the concatenation `’same__’//’word’` becomes `’same__word’` and `’bad’//’_’//’dog’` becomes `’bad_dog’`. Programs illustrating the reading and concatenating two strings are given in Fig. 4.13, and in the companion C++ code in the appendix.

Sometimes one needs to type in a non-printing character, such as a tab or a newline. To allow this, special transmissions have been allowed for, as summarized in Table 4.27.

Remember the ASCII character features: the uppercase letters correspond to numbers 65 through 90 in the list, while the lowercase letters are numbers 97 through 122, so that if we wanted to convert “G” to

```
program main
!  Compare two strings
!  Concatenate two character strings together
!  Get the combined length
  implicit none
  character(len=20) :: String1, String2
  character(len=40) :: String3
  integer           :: length

    print *,'Enter first string (20 char max):'
    read  '(a)', String1    ! formatted

    print *,'Enter second string (20 char max):'
    read  '(a)', String2    ! formatted

  ! compare
    if ( String1 == String2 ) then
      print *, "They are the same."
    else
      print *, "They are different."
    end if

  ! concatenate
    String3 = trim (String1) // trim (String2)

    print *,'The combined string is:', String3
    length = len_trim (String3)
    print *,'The combined length is:', length

end program main
!  Running with "red" and "bird" produces:
!  Enter first string (20 char max): red
!  Enter second string (20 char max): bird
!  They are different.
!  The combined string is: redbird
!  The combined length is: 7
!  Also "the red" and "bird" works
```

Figure 4.13: Using Two Strings in F90

Action	*ASCII Character*	F90 *Input*[a]	*C++ Input*
Alert (Bell)	7	Ctrl-G	\a
Backspace	8	Ctrl-H	\b
Carriage Return	13	Ctrl-M	\r
End of Transmission	4	Ctrl-D	Ctrl-D
Form Feed	12	Ctrl-L	\f
Horizontal Tab	9	Ctrl-I	\t
New Line	10	Ctrl-J	\n
Vertical Tab	11	Ctrl-K	\v

[a] "Ctrl-" denotes control action. That is, simultaneous pressing of the `CONTROL` key *and* the letter following.

Table 4.27: How to type non-printing characters.

"g" we could use commands such as:

```
character (len = 1) :: lower_g, UPPER_G
lower_g  = achar(iachar('G') + 32)
```

or visa versa:

```
UPPER_G  = achar(iachar('g') - 32)
```

since they differ by 32 locations. Likewise, since the zero character "0" occurs in position 48 of the ASCII set we could convert a single digit to the same numerical value with:

```
integer ::  number_5
number_5 = iachar('5') - 48
```

and so forth for all ten digits. To convert a string of digits, such as `'5623'`, to the corresponding number 5623, we could use a looping operation.

```
[ 1]  program  main
[ 2]  !  Convert a character string to an integer in F90
[ 3]    implicit none
[ 4]    character(len=5)  :: Age_Char
[ 5]    integer           :: age
[ 6]
[ 7]      print *, "Enter your age: "
[ 8]      read *, Age_Char                    ! a character string
[ 9]
[10]    ! convert using an internal file read
[11]      read (Age_Char, fmt = '(i5)') age  ! convert to integer
[12]
[13]      print *, "Your integer age is     ", age
[14]      print '(" Your binary age is      ", b8)', age
[15]      print '(" Your hexadecimal age is ", z8)', age
[16]      print '(" Your octal age is       ", o8)', age
[17]
[18]  end program main
[19]  !
[20]  ! Running gives:
[21]  ! Enter your age: 45
[22]  ! Your integer age is      45
[23]  ! Your binary age is       101101
[24]  ! Your hexadecimal age is      2D
[25]  ! Your octal age is            55
```

Figure 4.14: Converting a String to an Integer with F90

```
 character (len = 132) :: digits
 integer               :: d_to_n, power, number
!       Now build the number from its digits
 if (digits == ' ') then
   print *, 'warning, no number found'
   number = 0
 else
   number = 0
   k      = len_trim(digits)
   do m = k, 1, -1 ! right to left
     d_to_n = iachar(digits(m:m)) - 48
     power  = 10**(k-m)
     number = number + d_to_n*power
   end do ! over digits
   print *, 'number = ', number
```

However, since loops can be inefficient, it is better to learn that, in F90, an "internal file" can be (and should be) employed to convert one data type to another. Here we could simply code:

```
! internal file called convert
  write(convert, ''(A)'')  digit
  read(convert, ''(I4)'')  number
```

to convert a character to an integer (or real) number. Converting strings to integers is shown in the codes given in Fig. 4.14 (line 11) and the corresponding C++ appendix routine. Similar procedures would be used to convert strings to reals. The C++ version (see appendix) uses the intrinsic function "atoi" while the F90 version uses an internal file for the conversion.

One often finds it useful to change the case of a string of characters. Some languages provide intrinsic functions for that purpose. In C++ and MATLAB the function to convert a string to all lower case letters are called `tolower` and `lower`, respectively. Here we define a similar F90 function called `to_lower` which is shown in Fig. 4.15 along with a testing program in Fig. 4.16. Note that the testing program uses an interface to `tolower` (lines 4-13) assuming that routine was compiled and stored external to the testing program. The `tolower` function employs the intrinsic function `index` (line 16) to see if the k-th character of the input string is an upper case letter. The intrinsic function `len` is also used (line 8) to force the `new_string` to be the same length as the original string.

4.7 User Defined Data Types

Variables, as in mathematics, represent some quantity; unlike mathematics, many languages force the programmer to define what *type* the variable is. Generic kinds of type are integer, floating point (single, double, and quadruple precision), and complex-valued floating point. Table 4.2 (page 53) presents the data types inherent in the various languages. Most beginning programmers find the requirement most

```
function  to_lower (string)  result (new_string) ! like C
! -------------------------------------------------------------
!        Convert a string or character to lower case
!         (valid for ASCII or EBCDIC processors)
! -------------------------------------------------------------
  implicit none
  character (len = *), intent(in) :: string      ! unknown length
  character (len = len(string))   :: new_string  ! same length
  character (len = 26), parameter ::               &
            UPPER = 'ABCDEFGHIJKLMNOPQRSTUVWXYZ',  &
            lower = 'abcdefghijklmnopqrstuvwxyz'
  integer :: k    ! loop counter
  integer :: loc  ! position in alphabet
    new_string = string       ! copy everything
    do k = 1, len(string)     ! to change letters
      loc = index ( UPPER, string(k:k))              ! first upper
      if (loc /= 0 ) new_string(k:k) = lower(loc:loc) ! convert it
    end do ! over string characters
end function to_lower
```

Figure 4.15: Converting a String to Lower Case with F90

```
program up_down ! test character case inversion functions
  implicit none
  character (len = 24) :: test='ABCDefgh1234abcdZYXWzyxw'

    interface
      function to_lower (string) result (new_string)
        character (len = *), intent(in) :: string
        character (len = len(string))   :: new_string
      end function to_lower
      function to_upper (string) result (new_string)
        character (len = *), intent(in) :: string
        character (len = len(string))   :: new_string
      end function to_upper
    end interface

      print *,           test
      print *, to_lower (test)
      print *, to_upper (test)
end program     ! running gives
! ABCDefgh1234abcdZYXWzyxw
! abcdefgh1234abcdzyxwzyxw
! ABCDEFGH1234ABCDZYXWZYXW
```

Figure 4.16: Testing String Conversions with F90

languages impose of defining explicitly each variable's type to be tedious, unnecessary, and a source of bugs. It's tedious because the programmer must think not only about what the variable represents, but also how the computations calculate its value, unnecessary because mathematics doesn't work that way (the variable x represents a quantity regardless whether it turns out to be an integer or a complex value), and bug-creating because computations involving different types and assigned to a typed variable can yield nonmathematical results (for example, dividing the integers 1 with 3 and assigning the results to an integer yields a zero value).

MATLAB is one language in which variables are not explicitly typed. (Beginning programmers cheer!) Internally, MATLAB represents numbers in double precision floating point. If a variable's value corresponds to an integer, MATLAB will gleefully print it that way, effectively hiding its floating point representation. A surprise occurs when a calculation accidentality becomes complex: MATLAB will (silently) change what the variable represents from being real to being complex. For example, MATLAB will, without complaint, calculate `x=log(-1)` and assign the value $3.14159i$ to `x`. In many applications, the expression that yielded the value of -1 because of an error, and MATLAB will let the error propagate. (Beginning programmers sigh!) Most, if not all typed languages will immediately announce the evaluation of the logarithm of a negative number, and halt execution. By explicitly defining the kinds of values a variable will assume helps programming clarity and run-time debugging to some degree.

C++ has four intrinsic (i.e., built-in) types of data—integer, single and double precision reals, and character—and F90 has the similar set: integer, real, complex, logical, and character. F90 also allows the user to create a specific precision level for integer and real data. C++ has specified byte sizes for three character, six integer, one single precision real, and two double precision real data types for a total of twelve intrinsic data types.

C, C++	`Variable.component.sub_component`
F90	`Variable%component%sub_component`

Table 4.28: Referencing Defined Data Type Structure Components.

C, C++	<pre>struct data_tag { intrinsic_type_1 component_names; intrinsic_type_2 component_names; } ;</pre>
F90	<pre>type data_tag intrinsic_type_1 :: component_names; intrinsic_type_2 :: component_names; end type data_tag</pre>

Table 4.29: Defining New Types of Data Structure

C, C++	<pre>struct data_tag { intrinsic_type_1 component_names; struct tag_2 component_names; } ;</pre>
F90	<pre>type data_tag intrinsic_type :: component_names; type (tag_2) :: component_names; end type data_tag</pre>

Table 4.30: Nested Data Structure Definitions.

In addition to intrinsic types, C, C++ and F90 allow the formation of new types of data — *structures* — that are collections of values of not necessarily the same type. These procedures are named `struct` or `type` in C and F90, respectively.

To go along with this freedom, F90 allows you to define new operations to act on the derived types. While C++ retains the *struct* keyword, it is viewed as a *class* with only public data members and no functions. In other words, in C++ *class* is a generalization of *struct* and, thus, *class* is the preferred keyword to use. As an example of a task made easier by derived data, consider creating parts of a data structure to be used in an address book. We will need a variable that can have components and sub-components. They are referenced by a special syntax and defined as illustrated in Tables 4.28 and 4.29. This procedure for defining a new type of data structure can be "nested" by referring to other derived type entities defined earlier in the program. These concepts are shown in Table 4.30. One should declare the data type of all variables used in a program module. This is also true for user defined data structures. Table 4.31 outlines the forms of these statements, how structures are initialized, and how component values are assigned.

There are times when either the derived type variable or its components, or both, could be subscripted objects (i.e., arrays). Then care must be taken in the interpretation of which variable or component is being addressed. Table 4.32 illustrates the typical combinations with the F90 syntax.

As a concrete example, consider a `phone_type` and `address_type` definition.

C, C++	`struct data_tag variable_list; /* Definition */` `struct data_tag variable = {component_values}; /* Initialization */` `variable.component.sub_component = value; /* Assignment */`
F90	`type (data_tag) :: variable_list ! Definition` `variable = data_tag (component_values) ! Initialization` `variable%component%sub_component = value ! Assignment`

Table 4.31: Declaring, initializing, and assigning components of user-defined datatypes.

```
INTEGER, PARAMETER ::  j_max = 6
TYPE meaning_demo
    INTEGER, PARAMETER ::  k_max = 9, word = 15
    CHARACTER (LEN = word) ::  name(k_max)
END TYPE meaning_demo
TYPE (meaning_demo) derived(j_max)
```

Construct	Interpretation
`derived`	All components of all `derived`'s elements
`derived(j)`	All components of jth element of `derived`
`derived(j)%name`	All `k_max` components of `name` within jth element of `derived`
`derived%name(k)`	Component `k` of the `name` array for all elements of `derived`
`derived(j)%name(k)`	Component `k` of the `name` array of jth element of `derived`

Table 4.32: F90 Derived Type Component Interpretation.

F90

```
type phone_type
  integer :: area_code, number, extension
end type phone_type
type address_type
  integer :: number
  character (len = 35) :: street, city
  character (len =  2) :: state
  integer :: zip_code
end type address_type
```

C++

```
struct phone_type {
  int area_code, number, extension;
  };
struct address_type {
  int number;
  char street[35], city[35];
  char state[2];
  int zip_code;
  } ;
```

These could be used to define part of a `person_type`

F90

```
type person_type
  character (len = 50) :: name
  type (phone_type) :: phone
  type (address_type) :: address
  integer :: born_year
end type person_type
```

C++

```
struct person_type {
  char name[50];
  struct phone_type phone;
  struct address_type address;
  int born_year;
  };
```

We define two people with

F90

```
type (person_type) :: sammy, barney
```

C++

```
struct person_type sammy, barney;
```

or build an address book array filled with the above data structures by defining

F90

```
integer, parameter :: number = 99
type (person_type), dimension (number) :: address_book
```

C++

```
#define NUMBER 99
struct person_type address_book[NUMBER];
```

and then initialize, or "construct" sammy's phone and zip code as

F90

```
sammy%phone = phone_type (713, 5278100, 0)
sammy%zip_code = 770051892
```

C++

```
sammy.phone = {713, 5278100, 0};
sammy.zip_code = 770051892;
```

and print them with

F90

```
print *, sammy%phone
print *, sammy%address%zip_code
```

C++

```
printf("(%d)%d, extension %d",
  sammy.area_code,
  sammy.number,
  sammy.extension);
printf("%d", sammy.zip_code);
```

and then define specific members for barney with the "constructor"

F90

```
barney = person_type("Barn Owl", &
  phone_type(0,0,0), &
  sammy%address, 1892, "Sammy's cousin")
```

C++

```
barney = {"Barn Owl", {0,0,0},
  sammy.address, 1892,
  "Sammy's cousin"};
```

Note the difference in the defined type constructors. Two are actually used here because the second component must be defined as a `phone_type`. C++ just uses brackets to enclose the supplied components of each user defined type. F90 has an intrinsic functon that is created automatically by the type definition and it accepts all of the components required by the type. That is why the function name "phone_type" appears in the intrinsic constructor routine "person_type". Finally, put them in the book.

F90

```
address_book(1) = sammy
address_book(2) = barney
```

C++

```
address_book[1] = sammy;
address_book[2] = barney;
```

Fig. 4.17 presents a sample code for utilizing user defined structure types using F90 (there is a C++ version in the appendix). First a "person" structure is created (lines 4-7) by using only the intrinsic types of integers and characters. It then is used in turn within an additional data structure (line 10). The components of the structures are read (lines 18, 21, 24) and output (lines 26,27). For more general data, suggested in the comments, formatted input/output controls would be necessary.

4.7.1 Overloading Operators

As a complete short example of utilizing many of the new programming features that come with user defined data structures we will consider the use of a familiar old mathematics system, fractions. Recall that a fraction is the ratio of two integers. We will therefore define a new data type called *Fraction*. It

```
program  main ()
!  Define structures and components, via F90
  implicit none
  type  Person     ! define a person structure type
     character (len=20) ::  Name
     integer            ::  Age
  end type  Person

  type  Who_Where  ! use person type in a new structure
     type (Person)      ::  Guest
     character (len=40) ::  Address
  end type  Who_Where

  !  Fill a record of the Who_Where type components
     type  (Who_Where)  Record;

       print *,"Enter your name: "
       read  *, Record % Guest % Name

       print *,"Enter your city: "
       read  *, Record % Address

       print *,"enter your age: "
       read  *, Record % Guest % Age

       print *,"Hello ", Record % Guest % Age, " year old ", &
          Record % Guest % Name, " in ", Record % Address

end program main

!  Running with input: Sammy, Houston, 104 gives
!  Hello 104 year old Sammy in Houston
!
!  But try: Sammy Owl, Houston, 104 for a bug
```

Figure 4.17: Using Multiple Structures in F90

will simply consist of two integer types, named *num* and *denom*, respectively. New data types can be defined in any program unit. For maximum usefulness we will place the definition in a module named *Fractions*. To use this new data type we will want to have subprograms to define a fraction, list its components, and multiply two fractions together, and to equate one fraction to another. In addition to the intrinsic constructor function `fraction` we will create a manual constructor function called `assign` and it will have two arguments, the numerator value, and denominator value, and will use them to return a fraction type. The listing subroutine, called `list_Fraction`, simply needs the name of the fraction to be printed. The function, `mult_Fraction`, accepts two fraction names, and returns the third fraction as their product. Finally, we provide a function that equates the components of one fraction to those in a new fraction.

This data structure is presented in Fig. 4.18. There we note that the module starts with the definition of the new data type (lines 2-4), and is followed with the “contains” statement (line 12). The subprograms that provide the functionality of the fraction data type follow the “contains” statement and are thus coupled to the definition of the new type. When we have completed defining the functionality to go with the new data type we end the module.

In this example the program to invoke the fraction type follows in Fig. 4.19. To access the module, which defines the new data type and its supporting functions, we simply employ a “use” statement at the beginning of the program (line 2). The program declares three `Fraction` type variables (line 3): x, y, and z. The variable x is defined to be 22/7 with the intrinsic type constructor (line 5), while y is assigned a value of 1/3 by using the function `assign` (line 7). Both values are listed for confirmation. Then we form the new fraction, $z = 22/21$, by invoking the `mult_Fraction` function (line 9),

```
z = mult_Fraction (x, y)
```

which returns z as its result. A natural tendency at this point would be to simply write this as $z = x * y$. However, before we could do that we would have to tell the operators, “*” and ”=”, how to act when provided with this new data type. This is known as *overloading* an intrinsic operator. We had the foresight to do this when we set up the module by declaring which of the “module procedure”s were equivalent to each operator symbol. Thus from the “interface operator (*)” statement block the system now knows that the left and right operands of the “*” symbol correspond to the first and second arguments in the

```
module Fractions   ! F90 "Fraction" data structure and functionality
   implicit none
   type Fraction          ! define a data structure
      integer :: num, den ! with two "components"
   end type Fraction

   interface operator (*)  ! extend meaning to fraction
     module procedure mult_Fraction ; end interface

   interface assignment (=) ! extend meaning to fraction
     module procedure equal_Fraction ; end interface

contains ! functionality
  subroutine assign (name, numerator, denominator)
    type (Fraction), intent(inout) :: name
    integer, intent(in)            :: numerator, denominator

    name % num = numerator   ! % denotes which "component"
    if ( denominator == 0 ) then
          print *, "0 denominator not allowed, set to 1"
          name % den = 1
    else; name % den = denominator
    end if ; end subroutine assign

  subroutine list(name)
    type (Fraction), intent(in) :: name

    print *, name % num, "/", name % den ; end subroutine list

  function  mult_Fraction (a, b) result (c)
    type (Fraction), intent(in) :: a, b
    type (Fraction)             :: c

    c%num = a%num * b%num  ! standard = and * here
    c%den = a%den * b%den  ; end function  mult_Fraction

  subroutine equal_Fraction (new, name)
    type (Fraction), intent(out) :: new
    type (Fraction), intent(in)  :: name

    new % num = name % num  ! standard = here
    new % den = name % den  ; end subroutine equal_Fraction
end module Fractions
```

Figure 4.18: Overloading operations for new data types

function `mult_Fraction`. Likewise, the left and right operands of "=" are coupled to the first and second arguments, respectively, of subroutine `equal_Fraction`. The testing `main` and verification results are in Fig. 4.19 Before moving on note that the system does not yet know how to multiply a integer times a fraction, or visa versa. To do that one would have to add more functionality, such as a function, say `int_mult_frac`, and add it to the "module procedure" list associated with the "*" operator.

When considering which operators to overload for a newly defined data type one should consider those that are used in `sorting` operations, such as the greater-than, $>$, and less-than, $<$, operators. They are often useful because of the need to sort various types of data. If those symbols have been correctly overloaded then a generic sorting routine might be used, or require few changes.

4.7.2 User Defined Operators

In addition to the many intrinsic operators and functions we have seen so far, the F90 user can also define new operators or extend existing ones. User defined operators can employ intrinsic data types and/or user defined data types. The user defined operators, or extensions, can be unary or binary (i.e., have one or two arguments). The operator symbol must be included between two periods, such as '`.op.`'. Specific examples will be given in the next chapter.

4.8 Pointers and Targets

The beginning of every data item must be stored in computer memory at a specific address. The address of that data item is called a *pointer* to the data item, and a variable that can hold such an address is called a *pointer variable*. Often it is convenient to have a pointer to a variable, an array, or a sub-array. F90, C++ and MATLAB provide this sophisticated feature. The major benefits of the use of pointers is that

```
 program main
  use Fractions
   implicit none
   type (Fraction) :: x, y, z

   x = Fraction (22,7)      ! default constructor
   write (*,'("default   x  = ")', advance='no') ; call list(x)
   call assign(y,1,3)       ! manual constructor
   write (*,'("assigned  y  = ")', advance='no') ; call list(y)
   z = mult_Fraction (x,y)  ! function use
   write (*,'("x mult y = ")', advance='no') ; call list(z);
   print *, "Trying overloaded * and = for fractions:"
   write (*,'("y * x gives ")', advance='no') ; call list(y*x) ! multi
   z = x*y                  ! new operator uses
   write (*,'("z = x*y gives ")', advance='no') ; call list(z) ! add
 end program main                                  ! Running gives:
 ! default   x  = 22/7      ! assigned  y  = 1/3   ! x mult y = 22/21
 ! Trying overloaded * and = for fractions:
 ! y * x gives 22/21        ! z = x*y gives 22/21
```

Figure 4.19: Testing overloading for new data types

	C++	F90
Declaration	`type_tag *pointer_name;`	`type (type_tag), pointer :: pointer_name`
Target	`&target_name`	`type (type_tag), target :: target_name`
Examples	`char *cp, c;` `int *ip, i;` `float *fp, f;` `cp = & c;` `ip = & i;` `fp = & f;`	`character, pointer :: cp` `integer, pointer :: ip` `real, pointer :: fp` `cp => c` `ip => i` `fp => f`

Table 4.33: Definition of pointers and accessing their targets.

they allow dynamic data structures, such as “linked lists” and “tree structures,” and they allow recursive algorithms. Note that rather than containing data themselves, pointer variables simply exist to point to where some data are stored. Unlike C and MATLAB the F90 pointers are more like the “reference variables” of the C++ language in that they are mainly an alias or synonym for another variable, or part of another variable. They do not allow one to easily get the literal address in memory as does C. This is why programmers that write computer operating systems usually prefer C over F90. But F90 pointers allow easy access to array partitions for computational efficiency, which C++ does not. Pointers are often used to pass arguments by reference.

The item to which a pointer points is known as a *target* variable. Thus, every pointer has a logical status associated with it which indicates whether or not it is currently pointing to a target. The initial value of the association is `.false.`, or undefined.

4.8.1 Pointer Type Declaration

For every type of data object that can be declared in the language, including derived types, a corresponding type of pointer and target can be declared (Table 4.33).

While the use of pointers gives programmers more options for constructing algorithms, they also have a potential severely detrimental effect on the program execution efficiency. To ensure that compilers can produce code that execute efficiently, F90 restricts the variables, to which a pointer can point, to those specifically declared to have the attribute `target`. This, in part, makes the use of pointers in F90 and C++ somewhat different. Another major difference is that C++ allows arithmetic to be performed on the pointer address, but F90 does not.

So far, we have seen that F90 requires specific declarations of a `pointer` and an potential `target`. However, C++ employs two unary operators, `&` and `*`, to deal with pointers and targets, respectively. Thus, in C++ the operator `&variable_name` means “the address of” `variable_name`, and the C++ operator `*pointer_name` means “the value at the address of” `pointer_name`.

C, C++	`pointer_name = NULL`
F90	`nullify (list_of_pointer_names)`
F95	`pointer_name = NULL()`

Table 4.34: Nullifying a pointer to break target association.

```
program  pt_expression
!
!      F90 example of using pointers in expressions
   implicit none
   integer, POINTER :: p, q, r
   integer, TARGET  :: i = 1, j = 2, k = 3

   q => j                 ! q points to integer j
   p => i                 ! p points to integer i
!
!      An expression that "looks like" pointer arithmetic
!      automatically substitutes the target value:
!
   q = p + 2              ! means: j = i + 2 = 1 + 2 = 3
   print *, i, j, k       ! print target values
   p => k                 ! p now points to k
   print *, (q-p)         ! means print j - k = 3 - 3 = 0
!
!      Check associations of pointers
   print *, associated (r)    ! false
   r => k                     ! now r points to k, also
   print *, associated (p,i)  ! false
   print *, associated (p,k)  ! true
   print *, associated (r,k)  ! true
end program pt_expression
```

Figure 4.20: Using F90 Pointers in Expressions.

4.8.2 Pointer Assignment

F90 requires that a pointer be associated with a target by a single pointer assignment statement. C allows, but does not require, a similar statement. (See Table 4.33). After such a statement, the pointer has a new association status and one could employ the F90 intrinsic inquiry function `associated(pointer_name, target_name)` to return `.true.` as the logical return value. If one wishes to break or nullify a pointer's association with a target, but not assign it another target, one can nullify the pointer as shown in Table 4.34.

4.8.3 Using Pointers in Expressions

The most important rule about using pointers in F90 expressions is that, where ever a pointer occurs, it is treated as its associated target. That is, the target is automatically substituted for the pointer when the pointer occurs in an expression. For example, consider the actions in Fig. 4.20 (where the results are stated as comments).

4.8.4 Pointers and Linked Lists

Pointers are the simplest available mechanism for dynamic memory management of arrays such as stacks, queues, trees, and linked lists. These are extraordinarily flexible data structures because their size can grow or shrink during the execution of a program. For linked lists the basic technique is to create a derived type that consists of one or more data elements and at least one pointer. Memory is allocated to contain the data and a pointer is set to reference the next occurrence of data. If one pointer is present, the list is a singly-linked list and can only be traversed in one direction: head to tail, or vice versa. If two pointers are present: the list is a doubly-linked list and can be traversed in either direction. Linked lists allow the data of interest to be scattered all over memory and uses pointers to weave through memory, gathering data as required. Detailed examples of the use of linked lists are covered in Chapter 8.

As a conceptual example of when one might need to use linked-lists think of applications where one never knows in advance how many data entries will be needed. For example, when a surveyor determines the exact perimeter of a building or plot of land, critical measurements are taken at each angle. If the perimeter has N sides, the surveyor measures the length of each side and the interior angle each side forms with the next. Often the perimeter has visual obstructions and offsets around them must be made, recorded, and corrected for later. Regardless of how careful the surveyor is, errors are invariably introduced during the measurement process. However, the error in angle measurements can be bounded.

The program for implementing the recording and correcting of the angles in a survey could be written using a singly linked list. A linked list is chosen because the programmer has no idea how many sides the perimeter has, and linked lists can grow arbitrarily. Because of the linked list's ability to absorb a short or long data stream, the user does not have to be asked to count the number of legs in the traverse. The program begins by declaring a derived type that contains one angle measurement and a pointer to the next measurement. A count is kept of the number of legs in this loop and the forward pointer for the last angle read is cleared (set to null) to signal the end of list. After all the data are read, the entire list of angles is reviewed to get the total of the measurements. This starts by revisiting the head of the list and adding together all the angle measurements until a null pointer is encountered, signaling the end of list. Then the error can be computed and distributed equally among the legs of the traverse.

4.9 Accessing External Source Files and Functions

At times one finds it necessary, or efficient to utilize other software from libraries, other users, or different paths in your directories. Of course, you could always use the brute force approach and use a text editor to copy the desired source code into your program. However, this is unwise not only because it wastes storage, but more importantly gives multiple copies of a module that must all be found and changed if future revisions are needed or desired. Better methods of accessing such codes can be defined either inside your program, or external to it in the "linking" phase after compiling has been completed.

High level languages like C, C++, and F90 allow one or more approaches for accessing such software from within your code. One feature common to all these languages is the availability of an "include" statement which gives the system path to the desired code file. At compile time, and only then, a temporary copy of the indicated code from that file is literally copied and inserted into your program at the location of the corresponding "include" statement.

It is common practice, but not required, to denote such code fragments with name extensions of ".h" and ".inc", in C++ and F90, respectively. For example, to use a program called "class_Person" one could insert the following statement in your program:

```
C, C++: include <class_Person.h>
F90   : include 'class_Person.inc'
```

if the files, class_Person.h or class_Person.inc, were in the same directory as your program. Otherwise, it is necessary to give the complete system path to the file, such as,

```
include '/home/caam211/Include/inv.f90'
include '/home/caam211/Include/SolveVector.f90'
```

which give source links to the `caam211` course files for the function `inv(A)` for returning the inverse of a matrix `A`, and the function `SolveVector(A,B)` which returns the solution vector `X` for the matrix system `A*X = B`.

In F90 one can also provide a "module" that defines constants, user defined types, supporting subprograms, operators, etc. Any of those features can be accessed by first including such a F90 module before the main program and later invoking it with a "use" statement which cites the "module" name. For example, the F90 program segments:

```
include '/home/caam211/Include/caam211_operators.f90'
Program  Lab2_A_2
. . .
  call  test_matrix ( A, B, X )  ! form and invert test matrix
. . .
subroutine  test_matrix ( A, B, X )
 use caam211_operators              ! included above
  implicit none
  real :: A(:,:), B(:), X(:)
  real :: A_inv(size(A,1),size(A,1)) ! automatic array allocation
    A_inv = inv(A)
    X     = A .solve. B                ! like X = A \ B in Matlab
    . . .
```

gives a source link to the `caam211` course "module" source file named `caam211_operators.f90` which contains subprograms, such as the function `inv()`, and operator definitions like `.solve.` which is equivalent to the "\" operator in MATLAB.

In the last example the omission of the "include" statement would require a compiler dependent statement to allow the system to locate the module cited in the "use" statement. For the National Algorithms Group (NAG) F90 compiler that link would be given as

```
f90 -o go /home/caam211/Include/caam211_operators.f90 my.f90
```

if the above segment was stored in the file named `my.f90`, while for the Cray F90 compiler a path flag, `-p`, to the compiled version is required, such as:

```
f90 -o go -p /home/caam211/Include/caam211_op_CRAY.o my.f90
```

Either would produce an executable file, named "go" in this example.

4.10 Procedural Applications

In this section we will consider two common examples of procedural algorithms: fitting curves to experimental data, and sorting numbers, strings, and derived types. Sorting concepts will be discussed again in Chapter 7.

4.10.1 Fitting Curves to Data

We must ofter deal with measurements and what they result in: data. Measurements are never exact because they are limited by instrument sensitivity and are contaminated by noise. To determine trends (how measurements are related to each other), confirm theoretical predictions, and the like, engineers must frequently *fit* functions to data. The "curve" fit is intended to be smoother than a raw plot of the data, hopefully revealing more about the underlying relation between the variables than would otherwise be apparent.

Often, these functions take *parametric* form: The functional form is specified, but has unknown coefficients. Suppose you want to fit a straight line to a dataset. With y denoting the measurement and x the independent variable, we wish to fit the function $y = f(x) = mx + b$ to the data. The fitting process amounts to determining a few quantities of the assumed linear functional form—the parameters m and b—from the data. You know that two points define a straight line; consequently, only two of the (x, y) pairs need be used. But which two should be used? In virtually all real-world circumstances, the measurements do *not* precisely conform to the assumed functional form. Thus, fitting a curve by selecting a few values (two in the linear case) and solving for the function's parameters produces a circumspect "fit", to say the least. Instead, the most common approach is to use *all* the data in the curve fitting process. Because you frequently have much more data than parameters, you have what is known as an *over-determined* problem. In most cases, no parameter values produce a function that will fit all the data exactly. Over-determined problems can be solved by specifying an *error criterion* (what is an error and how large is the deviation of data from the assumed curve) and finding the set of parameter values that minimizes the error criterion. With this approach, we can justifiably claim to have found the best parameter choices.

The "Least Squares" Approach

Far and away the most common error criterion is the *mean-squared error*: Given measurement pairs (x_i, y_i), $i = 1, \ldots, N$, the mean squared error ϵ^2 equals the average across the dataset of $\big(y_i - f(x_i)\big)^2$, the squared error between the i^{th} measurement and the assumed parametric function $f(x_i)$.

$$\epsilon^2 = \frac{1}{N} \sum_{i=1}^{N} \big(y_i - f(x_i)\big)^2$$

Least squares fitting of functions to data amounts to minimizing the dataset's mean squared error with respect to the parameters.

To illustrate the least-squares approach, let's fit a linear function to a dataset. Substituting the assumed functional form $f(x) = mx + b$ into the expression for the mean-squared error, we have

$$\epsilon^2 = \frac{1}{N}\sum_{i=1}^{N}\bigl(y_i - (mx_i + b)\bigr)^2$$

We can find a set of equations for the parameters m and b that minimize this quantity by evaluating the derivative of ϵ^2 with respect to each parameter and setting each to zero.

$$\begin{aligned}\frac{d\epsilon^2}{dm} &= \frac{1}{N}\sum_{i=1}^{N} -2x_i\bigl(y_i - (mx_i + b)\bigr) = 0\\ \frac{d\epsilon^2}{db} &= \frac{1}{N}\sum_{i=1}^{N} -2\bigl(y_i - (mx_i + b)\bigr) = 0\end{aligned}$$

After some simplification, we find that we have two *linear* equations to solve for the fitting parameters.

$$\begin{aligned}m\cdot\left(\frac{1}{N}\sum_{i=1}^{N}x_i^2\right) + b\cdot\left(\frac{1}{N}\sum_{i=1}^{N}x_i\right) &= \frac{1}{N}\sum_{i=1}^{N}x_iy_i\\ m\cdot\left(\frac{1}{N}\sum_{i=1}^{N}x_i\right) + b &= \frac{1}{N}\sum_{i=1}^{N}y_i\end{aligned}$$

Thus, finding the least-squares fit of a straight line to a set of data amounts to solving a set of two linear equations, the coefficients of which are computed from the data. Note that the four summations in the last equation have the same range count (N) and could be evaluated in a single explicit loop.

An Aside

Because fitting data with a linear equation yields a set of two easily solved equations for the parameters, one approach to fitting *nonlinear* curves to data is to convert the nonlinear problem into a linear one. For example, suppose we want to fit a *power law* to the data: $f(x) = ax^b$. Instead of minimizing the mean squared error directly, we transform the data so that we are fitting it with a linear curve. In the power law case, the logarithm of the fitting curve is linear in the parameters: $\log f(x) = \log a + b \log x$. This equation is not linear in the parameter a. For purposes of least-squares fits, we instead treat $a' = \log a$ as the linear fit parameter, solve the resulting set of linear equations for a', and calculate $a = \exp a'$ to determine the power law fitting parameter. By evaluating the logarithm of x_i and y_i and applying the least squares equations governing the fitting of a linear curve to data, we can fit a power-law function to data. *Thus, calculating a linear least squares fit to data underlies general approximation of measurements by smooth curves.* For an insight to the types of relationships that can be determined, see the following summary.

x-axis	y-axis		Relationship
Linear	Linear	$y = mx + b$	linear
Linear	Logarithmic	$\log y = mx + b$	exponential: $y = e^b \cdot e^{mx}$
Logarithmic	Linear	$y = m \log x + b$	logarithmic
Logarithmic	Logarithmic	$\log y = m \log x + b$	power-law: $y = e^b \cdot x^m$

We can now specify the computations required by the least squares fitting algorithm mathematically.

Algorithm: Least-Squares Fitting of Straight Lines to Data

1. **Given** N pairs of data points (x_i, y_i)
2. **Calculate**[†] $a_{11} = \frac{1}{N}\sum_{i=1}^{N}x_i^2$, $a_{12} = \frac{1}{N}\sum_{i=1}^{N}x_i$, $a_{21} = \frac{1}{N}\sum_{i=1}^{N}x_i$, $a_{22} = 1$, $c_1 = \frac{1}{N}\sum_{i=1}^{N}x_iy_i$, and $c_2 = \frac{1}{N}\sum_{i=1}^{N}y_i$.

[†] Note that these calculations can be performed in one loop rather than four.

3. **Solve the set of linear equations**

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

which for two equations can be done by hand to yield

$$m = (a_{12} \cdot c_2 - N \cdot c_1)/(a_{12} \cdot a_{21} - N \cdot a_{11})$$

$$b = (c_2 - m \cdot a_{12})/N$$

4. **Calculate the mean squared error** $\epsilon^2 = \frac{1}{N} \sum_{i=1}^{N} \big(y_i - (mx_i + b)\big)^2$.

Implementing the Least Squares Algorithm

In F90, such calculations can be performed two different ways: one expresses the looping construct directly, the other uses more efficient intrinsic array routines inside F90. Assuming the $\{x_i\}$ are stored in the vector `x`, the coefficient `a12` can be calculated (at least) two ways.

1.
```
sum_x = 0
N = size(x)
do i = 1,N
   sum_x = sum_x + x(i)
end do
a12 = sum_x/N
```

2.
```
a12 = sum(x)/size(x)
```

Clearly, the second method produces a somewhat simpler expression than the first, and is vastly superior to the first. In the sample code that follows in Fig. 4.21 we use the intrinsic array functions but encourage the reader to check the results with a single loop that computes all six terms need to find `m` and `b`.

There are a few new features demonstrated in this example code. In line 6 we have specified a fixed unit number to associate with the data file to be specified by the user. But we did not do an INQUIRE to see if that unit was already in use. We will accept a user input filename (lines 8, 25 and 28) that contains the data to be fitted. An interface (lines 12-21) is provided to external routines that will determine the number of lines of data in the file and the read those data into the two arrays. Those two routines are given elsewhere. Of course, the memory for the data arrays must be dynamically allocated (line 35) before they can be read (line 37). After the least squares fit is computed (line 40) and printed the memory space for the data is freed (line 44).

In the `lsq_fit` subroutine (line 47) the three items of interest are passed in the array `fit`. (Routine `lsq_fit` could have been written as a function, try it.) Observe that `y` must be the same length as array `x` so the `size` intrinsic was used to ensure that (line 56). The data summations are evaluated with the `sum` intrinsic (lines 62-64) and it is used again to evaluate the mean squared error `mse` (line 72) as described in step 4 of the algorithm. The test data (lines 78-89) and results (lines 92-96) are given as comments as usual. Since no explicit loops have been used this form would be more efficient on vector computers and some parallel computers.

4.10.2 Sorting

One of the most useful computational routines is sorting: Ordering a sequence of data according to some rule. For example, the alphabetized list of filenames producted by a system directory command is far easier to read than an unsorted list would be. Furthermore, data can be fruitfully sorted in more than one way. As an example, you can sort system files by their creation date.

Sorting algorithms have been well studied by computer scientists in a quest to find the most efficient. We use here the *bubble sort algorithm*, perhaps the oldest, but not most efficient. This algorithm makes multiple passes over a list, going down the list interchanging adjacent elements in the list if needed to put them in order. For example, consider the list `[b, e, a, d, f, c]`, shown in Fig. 4.22, that we

```
program linear_fit
! ---------------------------------------------------
!     F90 linear least-squares fit on data in file
!             specified by the user.
! ---------------------------------------------------
implicit none
integer, parameter   :: filenumber = 1 ! RISKY
real, allocatable    :: x(:), y(:)     ! data arrays
character (len = 64) :: filename       ! name of file to read
integer              :: lines          ! number of input lines
real                 :: fit(3)         ! final results

interface
  function inputCount(unit) result(linesOfInput)
    integer, intent(in) :: unit         ! file unit number
    integer             :: linesOfInput ! result
  end function inputCount
  subroutine readData (inFile, lines, x, y)
    integer, intent(in)  :: inFile,   lines    ! file unit, size
    real,    intent(out) :: x(lines), y(lines) ! data read
  end subroutine readData
end interface

!   Get the name of the file containing the data.
  write (*,*) 'Enter the filename to read data from:'
  read  (*,'(A64)') filename

!   Open that file for reading.
  open (unit = filenumber, file = filename)

!   Find the number of lines in the file
  lines = inputCount (filenumber)
  write (*,*) 'There were ',lines,' records read.'

!   Allocate that many entries in the x and y array
  allocate (x(lines), y(lines))

  call readData (filenumber, lines, x, y)   ! Read data
  close (filenumber)

  call lsq_fit (x, y, fit)                 ! least-squares fit
  print *, "the slope is     ", fit(1) ! display the results
  print *, "the intercept is ", fit(2)
  print *, "the error is     ", fit(3)
  deallocate (y, x)
contains

```

Fig. 4.21, A Typical Least Squares Linear Fit Program (continued)

wish to sort to alphabetical order. In the first pass, the algorithm begins by examining the first two list elements `(b, e)`. Since they are in order, these two are left alone. The next two elements `(e, a)` are not in order; these two elements of the list are interchanged. In this way, we "bubble" the element `a` toward the top and `e` toward the bottom. The algorithm proceeds through the list, interchanging elements if need be until the last element is reached. Note that the bottom of the list at the end of the first pass contains the correct entry. This effect occurs because of the algorithm's structure: The "greatest" element will always propagate to the list's end. Once through the pass, we see that the list is in better, but not perfect, order. We must perform another pass just like the first to improve the ordering. Thus, the second pass need consider only the first $n-1$ elements, the third $n-2$, etc. The second pass does make the list better formed. After more passes, the list eventually becomes sorted. To produce a completely sorted list, the bubble-sort algorithm requires no more passes than the number of elements in the list minus one.

The following F90 routines illustrate some of the initial features of a simple procedural approach to a simple process like the bubble-sort algorithm. We begin by considering the sorting of a list of real numbers as shown in subroutine Sort_Reals in Fig. 4.22.

In line 1 we have passed in the size of the array, and the actual array (called database). Note that the database has intent (inout) because we plan to overwrite the original database with the newly sorted order, which is done in lines 18–20. For efficiency sake we have included an integer counter, swaps_Made, so that we can determine if the sort has terminated early. If we wished to apply the same bubble-sort algorithm to an integer array all we would have to do is change the procedure name and lines 6 and 10 that describe the type of data being sorted (try it).

```
  subroutine lsq_fit (x, y, fit)
! --------------------------------------------------------
!         Linear least-squares fit, A u = c
! --------------------------------------------------------
!  fit   = slope, intercept, and mean squared error of fit.
!  lines = the length of the arrays x and y.
!  x     = array containing the independent variable.
!  y     = array containing the dependent variable data.
  implicit none
  real,    intent(in)  :: x(:), y(size(x))
  real,    intent(out) :: fit(3)
  integer              :: lines
  real                 :: m,    b,     mse
  real                 :: sumx, sumx2, sumy, sumxy

!   Summations
    sumx  = sum ( x )     ; sumx2 = sum ( x**2 )
    sumy  = sum ( y )     ; sumxy = sum ( x*y )

!   Calculate slope intercept
    lines = size(x)
    m = (sumx*sumy - lines*sumxy)/(sumx**2 - lines*sumx2)
    b = (sumy - m*sumx)/lines

!   Predicted y points and the sum of squared errors.
    mse = sum ( (y - m*x - b)**2 )/lines
    fit(1) = m ; fit(2) = b ; fit(3) = mse      ! returned
  end subroutine lsq_fit

  end program linear_fit

! Given test set 1 in file lsq_1.dat:
! -5.000000 -2.004481
! -4.000000 -1.817331
! -3.000000 -1.376481
! -2.000000 -0.508725
! -1.000000 -0.138670
!  0.000000  0.376678
!  1.000000  0.825759
!  2.000000  1.036343
!  3.000000  1.815817
!  4.000000  2.442354
!  5.000000  2.636355
! Running the program yields:
!
! Enter the filename to read data from: lsq_1.dat
! There were  11  records read.
! the slope is      0.4897670746
! the intercept is  0.2988743484
! the error is      0.2139159478E-01
```

Figure 4.21: A Typical Least Squares Linear Fit Program

That is true because the compiler knows how to apply the $>$ operator to all the standard numerical types in the language. But what if we want to sort character strings, or other types of objects? Fortran has lexical operators (like LGE) to deal with strings, but user defined objects would require that we overload the $>$ operator, if the expected users would not find the overloading to be confusing. In other words, you could develop a fairly general sort routine if we changed lines 6 and 10 to be

```
[ 6]   type (Object), intent(inout) :: database (lines)
[10]   type (Object)                :: temp
```

and provided an overloading of $>$ so that line 17 makes sense for the defined Object (or for selected component of it).

To illustrate the sort of change that is necessary to sort character strings consider subroutine Sort_String Fig. 4.23:

To keep the same style as the previous algorithm and overload the $>$ operator we would have to have a procedure that utilizes the lexical operators in lines 24 and 25, along with the interface definition on lines 12 through 17, do define the meaning of $>$ in the context of a string. While the concept of a "template" for a code to carry out a bubble-sort on any list of objects it may not always be obvious what $>$ means when it is overloaded by you or some other programmer.

Note that in the two above sorting examples we have assumed that we had the authority to change the original database, and that it was efficient to do so. Often that is not the case. Imagine the case where the database represents millions of credit card users, each with a large number components of numbers,

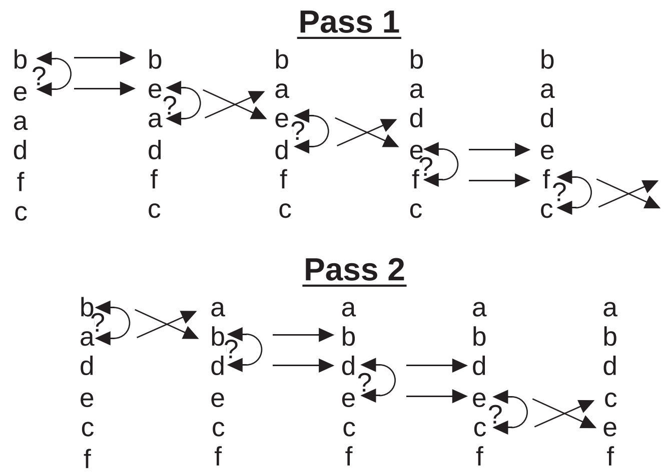


Figure 4.22: Example passes of the bubble-sort algorithm through data.

```
subroutine Sort_Reals (lines, database)
! Bubble Sort of (changed) Real Database

 implicit none
 integer, intent(in)    :: lines             ! number of records
 real,    intent(inout) :: database (lines)  ! records in database

 integer :: swaps_Made       ! number of swaps made in one pass
 integer :: count           ! loop variable
 real    :: temp            ! temporary holder for making swap

   do ! Repeat this loop forever... (until we break out of it)
     swaps_Made = 0             ! Initially, we've made no swaps
     ! Make one pass of the bubble sort algorithm
     do count = 1, (lines - 1)
       ! If item is greater than the one after it, swap them
       if ( database (count) > database (count + 1) ) then
              temp                = database (count)
              database (count)     = database (count + 1)
              database (count + 1) = temp
              swaps_Made           = swaps_Made + 1
        end if
      end do
      ! If we made no swaps, break out of the loop.
      if ( swaps_Made == 0 ) exit ! do count swaps
    end do
end subroutine Sort_Reals
```

Figure 4.23: Bubble Sort of a Real Array

character strings, or general objects. If many workers are accessing those data for various sorting needs you probably would not allow the original dataset to be changed for reasons of safety or security. Then we consider an alternative to moving around the actual database components. That is, we should consider using moving pointers to large data components, or pseudo-pointers such as an ordering array. The use of an ordering array is shown in Fig. 4.24 where subroutine Integer_Sort now includes an additional argument.

The third argument has intent (out), as shown in line 7, and is an integer array of the same length as the original database which has now been changed to intent (in) so the compiler will not allow us to change the original data. If the data are properly sorted as supplied then it should not be changed and the new order should be the same as the original sequential input. That is why line 13 initializes the return order to a sequential list. Then we slightly change the previous sort logic so that lines 19 through 23 now check whats in an ordered location, and change the order number when necessary, but never change the original data. After exiting this routine you could list the information, in sorted order, without changing the original data simply by using vector subscripts in a print statement like:

```
print *, database (order).
```

```
subroutine Sort_String (lines, database)
! Bubble Sort of (Changed) String Database
 implicit none

 integer,          intent(in)     :: lines            ! input size
 character(len=*), intent(inout)  :: database (lines) ! records

 character (len = len(database (1))) :: temp ! swap holder
 integer :: swaps_Made      ! number of swaps in a pass
 integer :: count           ! loop variable

   interface ! to_lower
     function  to_lower (string)  result (new_String)
       character (len = *), intent(in) :: string
       character (len = len(string))   :: new_String
     end function to_lower
   end interface ! to_lower

   do ! Repeat this loop forever... (until we break out of it)
     swaps_Made = 0            ! Initially, we've made no swaps
     ! Make one pass of the bubble sort algorithm
     do count = 1, (lines - 1)
       ! If the element is greater than the one after it, swap them
       if ( LGT (to_lower (database (count    )),
                 to_lower (database (count + 1))) ) then
           temp                 = database (count    )
           database (count    ) = database (count + 1)
           database (count + 1) = temp
           swaps_Made           = swaps_Made + 1
       end if
     end do
     ! If we made no swaps, berak out of the loop.
     if ( swaps_Made == 0) exit ! do count swaps
   end do
 end subroutine Sort_String
```

Figure 4.24: Bubble Sort of an Array of Character Strings

```
subroutine Integer_Sort (lines, database, order)
! Ordered Bubble Sort of (Unchanged) Integer Database

 implicit none
 integer, intent(in)  :: lines             ! number of records
 integer, intent(in)  :: database (lines)  ! records in database
 integer, intent(out) :: order    (lines)  ! the order array

 integer :: swaps_Made       ! number of swaps made in one pass
 integer :: count            ! loop variable
 integer :: temp             ! temporary holder for making swap

   order = (/ (count, count = 1, lines) /) ! default order
   do ! Repeat this loop forever... (until we break out of it)
     swaps_Made = 0             ! Initially, we've made no swaps
     ! Make one pass of the bubble sort algorithm
     do count = 1, (lines - 1)
       ! If item is greater than the one after it, swap them
       if ( database (order (count)) >     &
            database (order (count + 1)) ) then
              temp              = order (count)
              order (count)     = order (count + 1)
              order (count + 1) = temp
              swaps_Made        = swaps_Made + 1
        end if
      end do
      ! If we made no swaps, break out of the loop.
      if ( swaps_Made == 0 ) exit ! do count swaps
    end do
end subroutine Integer_Sort
```

Figure 4.25: An Ordered Bubble Sort of an Integer Array

Clearly you could write a very similar program using a true "pointer" array since they are now standard in Fortran.

Next we will start to generalize the idea of sorting to include the sorting of objects that may have numerous components. Assume the each record object to be read is defined as in Fig. 4.25.

There may be thousands, or millions, of such records to be read from a file, sorted by name and/or number, and then displayed in sorted order. Program test_bubble, in Fig. 4.26 illustrates one approach to such a problem. Here since the database of records are to read from a file we do not yet know how many

```
module record_Module
!-----------------------------------------------------------
! record_Module holds the "record" type
!-----------------------------------------------------------
  ! record is a data structure with two names and an id number.
  type record
    character (len=24) :: last_Name   ! last name
    character (len=24) :: first_Name  ! first name
    integer            :: id          ! id number
  end type record
end module record_Module
```

Figure 4.26: A Typical Record in a List to be Sorted

```
[ 1]  program test_bubble
[ 2]  !-----------------------------------------------------------
[ 3]  ! test_bubble asks for a filename for a file of names and id
[ 4]  ! numbers, loads in the data from a file into the database,
[ 5]  ! finds sorting orders, and prints sorted data
[ 6]  !-----------------------------------------------------------
[ 7]   use record_Module     ! need this to use the 'record' type
[ 8]    implicit none
[ 9]  ! We define the database as an allocatable array of records.
[10]    type (record), allocatable :: database (:)
[11]
[12]  ! These arrays hold the sorted order of the database entries.
[13]    integer, allocatable :: sort_by_Name   (:)
[14]    integer, allocatable :: sort_by_Number (:)
[15]
[16]    character (len = 64) :: file_Name   ! file to read data from
[17]    integer              :: lines       ! number of lines of input
[18]    integer              :: file_Number ! the input file number
[19]    integer              :: loop_Count  ! loop counter
[20]
[21]      file_Number = 1      ! arbitrarily set file_Number to 1
[22]
[23]      write (*,*) 'Enter the filename to read data from:'
[24]      read  (*,'(A64)') file_Name
[25]
[26]    ! Open our file and assign the number to 'file_Number'
[27]      open (unit = file_Number, file = file_Name)
[28]
[29]    ! Find the number of lines in the input file with input_Count.
[30]      lines = input_Count (file_Number)
[31]      write (*,*) 'There are ', lines,' records.'
[32]
[33]    ! Allocate that many entries in the database and order arrays
[34]      allocate ( database (lines) )
[35]      allocate ( sort_by_Name (lines), sort_by_Number (lines) )
[36]
[37]    ! Read the data from file into the database and close the file.
[38]      call read_Data (file_Number, lines, database)
[39]      close (file_Number)
[40]
[41]    ! Sort the database by name; the order will be in sort_by_Name.
[42]      call String_Sort (lines, database (:)%last_Name, sort_by_Name)
[43]      write (*,*); write (*,*) 'Data sorted by name: '; write (*,*)
[44]
[45]    ! Print out the data in the database sorted by name
[46]      call show_Data (lines, database, sort_by_Name)
[47]      write (*,*); write (*,*) 'Data sorted by number:'; write (*,*)
[48]
[49]    ! Sort the database by id numbers; new order is sort_by_Number.
[50]      call Integer_Sort (lines, database (:)%id, sort_by_Number)
[51]
[52]    ! Print out the data in the database sorted by number.
[53]      call show_Data (lines, database, sort_by_Number)
[54]  end program test_bubble
```

Figure 4.27: Testing of Ordered Bubble Sorts

there are to be stored. Therefore, it is declared allocatable in line 13, and allocated later in line 34 after we have evaluated the file size of a file named by the user. Although not generally necessary we have selected to have an order array for names and a different one for numbers. The are sort_by_Name, and sort_by_Number, respectively and are treated in a similar fashion to the database memory allocation as noted in lines 13–14, and line 35.

In line 21 we have arbitrarily set a unit number to be used for the file. That is okay for a very small code, but an unnecessary and unwise practice in general. The Fortran intrinsic inquire allows one to determine which units are inactive and we could create a function, say Get_Next_Unit, to select a safe unit number for our input operation. After accepting a file name we open the unit, and count the number of lines present in the file (see line 30). Had the database been on the standard input device, and not contained any non-printing control characters, we could have easily read it with the statement

```
read *, database
```

However, it does contain tabs (ASCII character number 9), and is in a user defined file instead of the standard input device so line 38 invokes subroutine read_Data to get the data base. Of course, once the tabs and commas have been accounted for and the names and id number extracted it uses an intrinsic constructor on each line to form its database entry like:

```
database (line_Count) = Record (last, first, id)
```

After all the records have been red into the database note that line 42 extracts all the last names with the syntax

```
database (:) last_Name
```

so they are copied into subroutine String_Sort, as its second argument, and the ordered list sort_by_Name) is returned to allow operations that need a last name sort. Likewise, subroutine Integer_Sort, shown above, is used in line 50 to sort the id numbers and save the data in order list sort_by_Number. The ordered lists are used in show_Data, in lines 46 and 53, to display the sorted information, without changing the original data.

If the supplied file, say namelist, contained data in the format of (String comma String tab Number) with the following entries:

```
Indurain, Miguel 5623
van der Aarden, Eric 1245
Rominger, Tony 3411
Sorensen, Rolf 341
Yates, Sean 8998
Vandiver, Frank 45
Smith, Sally 3821
Johnston, David 3421
Gillis, Malcolm 3785
Johns, William     7234
Johnston, Jonathan 7234
Johnson, Alexa 5190
Kruger, Charlotte 2345
Butera, Robert 7253
Armstrong, Lance 2374
Hegg, Steve 9231
LeBlanc, Lucien 23
Peiper, Alan 5674
Smith-Jones, Nancy 9082
```

The output would be:

```
! Enter the filename to read data from: namelist
! There are  19  records.
!
! Data sorted by name:
!
! Armstrong                 Lance                   2374
! Butera                    Robert                  7253
! Gillis                    Malcolm                 3785
! Hegg                      Steve                   9231
! Indurain                  Miguel                  5623
! Johns                     William                 7234
! Johnson                   Alexa                   5190
! Johnston                  David                   3421
! Johnston                  Jonathan                7234
! Kruger                    Charlotte               2345
! LeBlanc                   Lucien                    23
! Peiper                    Alan                    5674
! Rominger                  Tony                    3411
! Smith                     Sally                   3821
! Smith-Jones               Nancy                   9082
! Sorensen                  Rolf                     341
! van der Aarden            Eric                    1245
! Vandiver                  Frank                     45
! Yates                     Sean                    8998
!
```

and

```
! Data sorted by number:
!
! LeBlanc                  Lucien                    23
! Vandiver                 Frank                     45
! Sorensen                 Rolf                     341
! van der Aarden           Eric                    1245
! Kruger                   Charlotte               2345
! Armstrong                Lance                   2374
! Rominger                 Tony                    3411
! Johnston                 David                   3421
! Gillis                   Malcolm                 3785
! Smith                    Sally                   3821
! Johnson                  Alexa                   5190
! Indurain                 Miguel                  5623
! Peiper                   Alan                    5674
! Johns                    William                 7234
! Johnston                 Jonathan                7234
! Butera                   Robert                  7253
! Yates                    Sean                    8998
! Smith-Jones              Nancy                   9082
! Hegg                     Steve                   9231
```

Pass 1

Level 1	2	3	4	5	6
Sorted					
b	b	b	b	b	b
e	e	a	a	a	a
a	a	e	d	d	d
d	d	d	e	e	e
f	f	f	f	f	c
c	c	c	c	c	f
Is_Was*					
	1	1		1	1
	2	3		3	3
	3	2		4	4
	4	4		2	2
	5	5		5	6
	6	6		6	5

Pass 2

Level 1	2	3	4	5
Sorted				
b	a	a	a	a
a	b	b	b	b
d	d	d	d	d
e	e	e	e	c
c	c	c	c	e
f	f	f	f	f
Is_Was				
		1	3	3
		3	1	1
		4	4	4
		2	2	6
		6	6	2
		5	5	5

Pass 3

Level 1	2
Sorted	
a	a
b	b
d	c
c	d
e	e
f	f
Is_Was	
3	3
1	1
4	6
6	4
2	2
5	5

* Is_Was $(j) = k$. What is position j was position k.

Figure 4.28: Sorting via an Order Vector, Array (Is_Was) $\rightarrow$ a b c d e f

4.11 Exercises

1 Frequently we need to know how many lines exist in an external file that is to be used by our program. Usually we need that information to `dynamically allocate` memory for the arrays that will be constructed from the file data to be read. Write a F90 program or routine that will accept a unit number as input, `open` that unit, loop over the lines of data in the file connected to the unit, and return the number of lines found in the file. (A external file ends when the `iostat` from a read is less than zero.)

2 A related problem is to read a table of data from an external file. In addition to knowing the number of lines in the file it is necessary to know the number of entities (columns) per line and to verify that all lines of the file have the same number of columns. Develop a F90 program for that purpose. (This is the sort of checking that the MATLAB `load` function must do before loading an array of data.)

3 Write a program that displays the current date and time and uses the module `tic_toc`, in Fig. 4.10, to display the CPU time required for a calculation.

4 Develop a companion function called `to_upper` that converts a string to all upper case letters. Test it with the above program.

5 Develop a function that will take an external file unit number and count the number of lines in the file connected to that unit. This assumes that the file has been “opened” on that unit. The interface to the function is to be:

```
interface
  function inputCount(unit) result(linesOfInput)
    integer, intent(in) :: unit         ! file unit number
    integer             :: linesOfInput ! result
  end function inputCount
end interface
```

6 Assume the file in the previous problem contains two real values per line. Develop a subroutine that will read the file and return two vectors holding the first and second values, respectively. The interface to the subroutine is to be:

```
interface
  subroutine readData (inFile, lines, x, y)
    integer, intent(in)  :: inFile,   lines    ! file unit, size
    real,    intent(out) :: x(lines), y(lines) ! data read
  end subroutine readData
end interface
```

7 Written replies to the questions given below will be required. All of the named files are provided in source form as well as being listed in the text. The cited Figure number indicates where some or all of the code is discussed in the text.

(a) *Figure 1.3* — `hello.f90`
What is necessary to split the printing statement so that “Hello,” and “world” occur on different program lines? That is, to continue it over two lines?

(b) *Figure 4.1* — `arithmetic.f90`
What is the meaning of the symbol (`mod`) used to get the Mod_Result?
What is the meaning of the symbol (`**`) used to get the Pow_Result?

(c) *Figure 4.3* — `array_index.f90`
Is it good practice to use a loop index outside the loop? Why?

(d) *Figure 4.4* — `more_or_less.f90`
What does the symbol (>) mean here?
What does the symbol (==) mean here?

(e) *Figure 4.5* — `if_else.f90`
What does the symbol (`.and.`) mean here? Can its preceding and following arguments be interchanged (is it commutative)?

(f) *Figure 4.6* — `and_or_not.f90`
What does the symbol (`.not.`) mean here?
What does the symbol (`.or.`) mean here? Can its preceding and following arguments be interchanged (is it commutative)?

(g) *Figure 4.7* — `clip.f90`
What does the symbol (<=) mean here?

(h) *Figure 4.8* — `maximum.f90`
What are the input and output arguments for the maxint function?

8 The vertical motion of a projectile at any time, t, has a position given by $y = y_0 + V_0 * t - 1/2 * g * t^2$, and a velocity of $V = V_0 - g * t$ when upward is taken as positive, and where the initial conditions on the starting position and velocity, at $t = 0$, are y_0 and V_0, respectively. Here the gravitational acceleration term, g, has been taken downward. Recall that the numerical value of g depends on the units employed. Use metric units with $g = 9.81 m/s^2$ for distances measured in meters and time in seconds.

Write a C++ or F90 program that will accept initial values of y_0 and V_0, and then compute and print y and V for each single input value of time, t. Print the results for $y_0 = 1.5$ meters and $V_0 = 5.0 m/s$ for times $t = 0.5$, 2.0, and 4.0 seconds.

9 Modify the projectile program written in Problem 2 to have it print the time, position, and velocity for times ranging from 0.0 to 2.0 seconds, in increments of 0.05 seconds. If you use a direct loop do not use real loop variables. Conclude the program by having it list the approximate maximum (positive) height reached and the time when that occurred. The initial data will be the same, but should be printed for completeness. The three columns of numbers should be neat and right justified. In that case the default print format (print * in F90) will usually not be neat and one must employ a "formatted" print or write statement.

10 The Greatest Common Divisor of two positive integers can be computed by at least two different approaches. There is a looping approach known as the Euclidean Algorithm which has the following pseudocode:

```
Rank two positive integers as max and min.
do while min > 0
  Find remainder of max divided by min.
  Replace max by min.
  Replace min by the remainder
end do
Display max as the greatest common divisor.
```

Implement this approach and test with $max = 532 = 28 * 19$ and $min = 112 = 28 * 8$. The names of the remainder functions are given in Table 4.7.

Another approach to some algorithms is to use a "recursive" method which employs a subprogram which calls itself. This may have an advantage in clarifying the algorithm, and/or in reducing the round off error associated with the computations. For example, in computer graphics Bernstein Polynomials are often used to display curves and surfaces efficiently by using a recursive definition in calculating their value at a point.

The Greatest Common Divisor evaluation can also be stated in terms of a recursive function, say gcd, having max and min as its initial two arguments. The following pseudocode defines the function:

```
gcd(max, min) is
  a) max if min = 0, otherwise
  b) gcd(min, remainder of max divided by min) if min > 0
```

Also implement this version and verify that it gives the same result as the Eulerian Algorithm. Note that F90 requires the use of the word "recursive" when defining the subprogram statement block. For example,

```
recursive function gcd(...) result(g)
  ....
end function gcd
```

11 It is not uncommon for data files to be prepared with embedded tabs. Since it is a non-printing control character you can not see it in a listing. However, if you read the file expecting an integer, real, or complex variable the tab will cause a fatal read error. So one needs a tool to clean up such a file.

Write a program to read a file and output a duplicate copy, except that all tabs are replaced with a single space. One could read a complete line and check its characters, or read the file character by character. Remember that C++ and F90 have opposite defaults when advancing to a new line. That is, F90 advances to the next line, after any read or write, unless you include the format control, `advance = 'no'`, while C++ does not advance unless you include the new line control, "<< endl", and C does not advance unless you include the new line control, "\n".

12 Engineering data files consisting of discrete groups of variable types often begin with a control line that lists the number of rows and columns of data, of the first variable type, that follow beginning with the next line. At the end of the data block, the format repeats: control line, variable type data block, etc. until all the variable types are read (or an error occurs where the end of file is encountered). Write a program that reads such a file which contains an integer set, a real set, and a second real set.

13 Neither C++ or F90 provides an inverse hyperbolic tangent function. Write such a function, called `arctanh`. Test it with three different arguments against the values given by MATLAB.

14 Often if one is utilizing a large number of input/output file units it may be difficult to keep up with which one you need. One approach to dealing with that problem may be to define a unit_Class or to create an units_Module to provide functionality and global access to file information. In the latter case assume that we want to provide a function to simply find a unit number that is not currently in use and utilize it for our input/output action:

```
interface
  function get_next_io_unit () result (next)
    integer :: next   ! the next available unit number
  end function get_next_io_unit
end interface
```

Use the Fortran INQUIRE statement to build such a utility. If you are familiar with Matlab you will see this is similar to its fopen feature.

Chapter 5

Object Oriented Methods

5.1 Introduction

In Section 1.7 we outlined procedures that should be considered while conducting the object-oriented analysis and object-oriented design phases that are necessary before the OOP can begin. Here we will expand on those concepts, but the reader is encouraged to read some of the books on those subjects. Many of the references on OOA and OOD rely heavily on detailed graphical diagrams to describe the classes, their attributes ans states, and how they interact with other classes. Often those OO methods do not go into any programming language specific approaches. Our interest is on OOP so we usually will assume that the OOA and OOD have been completed and supplied to us as a set of tables that describe the application, and possibly a software interface contract. Sometimes we will use a subset of the common OO methods diagrams to graphically represent the attributes and members of our classes. Since they being used for OOP the graphical representations will contain, in part, the intrinsic data type descriptions of the language being employed, as well as the derived types created with them.

5.2 The Drill Class

Our first illustration of typical OO methods will be to apply them to a common electric drill. It feeds a rotating cutting bit through a workpiece, thereby removing a volume of material. The effort (power or torque) required to make the hole clearly depends on the material of the workpiece, as well as the attributes of the drill.

Table 5.1 contains a summary of the result of an OO analysis for the drill object. They are further processed in Table 5.2 which gives the results of the OO design phase. When the OOD phase is complete we can create the graphical representation of our `Drill` class as shown in Fig. 5.1. At this point one can begin the actual OOP in the target language. The coding required for this object is so small we could directly put it all together in one programming session. However, that is usually not the case. Often segments of the coding will be assigned to different programming groups that must interface with each other to produce a working final code. Often this means that the OOP design starts with defining the interfaces to each member function. That is, all of the given and return arguments must be defined with respect to their type, whether they are changed by the member, etc. Such an interface can be viewed as a contract between a software supplier and a client user of the software. Once the interface has been finalized, it can be written and given to the programmer to flesh out the full routine, but the interface itself can not be changed.

The interface prototype for our drill object members are given in Fig. 5.2. In this case the remaining coding is defined by a set of equations that relate the object attributes, selected member results, material data, and a few conversion constants to obtain the proper units. Those relationships are given as:

Attributes
What knowledge does it possess or require?

- Rotational speed (revolutions per minute)
- Feed rate per revolution (mm/rev)
- Diameter of the bit (mm)
- Power consumed (W)

Behavior
What questions should it be able to answer?

- What is the volumetric material removal rate? (mm^3/s)
- What is the cutting torque? (N·m)
- What is the material being removed?

Interfaces
What entities need to be input or output?

- Material data
- Torque produced
- Power

Table 5.1: Electric Drill OO Analysis

Area :	$A = \pi\ \text{d}^2\ /4$	(mm^2)
Angular velocity :	$\omega\ ,\ 1\ \text{rev}/\text{min} = \frac{2\pi}{60}$ rad/s	(rad/s)
Material removal rate :	$M = A \cdot \text{feed} \cdot \omega$	(mm^3/s)
Power :	$P = m \cdot u = T \cdot \omega$	(W)
Torque :	$T = P/\omega\ ,$ 1 m = 1000 mm	(N·mm)
Diameter :	d	(mm)
Feed rate :	feed	(mm/rev)
Material dissipation :	u	(W·s/mm^3)

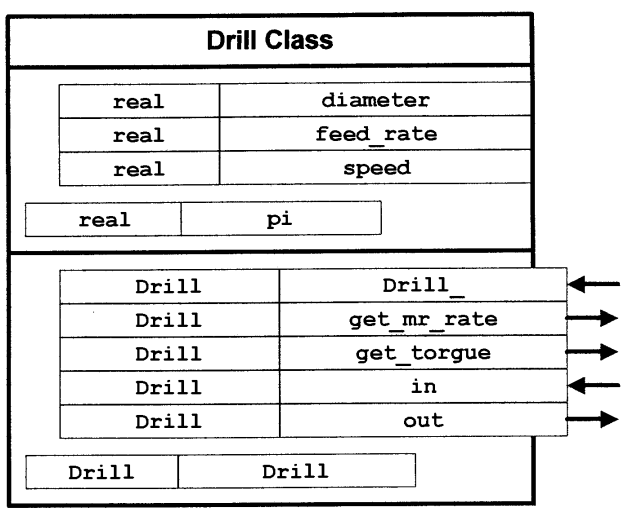


Figure 5.1: Graphical Representation of an Electric Drill Class

The full implementation of the drill class is given in Fig. 5.3, and a `main` program to test the drill class is given in Fig. 5.4. When we wrote the manual constructor, `Drill_`, in this example we chose to

```
interface
! type (Drill) :: x ; x = Drill (d, f, s)  ! intrinsic constructor

  function Drill_ (d, f, s) result (x) ! default constructor
    real, optional :: d, f, s           ! given diameter, feed, speed
    type (Drill)   :: x                 ! the Drill instance
  end function Drill_

  function get_mr_rate (x) result (r) ! material removal rate
    type (Drill), intent(in) :: x     ! a given drill instance
    real                     :: r     ! volume cut rate
  end function get_mr_rate

  function get_torque (x, unit_Power) result (t) ! torque from power
    type (Drill), intent(in) :: x            ! given drill instance
    real,         intent(in) :: unit_Power  ! dissipated in cutting
    real                     :: t            ! resulting torque
  end function get_torque

  subroutine in (x)                          ! read a Drill instance
    type (Drill), intent(out) :: x           ; end subroutine in

  subroutine out (x)                         ! output a Drill instance
    type (Drill), intent(in) :: x            ! given drill instance
  end subroutine out
end interface
```

Figure 5.2: Drill Object Contract Interface Prototype

```
module class_Drill                       ! class name
  implicit none                          ! enforce strong typing
  real, parameter :: pi = 3.141592654    ! or use math_constants
  public          :: Drill, Drill_, get_mr_rate, get_torque
  real, private   :: diameter, feed, speed

  type Drill                              ! defined type, private data
    real :: diameter, feed, speed ; end type

contains ! member functions, overloaded & new operators

! type (Drill) :: x ; x = Drill (d, f, s)  ! intrinsic constructor

  function Drill_ (d, f, s) result (x) ! default constructor
    real, optional :: d, f, s           ! given diameter, feed, speed
    type (Drill)   :: x                 ! the Drill instance
     if ( present(d) .and. present(f) .and. present(s) ) then
       x = Drill (d, f, s)              ! intrinsic constructor
     else                               ! check various input options
       if ( .not. ( present(d) ) ) then ! no diameter given
          x = Drill (10., 0., 0.)       ! default 10mm, at rest zero
       end if ! default form
     end if ! full form
  end function Drill_

  function get_mr_rate (x) result (r) ! material removal rate, mm3̂/sec
    type (Drill), intent(in) :: x  ! a given drill instance
    real                     :: r  ! volume cut rate
     r = 0.25 * pi * x%diameter * x%diameter * x%feed * x%speed/60.
  end function get_mr_rate

  function get_torque (x, unit_Power) result (t) ! torque from power
    type (Drill), intent(in) :: x            ! given drill instance
    real, intent(in)         :: unit_Power  ! dissipated in cutting
    real                     :: t            ! resulting torque
    real                     :: rad_per_sec ! radians per second
     rad_per_sec = 2 * pi * x%speed / 60.
     t = get_mr_rate(x) * unit_Power / rad_per_sec    ! torque
  end function get_torque

  subroutine in (x)                          ! input a Drill instance
    type (Drill), intent(out) :: x           ! given drill instance
     read *, x                               ! get intrinsic data
  end subroutine in

  subroutine out (x)                         ! output a Drill instance
    type (Drill), intent(in) :: x            ! given drill instance
     print *,"Drill"; print *, " Diameter: ",x % diameter
     print *," Feed    : ",x % feed; print *," Speed   : ",x % speed
  end subroutine out
end module class_Drill                      ! close class definition
```

Figure 5.3: A Electrical Drill Class

Attributes

Name	*Type*	*Private*	*Description*
diameter	real	Y	Bit diameter (mm)
feed	real	Y	Bit feed rate (mm/rev)
speed	real	Y	Bit rotational speed (rpm)

Behavior

Name	*Private*	*Description*
drill_	N	Default constructor using all attributes, or none
get_mr_rate	N	Material removal rate (mm^3/sec)
get_torque	N	Required torque (N·m)
power	N	Required power (W)

Data

Name	*Description*
u	Material power description per unit volume (W s/mm^3)

Interfaces

Name	*Description*
read	Input drill and material data
print	Output object results

Table 5.2: Electric Drill OO Design

utilize the intrinsic constructor `Drill` (in lines 18 and 21) rather than including lines to assign values to each of the components of our data type. If at some later time we add or delete a component in the type declaration then the number of required arguments for the intrinsic constructor would also change. That would require the revision of all members that used the intrinsic constructor. An advantage of the object-oriented approach to programming is that we know that all such routines (that can access the intrinsic constructor) are encapsulated within this class declaration module, and we can be sure that no other code segments must be changed to remain consistent with the new version. That is, OOP helps with code maintance.

5.3 Global Positioning Satellite Distances

Consider the problem of traveling by ship or airplane between two points on the earth. Here we assume that there are no physical obstructions that prevent the vehicle from following the shortest path, which is an arc of a ”great circle” on the earth’s surface. We will neglect the altitude of the airplane in comparison to the earth’s radius. The original and final positions are to be defined in terms of their angles of latitude (measured N or S from the equator) and longitude (measured E or W from Greenwich, England). These two attributes define an angular position from a defined reference point on the spherical surface of the earth. They are measured in terms of whole degrees, whole minutes (1 degree = 60 minutes), and seconds (1 minute = 60 seconds). Historically, whole seconds are usually used, but they give positions that are only accurate to about 300 meters. Thus, we will use a real variable for the seconds to allow for potential reuse for the software for applications that require more accuracy, such as those using Global Positioning Satellite (GPS) data. Recall that latitude and longitude have associated directional information of North or South, and East or West, respectively. Also in defining a global position point it seems logical to include a name for each position. Depending on the application the name may identify a city or port, or a ”station number” in a land survey, or a ”path point number” for a directed robot motion.

Eventually, we want to compute the great arc distance between given pairs of latitude and longitude. That solid geometry calculation requires that one use angles that are real numbers measured in radians ($2pi$ = 360 degrees). Thus our problem description begins with an `Angle` class as its basic class. Both latitude and longitude will be defined to be of the `Position_Angle` class and we observe that a `Position_Angle` is a ”Kind-Of” `Angle`, or a `Position_Angle` has an ”Is-A” relationship to an `Angle`. The positions we seek are on a surface so only two measures (latitude and longitude) are needed

```
program main               ! test the Drill class
 use class_Drill          ! i.e., all public members and public data
 implicit none
 type (Drill) :: drill_A, drill_B, drill_C
 real         :: unit_Power
  print *, "Enter diameter (mm), feed (mm/rev), speed (rpm):"
  call in (drill_A)
  print *, "Enter average power unit for material ( W.s/mm**3):"
  read *, unit_Power ; call out (drill_A)               ! user input
  print *, "Material removal rate is: ", get_mr_rate(drill_A), &
           " mm**3/sec"
  print *, "Torque in this material is: ",  &
           & get_torque (drill_A, unit_Power), " W.s"
  drill_B = Drill_ (5., 4., 3.); call out (drill_B) ! manual
  drill_C = Drill_ ();           call out (drill_C) ! default
end program                                       ! Running gives
! Enter diameter (mm), feed (mm/rev), speed (rpm): 10 0.2 800
! Enter average power unit for material ( W.s/mm**3): 0.5
! Drill
!  Diameter: 10.
!  Feed    : 0.200000003
!  Speed   : 800.
! Material removal rate is: 209.439514 mm**3/sec
! Torque in this material is: 1.25 W.s
! Drill
!  Diameter: 5.
!  Feed    : 4.
!  Speed   : 3.
! Drill
!  Diameter: 10.
!  Feed    : 0.E+0
!  Speed   : 0.E+0
```

Figure 5.4: Testing a Electrical Drill Class

to uniquely define the location, which we will refer to as the `Global_Position`. Here we see that the two `Position_Angle` object values are a ”Part-Of” the `Global_Position` class, or we can say that a `Global_Position` ”Has-A” `Position_Angle`.

The sort of relationships between classes that we have noted above are quite common and relate to the concept of inheritance as a means to reuse code. In an ”Is-A” relationship, the derived class is a variation of the base class. Here the derived class `Position_Angle` forms an ”Is-A” relation to the base class, `Angle`. In a ”Has-A” relationship, the derived class has an attribute or property of the base class. Here the derived class of `Global_Position` forms a Has-A relation to its base class of `Position_Angle`. Also, the `Great_Arc` class forms a ”Has-A” relation to the `Global_Position` class.

Looking back at previous classes, in Chapter 3, we observe that the class Student ”Is-A” variation of the class `Person` and the class `Person` forms at least one ”Has-A” relationship with the class `Date`. In general we know that a graduate student is a ”Kind-Of” student, but not every student is a graduate student. This subtyping, or ”Is-A” relationship is also called interface inheritance. Likewise, complicated classes can be designed from simpler or composition inheritance.

The OO Analysis Tables for the classes of `Great_Arc`, `Global_Position`, `Position_Angle`, and `Angle` are given in Tables 5.3 through 5.6, respectively. Historically people have specified latitude and longitude mainly in terms of whole (integer) degrees, minutes, and seconds. Sometimes you find navigation charts that give positions in whole degrees and decimal minutes. Today GPS data are being used for various high accuracy positioning such as land surveys, or the control of robots as they move over distances of a few meters. The latter will clearly need decimal seconds values in their constructor. Thus, we will create a number of constructors for the position angles. In the next chapter we will review how to access any of them, based on the signature of their arguments, through the use of a single polymorphic routine name. These considerations and the OOA tables lead to the construction of the corresponding set of OO Design Tables given in Tables 5.7 through 5.10. Those OOD tables could lead to software interface contracts to be distributed to the programming groups. When combined and tested they yield the corresponding class modules which are shown for the classes `Angle, Position_Angle, Global_Position,` and `Great_Arc` in Figs. 5.6 to 5.12, respectively. They in turn are verified by the `main` program given in Fig. 5.13 along with its output.

Attributes
What knowledge does it possess or require?
- Global position 1 (latitude, longitude)
- Global position 2 (latitude, longitude)
- Smallest arc (km)
- Radius of the earth (km)

Behavior
What questions should it be able to answer?
- What is the (smallest) great arc between the points

What services should it provide?
- Default value (Greenwich, Greenwich, 0.0)
- Initialize for two positions
- Convert kilometers to miles

Relationships
What are its related classes?
- Has-A pair of Global_Positions

Interfaces
What entities need to be input or output?
- The distance between two positions.

Table 5.3: Great Arc OO Analysis

Attributes
What knowledge does it possess or require?
- Latitude (degrees, minutes, seconds, and direction)
- Longitude (degrees, minutes, seconds, and direction)

Behavior
What questions should it be able to answer?
- What is the latitude of the location
- What is the longitude of the location

What services should it provide?
- Default position (Greenwich)
- Initialize a position (latitude and longitude)

Relationships
What are its related classes?
- Part-Of GreatArc
- Has-A pair of Position_Angles

Interfaces
What entities need to be input or output?
- The latitude and longitude, and a position name.

Table 5.4: Global Position OO Analysis

Attributes
What knowledge does it possess or require?
- Magnitude (degrees, minutes, seconds)
- Direction (N or S or E or W)

Behavior
What questions should it be able to answer?
- What is its magnitude and direction

What services should it provide?
- Default value (0, 0, 0.0, N)
- Initialization to input value

Relationships
What are its related classes?
- Part-Of Global_Positions
- Is-A Angle

Interfaces
What entities need to be input or output?
- None

Table 5.5: Position Angle OO Analysis

Attributes
What knowledge does it possess or require?
- Signed value (radians)

Behavior
What questions should it be able to answer?
- What is the current value

What services should it provide?
- default values (0.0)
- Conversion to signed decimal degrees
- Conversion to signed degree, minutes, and decimal seconds
- Conversion from signed decimal degrees
- Conversion from signed degree, minutes, and decimal seconds

Relationships
What are its related classes?
- Base Class for Position_Angle

Interfaces
What entities need to be input or output?
- None

Table 5.6: Angle OO Analysis

Attributes

Name	*Type*	*Private*	*Description*
point_1	Global_Position	Y	Lat-Long-Name of point 1
point_2	Global_Position	Y	Lat-Long-Name of point 2
arc	real	Y	Arc distance between points

Behavior

Name	*Private*	*Description*
Great_Arc_	N	Constructor for two position points
get_Arc	N	Compute great arc between two points

Data

Name	*Description*
Earth_Radius_Mean	Conversion factor
m_Per_Mile	Conversion factor

Interfaces

Name	*Description*
List_Great_Arc	Print arc values (two positions and distance)
List_Pt_to_Pt	Print distance and two points

Table 5.7: Class Great_Arc OO Design

Attributes

Name	*Type*	*Private*	*Description*
latitude	Position_Angle	Y	Latitude
longitude	Position_Angle	Y	Longtitude
name	characters	Y	Point name

Behavior

Name	*Private*	*Description*
Global_Position_	N	Constructor for d-m-s pairs and point name
set_Lat_and_Long_at	N	Constructor for lat-long-name set
get_Latitude	N	Return latitude of a point
get_Longitude	N	Return longitude of a point
set_Latitude	N	Insert latitude of a point
set_Longitude	N	Insert longitude of a point

Data

Name	*Description*
None	

Interfaces

Name	*Description*
List_Position	Print name and latitude, longitude of a position

Table 5.8: Class Global_Position OO Design

Attributes

Name	*Type*	*Private*	*Description*
deg	integer	Y	Degrees of angle
min	integer	Y	Minutes of angle
sec	real	Y	Seconds of angle
dir	character	Y	Compass direction

Behavior

Name	*Private*	*Description*
Default_Angle	N	Default constructor
Decimal_min	N	Constructor for decimal minutes
Decimal_sec	N	Constructor for decimal seconds
Int_deg	N	Constructor for whole deg
Int_deg_min	N	Constructor for whole deg, min
Int_deg_min_sec	N	Constructor for whole deg, min, sec
to_Decimal_Degrees	N	Convert position angle values to decimal degree
to_Radians	N	Convert position angle values to decimal radian

Data

Name	*Description*
None	

Interfaces

Name	*Description*
List_Position_Angle	Print values for position angle
Read_Position_Angle	Read values for position angle

Table 5.9: Class Position_Angle OO Design

Attributes

Name	*Type*	*Private*	*Description*
rad	real	Y	Radian measure of the angle (rad)

Behavior

Name	*Private*	*Description*
Angle_	N	A generic constructor
List_Angle	N	List angle value in radians and degrees

Data

Name	*Description*
Deg_per_Rad	Unit conversion parameter

Table 5.10: Class Angle OO Design

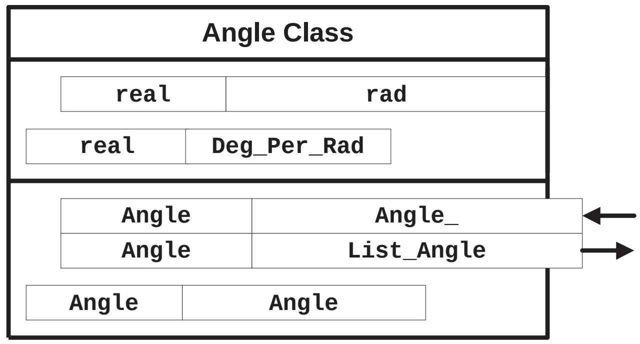


Figure 5.5: Graphical Representation of an Angle Class

```
module class_Angle      ! file: class_Angle.f90
 implicit none
  type Angle             ! angle in (signed) radians
    private
    real :: rad          ! radians
  end type
  real, parameter:: Deg_Per_Rad = 57.2957795130823209d0
contains

 function Angle_ (r) result (ang) ! public constructor
   real, optional :: r            ! radians
   type (Angle)   :: ang
     if ( present(r) ) then
            ang = Angle (r)    ! intrinsic constructor
     else ; ang = Angle (0.0)  ! intrinsic constructor
     end if ; end function Angle_

  subroutine List_Angle (ang)
    type (Angle), intent(in) :: ang
      print *, 'Angle = ', ang % rad, ' radians (', &
                         Deg_Per_Rad * ang % rad, ' degrees)'
  end subroutine List_Angle
end module class_Angle
```

Figure 5.6: A Definition of the Class Angle

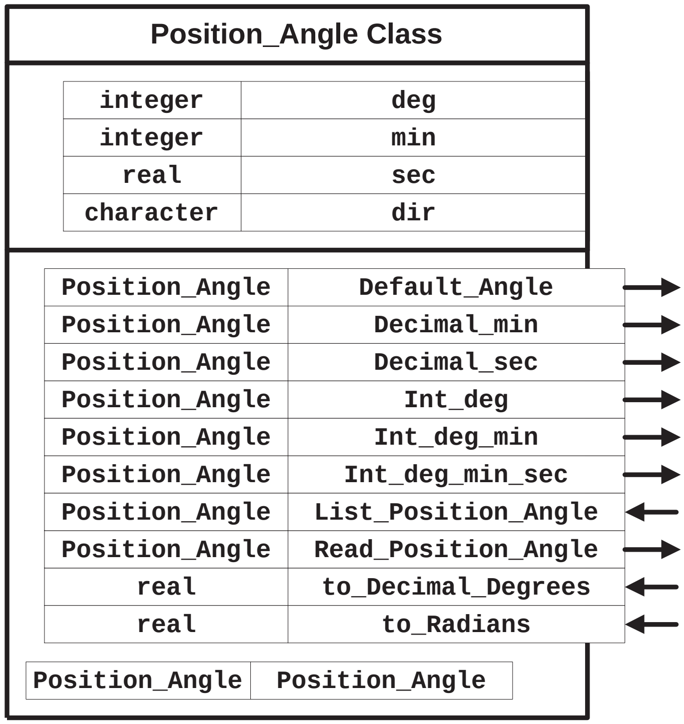


Figure 5.7: Graphical Representation of a Position Angle Class

```
module class_Position_Angle ! file: class_Position_Angle.f90
  use class_Angle
  implicit none
  type Position_Angle       ! angle in deg, min, sec
    private
    integer   :: deg, min    ! degrees, minutes
    real      :: sec         ! seconds
    character :: dir         ! N | S, E | W
  end type
contains

 function Default_Angle () result (ang) ! default constructor
   type (Position_Angle) :: ang
     ang = Position_Angle (0, 0, 0., ’N’)  ! intrinsic
 end function Default_Angle

 function Decimal_min (d, m, news) result (ang) ! public
   integer,   intent(in)  :: d              ! degrees
   real,      intent(in)  :: m              ! minutes
   character, intent(in)  :: news           ! N | S, E | W
   type (Position_Angle)  :: ang            ! angle out
   integer                :: min            ! minutes
   real                   :: s              ! seconds
     min = floor ( m ) ; s = (m - min)*60.  ! convert
     ang = Position_Angle (d, m, s, news)  ! intrinsic
 end function Decimal_min

 function Decimal_sec (d, m, s, news) result (ang) ! public
   integer,   intent(in)  :: d, m           ! degrees, minutes
   real,      intent(in)  :: s              ! seconds
   character, intent(in)  :: news           ! N | S, E | W
   type (Position_Angle) :: ang             ! angle out
     ang = Position_Angle (d, m, s, news)   ! intrinsic
 end function Decimal_sec

```

(Fig. 5.8, A Definition of the Class Position Angle (Continued))

```
  function Int_deg (d, news) result (ang)   ! public
    integer,   intent(in)  :: d             ! degrees, minutes
    character, intent(in)  :: news          ! N | S, E | W
    type (Position_Angle) :: ang            ! angle out
      ang = Position_Angle (d, 0, 0.0, news)  ! intrinsic
  end function Int_deg

  function Int_deg_min (d, m, news) result (ang) ! public
    integer,   intent(in)  :: d, m            ! degrees, minutes
    character, intent(in)  :: news            ! N | S, E | W
    type (Position_Angle) :: ang              ! angle out
      ang = Position_Angle (d, m, 0.0, news)  ! intrinsic
  end function Int_deg_min

  function Int_deg_min_sec (d, m, s, news) result (ang) ! public
    integer,   intent(in)  :: d, m, s         ! deg, min, seconds
    character, intent(in)  :: news            ! N | S, E | W
    type (Position_Angle) :: ang             ! angle out
      ang = Position_Angle (d, m, real(s), news)  ! intrinsic
  end function Int_deg_min_sec

  subroutine List_Position_Angle (a)
   type (Position_Angle) :: a   ! angle
     print 5, a ; 5 format (i3, " ", i2,"' ", f8.5, '" ', a1)
  end subroutine

  subroutine Read_Position_Angle (a)
   type (Position_Angle) :: a   ! angle
     read *, a%deg, a%min, a%sec, a%dir ; end subroutine

  function to_Decimal_Degrees (ang) result (degrees)
    type (Position_Angle), intent(in) :: ang
    real                              :: degrees
      degrees = ang%deg + ang%min/60. + ang%sec/60.
      if (ang%dir == "S" .or. ang%dir == "s" .or. &
          ang%dir == "W" .or. ang%dir == "w") degrees = -degrees
  end function to_Decimal_Degrees

  function to_Radians (ang) result (radians)
    type (Position_Angle), intent(in) :: ang
    real                              :: radians
      radians = (ang%deg + ang%min/60. + ang%sec/60.)/Deg_Per_Rad
      if (ang%dir == "S" .or. ang%dir == "s" .or. &
          ang%dir == "W" .or. ang%dir == "w") radians = -radians
  end function to_Radians
end module class_Position_Angle
```

Figure 5.8: A Definition of the Class Position Angle

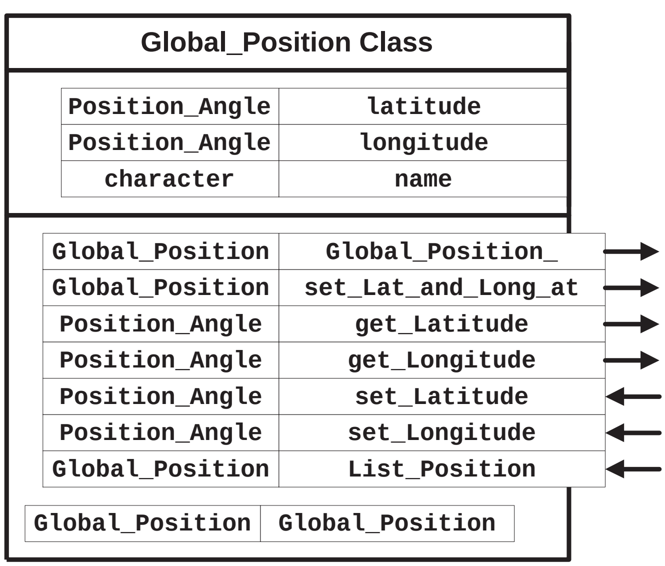


Figure 5.9: Graphical Representation of a Global Position Class

```
module class_Global_Position
  use class_Position_Angle
  implicit none
  type Global_Position
    private
    type (Position_Angle) :: latitude, longitude
    character (len=31)    :: name
  end type Global_Position
contains

  function Global_Position_ (d1, m1, s1, c1,  &  ! constructor
                             d2, m2, s2, c2, n) result (GP)
   integer,    intent(in)  :: d1, m1, s1     ! deg, min, sec
   integer,    intent(in)  :: d2, m2, s2     ! deg, min, sec
   character,  intent(in)  :: c1, c2         ! compass
   character (len=*)       :: n              ! name
   type (Global_Position) :: GP             ! returned position
     GP % latitude  =  Int_deg_min_sec (d1, m1, s1, c1)
     GP % longitude =  Int_deg_min_sec (d2, m2, s2, c2)
     GP % name      = n  ; end function Global_Position_

  function set_Lat_and_Long_at (lat, long, n) result (GP) ! cons
    type (Position_Angle), intent(in) :: lat, long         ! angles
    character (len=*),      intent(in) :: n                 ! name
    type (Global_Position)            : GP                 ! position
      GP % latitude = lat   ; GP % longitude = long
      GP % name     = n     ; end function set_Lat_and_Long_at

  function get_Latitude (GP) result (lat)
    type (Global_Position), intent(in) :: GP
    type (Position_Angle)              :: lat
      lat = GP % latitude ; end function get_Latitude

  function get_Longitude (GP) result (long)
    type (Global_Position), intent(in) :: GP
    type (Position_Angle)              :: long
      long = GP % longitude ; end function get_Longitude

  subroutine set_Latitude (GP, lat)
    type (Global_Position), intent(inout) :: GP
    type (Position_Angle), intent(in)     :: lat
      GP % latitude = lat ; end subroutine set_Latitude

  subroutine set_Longitude (GP, long)
    type (Global_Position), intent(inout) :: GP
    type (Position_Angle), intent(in)     :: long
      GP % longitude = long ; end subroutine set_Longitude

  subroutine List_Position (GP)
    type (Global_Position), intent(in) :: GP
      print *, 'Position at ', GP % name
      write (*,'(" Latitude:  ")', advance = "no")
      call List_Position_Angle (GP % latitude)
      write (*,'(" Longitude: ")', advance = "no")
      call List_Position_Angle (GP % longitude)
  end subroutine List_Position
end module class_Global_Position
```

Figure 5.10: A Definition of the Class Global Position

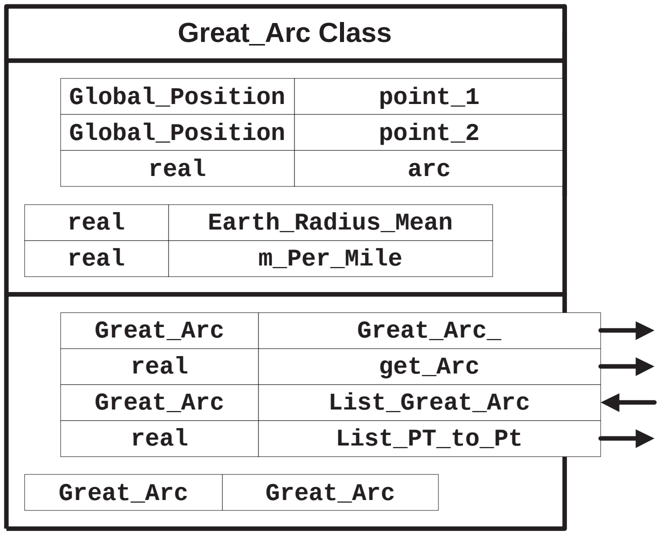


Figure 5.11: Graphical Representation of a Great Arc Class

```
module class_Great_Arc
 use class_Global_Position
  implicit none
  real, parameter :: Earth_Radius_Mean = 6.371d6 ! meters
  real, parameter :: m_Per_Mile        = 1609.344
  type Great_Arc
    type (Global_Position) :: point_1, point_2
    real                   :: arc
  end type Great_Arc
contains

  function Great_Arc_ (GP1, GP2) result (G_A)        ! constructor
    type (Global_Position), intent(in) :: GP1, GP2   ! points
    type (Great_Arc)                   :: G_A        ! earth arc
      G_A = Great_Arc (GP1, GP2, get_Arc (GP1, GP2)) ! intrinsic
  end function Great_Arc_

  function get_Arc (GP1, GP2) result (dist)
    type (Global_Position), intent(in) :: GP1, GP2
    real                               :: dist
    real :: lat1, lat2, long1, long2
    !  convert latitude, longitude to radians
      lat1  = to_Radians (get_Latitude (GP1))
      lat2  = to_Radians (get_Latitude (GP2))
      long1 = to_Radians (get_Longitude (GP1))
      long2 = to_Radians (get_Longitude (GP2))
    !  compute great circle arc of earth
      dist = 2 * Earth_Radius_Mean                            &
           * asin( sqrt ( (sin((lat1 - lat2)/2.))**2          &
           + cos(lat1)*cos(lat2)*(sin((long1-long2)/2.))**2 ) )
  end function get_Arc

  subroutine List_Great_Arc (A_to_B)
    type (Great_Arc), intent(in) :: A_to_B
    real                         :: dist      ! in meters
      print * ; print *, "The great circle arc between"
      call List_Position (A_to_B % point_1)
      call List_Position (A_to_B % point_2)
      dist = A_to_B % arc                   ! convert to km and miles
      print *, "is ", dist/1000, " km  (", dist/m_Per_Mile, "miles)."
  end subroutine List_Great_Arc

  subroutine List_Pt_to_Pt (GP1, GP2)                    ! alternate
    type (Global_Position), intent(in) :: GP1, GP2       ! points
    real                               :: arc            ! distance
      print * ; print *, "The great circle arc between"
      call List_Position (GP1) ; call List_Position (GP2)
      arc = get_Arc (GP1, GP2)                            ! in meters
      print *, "is ", arc/1000, " km  (", arc/m_Per_Mile, "miles)"
  end subroutine List_Pt_to_Pt
end module class_Great_Arc
```

Figure 5.12: Definition of the Class Great Arc

```
program main
 use class_Great_Arc
 implicit none
 type (Great_Arc)       :: arc
 type (Global_Position) :: g1, g2
 type (Position_Angle)  :: a1, a2
 type (Angle)           :: ang
 real                   :: deg, rad
   a1 = Decimal_sec     (10, 30, 0., "N"); call List_Position_Angle(a1
   a1 = Int_deg_min_sec(10, 30, 0,  "N"); call List_Position_
   a1 = Int_deg_min     (10, 30,    "N"); call List_Position_An
   a1 = Int_deg         (20,        "N"); call List_Position_Angle(a1
!   call Read_Position_Angle (a2)
   a2 = Decimal_sec     (30, 48, 0., "E"); call List_Position_Angle(a2
   ang = Angle_ (1.0)              ; call List_Angle (ang)
   deg = to_Decimal_Degrees (a1) ; print *, deg, deg/Deg_Per_Rad
   rad = to_Radians (a1)           ; print *, rad
!
   g1 = set_Lat_and_Long_at (a1, a2, 'g1')
   call List_Position (g1)
   g2 = Global_Position_ (20, 5, 40, "S", 75, 0, 20, "E", 'g2')
   call List_Position (g2)
   print *, "Arc = ", get_Arc (g1, g2), " (meters)"
   g1 = Global_Position_ ( 0, 0, 0, "N", 0, 0, 0, "E", 'equator')
   g2 = Global_Position_ (90, 0, 0, "N", 0, 0, 0, "E", 'N-pole')
   call List_Pt_to_Pt (g1, g2)
   arc = Great_Arc_ (g1, g2) ; call List_Great_Arc (arc)
end program main                              ! running gives:
! 10 30'  0.00000" N  ; ! 10 30'  0.00000" N ; ! 10 30'  0.00000" N
! 20  0'  0.00000" N  ; ! 30 48'  0.00000" N
! Angle =  1.000000000  radians ( 57.29578018  degrees)
! 20.00000000 0.3490658402        ; ! 0.3490658402
! Position at g1                  ; ! Position at g2
! Latitude:   20  0'  0.00000" N  ; ! Latitude:   20  5' 40.00000" S
! Longitude:  30 48'  0.00000" E  ; ! Longitude:  75  0' 20.00000" E
! Arc =  6633165.000  (meters)
!
! The great circle arc between
! Position at equator             ; ! Position at N-pole
! Latitude:    0  0'  0.00000" N  ; ! Latitude:   90  0'  0.00000" N
! Longitude:   0  0'  0.00000" E  ; ! Longitude:   0  0'  0.00000" E
! is  10007.54297  km  ( 6218.398926 miles)
!
! The great circle arc between
! Position at equator             ; ! Position at N-pole
! Latitude:    0  0'  0.00000" N  ; ! Latitude:   90  0'  0.00000" N
! Longitude:   0  0'  0.00000" E  ; ! Longitude:   0  0'  0.00000" E
! is  10007.54297  km  ( 6218.398926 miles)
```

Figure 5.13: Testing the Great Arc Class Interactions

5.4 Exercises

1. Referring to Chapter 3, develop OOA and OOD tables for the a) `Geometric` class, b) `Date` class, c) `Person` class, d) `Student` class.

2. Develop the graphical representations for the classes in the a) drill study, b) global position study.

3. Use the classes in the GPS study to develop a main program that will read a list (vector) of `Global_Position` types and use them to output a square table of great arc distances from one site to each of the others. That is, the table entry in row `j`, column `k` gives the arc from site `j` to site `k`. Such a table would be symmetric (with zeros along one diagonal) so you may want to give only half of it.

4. Modify the given `Class_Position_Angle` to provide a polymorphic interface for a constructor `Position_Angle_` that will accept decimal, integer or no data for the seconds value. Also allow for the omission of the minutes value.

Chapter 6

Inheritance and Polymorphism

6.1 Introduction

As we have seen earlier in our introduction to OOP *inheritance* is a mechanism for deriving a new class from an older *base class*. That is, the base class, sometimes called the *super class*, is supplemented or selectively altered to create the new *derived class*. Inheritance provides a powerful code reuse mechanism since a hierarchy of related classes can be created that share the same code. A class can be derived from an existing base class using the module construct illustrated in Fig. 6.1.

We note that the inheritance is invoked by the USE statement. Sometimes an inherited entity (attribute or member) needs to be slightly amended for the purposes of the new classes. Thus, at times one may want to selectively bring into the new class only certain entities from the base class. The modifier ONLY in a USE statement allows one to select the desired entities from the base class as illustrated below in Fig. 6.2. It is also common to develop name conflicts when combining entities from one or more related classes. Thus a rename modifier, =>, is also provided for a USE statement to allow the programmer to pick a new *local* name for an entity onherited from the base class. The form for that modifier is given in Fig. 6.3.

It is logical to extend any or all of the above inheritance mechanisms to produce multiple inheritance. *Multiple Inheritance* allows a derived class to be created by using inheritance from more than a single base class. While multiple inheritance may at first seem like a panacea for efficient code reuse, experience has shown that a heavy use of multiple inheritance can result in entity conflicts and be otherwise counterproductive. Nevertheless it is a useful tool in OOP. In F90 the module form for selective multiple inheritance would combine the above USE options in a single module as illustrated in Fig. 6.4.

```
module derived_class_name
    use base_class_name
! new attribute declarations, if any
            . . .
contains

   ! new member definitions
            . . .
end module derived_class_name
```

Figure 6.1: F90 Single Inheritance Form.

```
module derived_class_name
      use  base_class_name, only: list_of_entities
! new attribute declarations, if any
               . . .
contains

    ! new member definitions
               . . .
end module derived_class_name
```

Figure 6.2: F90 Selective Single Inheritance Form.

```
module derived_class_name
      use  base_class_name, local_name => base_entity_name
! new attribute declarations, if any
               . . .
contains

    ! new member definitions
               . . .
end module derived_class_name
```

Figure 6.3: F90 Single Inheritance Form, with Local Renaming.

```
module derived_class_name
      use  base1_class_name
      use  base2_class_name
      use  base3_class_name, only: list_of_entities
      use  base4_class_name, local_name => base_entity_name
! new attribute declarations, if any
               . . .
contains

      ! new member definitions
               . . .
end module derived_class_name
```

Figure 6.4: F90 Multiple Selective Inheritance with Renaming.

```
module class_Professor    ! file: class_Professor.f90
  implicit none
  public  :: print, name
  private :: publs
    type Professor
       character (len=20) :: name
       integer            :: publs  ! publications
    end type Professor
contains
    function  make_Professor (n, p) result (who)
      character (len=*), optional, intent(in) :: n
      integer,           optional, intent(in) :: p
      type (Professor)                       :: who ! out
        who%name        = " "             ! set defaults
        who%publs       = 0.0
        if ( present(n) ) who%name  = n  ! construct
        if ( present(p) ) who%publs = p
    end function  make_Professor

    function  print (who)
      type (Professor), intent(in) :: who
        print *, "My name is ", who%name,  &
         ", and I have ", who%publs, " publications."
    end function  print
end module class_Professor
```

Figure 6.5: A Professor Class

6.2 Example Applications of Inheritance

6.2.1 The Professor Class

In the introductory examples of OOP in Chapter 3 we introduced the concepts of inheritance and multiple inheritance by the use of the `Date` class, `Person` class, and `Student` class. To reinforce those concepts we will reuse those three classes and will have them be inherited by a Professor class. Acknowledging the common "publish or perish" aspect of academic life the professor class must keep up with the number of publications of the professor. The new class is given in Fig. 6.5 along with a small validation program in Fig. 6.6.

Note that the validation program brings in three different versions of the "print" member (lines 7-9) and renames two of them to allow a polymorphic print statement (lines 12-14) that selects the proper member based solely on the class of its argument. Observe that the previous `Date` class is brought into the `main` through the use of the `Person` class (in line 7). Of course, it is necessary to have an interface defined for the overloaded member name so that the compiler knows which candidate routines to search at run time. This example also serves to remind the reader that Fortran does *not* have *keywords* that are not allowed to be used by the programmer. In this case the print function (lines 19, 22, 25) has automatically replaced the intrinsic print function of Fortran. Most languages, including C++ do not allow one to do that.

6.2.2 The Employee and Manager Classes

Next we will begin the popular employee-manager classes as examples of common related classes that demonstrate the use of inheritance. Once again the idea behind encapsulating these data and their associated functionality is to model a pair of real world entities - an employee and a manager. As we go through possible relations between these two simple classes it becomes clear that there is no unique way to establish the classes and how they should interact. We begin with a minimal approach and then work through two alternate versions to reach the point where an experienced OO programmer might have begun. The first `Employee` class, shown in Fig. 6.7 has a name and pay rate as its attributes. Only the intrinsic constructor is used within the member `setDataE` to concatenate a first name and last name to form the complete name attribute and to accept the pay rate. To query members `getNameE` and `getRate` are provided to extract either of the desired attributes. Finally, member `payE` is provided to compute the pay earned by an employee. It assumes that an employee is paid by the hour. A simple testing main program is shown in Fig. 6.8 It simply defines two employees (`empl1` and `empl2`), assigns their names and pay rates, and then computes and displays their pay based on the respective number of hours worked.

```
! Multiple Inheritance and Polymorphism of the "print" function
include 'class_Person.inc'       ! also brings in class_Date
include 'class_Student.inc'
include 'class_Professor.inc'

program main
  use class_Person                               ! no changes
  use class_Student,   print_S => print ! renamed to print_S
  use class_Professor, print_F => print ! renamed to print_F
  implicit none

!  Interface to generic routine, print, for any type argument
   interface  print  ! using renamed type dependent functions
     module procedure print_Name, print_S, print_F
   end interface

   type (Person) :: x; type (Student) :: y; type (Professor) :: z

      x = Person ("Bob"); ! default constructor
      call print(x);      ! print person type

      y = Student ("Tom", 3.47); ! default constructor
      call print(y);      ! print student type

      z = Professor ("Ann", 7); ! default constructor
      call print(z);      ! print professor type
      ! alternate constructors not used
end program main            ! Running gives:
! Bob
! My name is Tom, and my G.P.A. is 3.4700000.
! My name is Ann, and I have 7 publications.
```

Figure 6.6: Bringing Four Classes and Three Functions Together

```
module class_Employee
! The module class_Employee contains both the
! data and functionality of an employee.
!
  implicit none
  public :: setDataE, getNameE, payE  ! the Functionality

  type Employee                   ! the Data
    private
    character(30) :: name
    real          :: payRate ; end type Employee

contains ! inherited internal variables and subprograms

  function setDataE (lastName, firstName, newPayRate) result (E)
    character(*), intent(in) :: lastName
    character(*), intent(in) :: firstName
    real,         intent(in) :: newPayRate
    type (Employee)          :: E            ! employee
                ! use intrinsic constructor
      E = Employee((trim(firstName)//" "//trim(lastName)),newPayRate)
  end function setDataE

  function getNameE ( Person ) result (n)
    type (Employee), intent(in) :: Person
    character(30)               :: n         ! name
      n = Person % name ; end function getNameE

  function getRate ( Person ) result ( r )
    type (Employee), intent(in) :: Person
    real                        :: r         ! rate
      r = Person % payRate ; end function getRate

  function payE ( Person, hoursWorked ) result ( amount )
    type (Employee), intent(in) :: Person
    real,            intent(in) :: hoursWorked
    real                        :: amount
      amount = Person % payRate * hoursWorked ; end function payE
end module class_Employee
```

Figure 6.7: First Definition of an Employee Class

Note that both `empl1` and `empl2` are each an instance of a class, and therefore they are objects and thus distinctly different from a class.

```
program main
! Example use of employees
  use class_Employee
  type (Employee)  empl1, empl2

! Set up 1st employee and print out his name and pay
    empl1 = setDataE ( "Jones", "Bill", 25.0 )
    print *, "Name: ", getNameE ( empl1 )
    print *, "Pay: ", payE ( empl1, 40.0 )

! Set up 2nd employee and print out her name and pay
    empl2 = setDataE ( "Doe", "Jane", 27.5 )
    print *, "Name: ", getNameE ( empl2 )
    print *, "Pay: ", payE ( empl2, 38.0 )
end program main      ! Running produces;
!  Name: Bill Jones   !  Pay:    1000.
!  Name: Jane Doe     !  Pay:    1045.
```

Figure 6.8: First Test of an Employee Class

Next we deal with a manager which Is-A "kind of" employee. One difference is that some managers may be paid a salary rather than an hourly rate. Thus we have the `Manager` class inherit the attributes of the `Employee` class and add a new logical attribute `isSalaried` which is true when the manager is salary based. To support such a case we must add a new member `setSalaried` which can turn the new attribute on or off, and a corresponding member `payM` that uses the `isSalaried` flag when computing the pay. The `class_Manager` module is shown in Fig. 6.9 Note that the constructor `Manager_` defaults to an hourly worker (line 33) and it uses the inherited employee constructor (line 31). Figure 6.10 shows a test program to validate the manager class (and indirectly the employee class). It defines a salaried manager, `mgr1`, an hourly manager `mgr2`, and prints the name and weekly pay for both. (Verify these weekly pay amounts.)

With these two classes we have mainly used different program names for members that do similar things in each class (the author's preference). However, many programmers prefer to use a single member name for a typical operation, regardless of the class of the operand. We also restricted all the attributes to `private` and allowed all the members to be `public`. We could use several alternate approaches to building our `Employee` and `Manager` classes. For example, assume we want a single member name called `pay` to be invoked for an employee, or manager (or executive). Furthermore we will allow the attributes to be `public` instead of `private`. Lowering the access restrictions to the attributes makes it easier to write an alternate program, but it is not a recommended procedure since it breaks the data hiding concept that has been shown to be important to OO software maintenance and reliability. The alternate `Employee` and `Manager` classes are shown in Figs. 6.11 and 6.12, respectively. Note that they both have a `pay` member but their arguments are of different classes and their internal calculations are different. Now we want a validation program that will create both classes of individuals, and use a single member name, `PrintPay`, to print the proper pay amount from the single member name `pay`. This can be done in different ways. One problem that arises in our plan to reuse the code in the two alternate class modules is that neither contained a pay printing member. We will need two new routines, `PrintPayEmployee` and `PrintPayManager`, and a generic or polymorphic interface to them. We have at least three ways to do this. One way is to place the two routines in an external file (or external to main if in the same file), leave the two class modules unchanged, and have the `main` program begin with (or INCLUDE) an external interface prototype. This first approach to `main` is shown in Fig. 6.13. Note that the two new external routines must each `use` their respective class module.

A second approach would be to have the two new routines become internal to the `main`, after line 30, and occur before `end program`. Another change would be that each routine would have to omit its `use` statement (such as lines 34 and 41). Why? Because they are now internal to `main` and it has already made `use` of the two classes (in line 2). That approach is shown in Figs. 6.13

A third approach would be the most logical and consistent with OOP principles. It is to make all the class attributes `private`, place the print members in each respective class, insert a single generic name interface in each class, and modify the `main` program to use the polymorphic name regardless of the class of the argument it acts upon. The improved version of the classes are given below in Figs. 6.14, 6.15, and 6.16. Observe that generic interfaces for `PrintPay` and `getName` have been added, but that we could

```
module class_Manager
! Gets class_Employee and add additional functionality
  use class_Employee
  implicit none
  public :: setSalaried, payM

  type Manager              ! the Data
    private
    type (Employee) :: Person
    integer         :: isSalaried    ! ( or logical )
  end type Manager

contains ! inherited internal variables and subprograms

  function getEmployee ( M ) result (E)
    type (Manager ), intent(in) :: M
    type (Employee)             :: E
      E = M % Person ; end function getEmployee

  function  getNameM ( M ) result (n)
    type (Manager ), intent(in) :: M
    type (Employee)             :: E
    character(30)               :: n         ! name
      n = getNameE(M % Person); end function getNameM

  function Manager_ (lastName, firstName, newPayRate) result (M)
    character(*), intent(in) :: lastName
    character(*), intent(in) :: firstName
    real,         intent(in) :: newPayRate
    type (Employee)          :: E         ! employee
    type (Manager )          :: M         ! manager constructor
      E = setDataE (lastName, firstName, newPayRate)
                  ! use intrinsic constructor
      M = Manager(E, 0) ! default to no salary
  end function Manager_

  function setDataM (lastName, firstName, newPayRate) result (M)
    character(*), intent(in) :: lastName
    character(*), intent(in) :: firstName
    real,         intent(in) :: newPayRate
    type (Employee)          :: E             ! employee
    type (Manager )          :: M             ! manager
      E = setDataE (lastName, firstName, newPayRate)
      M % Person = E
  end function setDataM

  subroutine setSalaried ( Who, salariedFlag )
    type (Manager), intent(inout) :: Who
    integer,        intent(in)    :: salariedFlag
      Who % isSalaried = salariedFlag ; end subroutine setSalaried

  function payM ( Human, hoursWorked ) result ( amount )
    type (Manager), intent(in) :: Human
    real,           intent(in) :: hoursWorked
    real                       :: amount, value
      value = getRate( getEmployee(Human) )
      if ( Human % isSalaried == 1 ) then  ! (or use logical)
        amount = value
      else
        amount = value * hoursWorked
      end if ; end function payM
end module class_Manager
```

Figure 6.9: A First Declaration of a Manager Class

not do that for a corresponding `setData`; do you know why? A final improvement will be given as an assignment.

6.3 Polymorphism

Fortran 90 and 95 do not include the full range of polymorphism abilities that one would like to have in an object-oriented language. It is expected that the Fortran 2000 standard will add those abilities.

Some of the code "re-use" features can be constructed through the concept of subprogram "templates," which will be discussed below. The lack of a standard "Is_A" polymorphism can be overcome in F90/95 by the use of the `SELECT CASE` feature to define "sub-types" of objects. This approach of subtyping programming provides the desired additional functionality, but it is clearly not as easy to change or extend as an inheritance feature built into the language standard. A short example will be provided.

```
program main ! Example use of managers
  use class_Manager
  implicit none
  type (Manager)  mgr1, mgr2

  ! Set up 1st manager and print out her name and pay

    mgr1 = setDataM ( "Smith", "Kimberly", 1900.0 )
    call setSalaried ( mgr1, 1 )  ! Has a salary

    print *, "Name: ", getNameM ( mgr1)
    print *, "Pay: ", payM ( mgr1, 40.0 )

  ! Set up 2nd manager and print out his name and pay

    ! mgr2 = setDataM ( "Danish", "Tom", 46.5 )
    ! call setSalaried ( mgr2, 0 )  ! Doesn't have a salary
    !                  or
    mgr2 = Manager_ ( "Danish", "Tom", 46.5 )

    print *, "Name: ", getNameM ( mgr2)
    print *, "Pay: ", payM ( mgr2, 40.0 )
end program main           ! Running produces;
!  Name: Kimberly Smith                !  Pay: 1900.
!  Name: Tom Danish                    !  Pay: 1860.
```

Figure 6.10: First Test of a Manager Class

```
module class_Employee  ! Alternate
  implicit none
  public :: setData, getName, pay  ! the Functionality

  type  Employee                   ! the Data
    character(30) :: name
    real          :: payRate
  end type  Employee

contains ! inherited internal variables and subprograms

  subroutine setData ( Person, lastName, firstName, newPayRate )
    type (Employee) :: Person
    character(*)    :: lastName
    character(*)    :: firstName
    real            :: newPayRate
      Person % name    = trim (firstName) // " " // trim (lastName)
      Person % payRate = newPayRate
  end subroutine setData

  function  getName ( Person )
    character(30)   :: getName
    type (Employee) :: Person
      getName = Person % name
  end function getName

  function  pay ( Person, hoursWorked )
    real            :: pay
    type (Employee) :: Person
    real            :: hoursWorked
      pay = Person % payRate * hoursWorked
  end function pay
end module class_Employee
```

Figure 6.11: Alternate Public Access Form of an Employee Class

6.3.1 Templates

One of our goals has been to develop software that can be reused for other applications. There are some algorithms that are effectively independent of the object type on which they operate. For example, in a sorting algorithm one often needs to interchange, or swap, two objects. A short routine for that purpose follows:

```
subroutine swap_integers (x, y)
  implicit none
  integer, intent(inout) :: x, y
  integer                :: temp
    temp = x
    x    = y
    y    = temp
end subroutine swap_integers
```

```
module class_Manager  ! Alternate
  use class_Employee, payEmployee => pay ! renamed
  implicit none
  public :: setSalaried, payManager

  type  Manager              ! the Data
    type (Employee) :: Person
    integer         :: isSalaried    ! ( or logical )
  end type  Manager

contains ! inherited internal variables and subprograms

  subroutine setSalaried ( Who, salariedFlag )
    type (Manager) :: Who
    integer        :: salariedFlag
      Who % isSalaried = salariedFlag
  end subroutine setSalaried

  function  pay ( Human, hoursWorked )
    real           :: pay
    type (Manager) :: Human
    real           :: hoursWorked

      if ( Human % isSalaried == 1 ) then  ! (or use logical)
        pay = Human % Person % payRate
      else
        pay = Human % Person % payRate * hoursWorked
      end if
  end function pay
end module class_Manager
```

Figure 6.12: Alternate Public Access Form of a Manager Class

Observe that in this form it appears necessary to have one version for integer arguments and another for real arguments. Indeed we might need a different version of the routine for each type of argument that you may need to swap. A slightly different approach would be to write our swap algorithm as:

```
subroutine swap_objects (x, y)
  implicit none
  type (Object), intent(inout) :: x, y
  type (Object)                :: temp
    temp = x
    x    = y
    y    = temp
end subroutine swap_objects
```

which would be a single routine that would work for any `Object`, but it has the disadvantage that one find a way to redefine the `Object` type for each application of the routine. That would not be an easy task. (While we will continue with this example with the algorithm in the above forms it should be noted that the above approaches would not be efficient if `x` and `y` were very large arrays or derived type objects. In that case we would modify the algorithm slightly to employ pointers to the large data items and simply swap the pointers for a significant increase in efficiency.)

Consider ways that we might be able to generalize the above routines so that they could accept and swap any specific type of arguments. For example, the first two versions could be re-written in a so called `template` form as:

```
subroutine swap_Template$ (x, y)
  implicit none
  Template$, intent(inout) :: x, y
  Template$                :: temp
    temp = x
    x    = y
    y    = temp
end subroutine swap_Template$
```

In the above template the dollar sign ($) was includes in the “wild card” because while it is a valid member of the F90 character set it is not a valid character for inclusion in the name of a variable, derived type, function, module, or subroutine. In other words, a template in the illustrated form would not compile, but such a name could serve as a reminder that its purpose is to produce a code that can be compiled after the “wild card” substitutions have been made.

With this type of template it would be very easy to use a modern text editor to do a global substitution of any one of the intrinsic types `character, complex, double precision, integer, logical,` or `real` for the “wild card” keyword `Template$` to produce a source code to swap any or all of

```
program main ! Alternate employee and manager classes
  use class_Manager  ! and thus Employee
  implicit none
 !    supply interface for external code not in classes
  interface PrintPay ! For TYPE dependent arguments
    subroutine PrintPayManager ( Human, hoursWorked )
      use class_Manager
      type (Manager) :: Human
      real           :: hoursWorked
    end subroutine
    subroutine PrintPayEmployee ( Person, hoursWorked )
      use class_Employee
      type (Employee) :: Person
      real            :: hoursWorked
    end subroutine
  end interface

  type (Employee) empl   ;  type (Manager)  mgr

  ! Set up an employee and print out his name and pay
    call setData ( empl, "Burke", "John", 25.0 )

    print *, "Name: ", getName ( empl )
    call PrintPay ( empl, 40.0 )

  ! Set up a manager and print out her name and pay
    call setData ( mgr % Person, "Kovacs", "Jan", 1200.0 )
    call setSalaried ( mgr, 1 )  ! Has a salary

    print *, "Name: ", getName ( mgr % Person )
    call PrintPay ( mgr, 40.0 )
end program

  subroutine PrintPayEmployee ( Person, hoursWorked )
   use class_Employee
    type (Employee) :: Person
    real            :: hoursWorked
      print *, "Pay: ", pay ( Person, hoursworked )
  end subroutine

  subroutine PrintPayManager ( Human, hoursWorked )
   use class_Manager
    type (Manager) :: Human
    real           :: hoursWorked
      print *, "Pay: ", pay ( Human , hoursworked )
  end subroutine
! Running produces;
! Name: John Burke
! Pay:    1000.
! Name: Jan Kovacs
! Pay:    1200.
```

Figure 6.13: Testing the Alternate Employee and Manager Classes

the intrinsic data types. There would be no need to keep up with all the different routine names if we placed all of them in a single module and also created a generic `interface` to them such as:

```
module swap_library
  implicit none
  interface swap    ! the generic name
    module procedure swap_character, swap_complex
    module procedure swap_double precision, swap_integer
    module procedure swap_logical, swap_real
  end interface
contains
  subroutine swap_characters (x, y)
   . . .
  end subroutine swap_characters
  subroutine swap_ . . .
   . . .
end module swap_library
```

The use of a text editor to make such substitutions is not very elegant and we expect that there may be a better way to pursue the concept of developing a reuseable software template. The concept of a text editor substitution also fails when we go to the next logical step and try to use a derived type argument instead of any of the intrinsic data types. For example, if we were to replace the “wild card” with our previous `type (chemical_element)` that would create:

```
subroutine swap_type (chemical_element) (x,y)
  implicit none
```

```
module class_Employee                ! the base class
 implicit none                       ! strong typing
 private :: PrintPayEmployee, payE   ! private members
  type Employee                      ! the Data
    private                          ! all attributes private
    character(30) :: name
    real          :: payRate ; end type Employee

  interface PrintPay                  ! a polymorphic member
    module procedure PrintPayEmployee ; end interface
  interface getName                   ! a polymorphic member
    module procedure getNameE         ; end interface
! NOTE: can not have polymorphic setData. Why ?

contains ! inherited internal variables and subprograms

  function setDataE (lastName, firstName, newPayRate) result (E)
    character(*), intent(in) :: lastName
    character(*), intent(in) :: firstName
    real,         intent(in) :: newPayRate    ! amount per period
    type (Employee)          :: E             ! employee
                 ! use intrinsic constructor
      E = Employee((trim(firstName)//" "//trim(lastName)),newPayRate)
  end function setDataE

  function getNameE ( Person ) result (n)
    type (Employee), intent(in) :: Person
    character(30)               :: n         ! name
      n = Person % name ; end function getNameE

  function getRate ( Person ) result ( r )
    type (Employee), intent(in) :: Person
    real                        :: r         ! rate of pay
      r = Person % payRate ; end function getRate

  function payE ( Person, hoursWorked ) result ( amount )
    type (Employee), intent(in) :: Person
    real,            intent(in) :: hoursWorked
    real                        :: amount
      amount = Person % payRate * hoursWorked ; end function payE

  subroutine PrintPayEmployee ( Person, hoursWorked )
    type (Employee) :: Person
    real            :: hoursWorked
       print *, "Pay: ", payE ( Person, hoursworked )
  end subroutine
end module class_Employee
```

Figure 6.14: A Better Private Access Form of an Employee Class

```
module class_Manager             ! the derived class
!   Get class_Employee, add additional attribute & members
 use class_Employee              ! inherited base class
 implicit none                  ! strong typing
 private :: PrintPayManager, payM, getNameM  ! private members

  type Manager                       ! the Data
    private                          ! all attributes private
    type (Employee) :: Person
    integer         :: isSalaried    ! 1 if true (or use logical)
  end type Manager

  interface PrintPay                 ! a polymorphic member
    module procedure PrintPayManager ; end interface
  interface getName                  ! a polymorphic member
    module procedure getNameM        ; end interface
```

Fig. 6.15: A Better Private Access Form of a Manager Class (continued)

```
     type (chemical_element), intent (inout)::x,y
     type (chemical_element)               ::temp
           temp = x
           x    = y
           y    = temp
   end subroutine swap_type (chemical_element)
```

This would fail to compile because it violates the syntax for a valid function or subroutine name, as well as the end function or end subroutine syntax. Except for the first and last line syntax errors this would be a valid code. To correct the problem we simply need to add a little logic and omit the characters `type`

```
    contains ! inherited internal variables and subprograms

      function getEmployee ( M ) result (E)
        type (Manager ), intent(in) :: M
        type (Employee)             :: E
          E = M % Person ; end function getEmployee

      function  getNameM ( M ) result (n)
        type (Manager ), intent(in) :: M
        type (Employee)             :: E
        character(30)               :: n         ! name
          n = getNameE(M % Person); end function getNameM

      function Manager_ (lastName, firstName, newPayRate) result (M)
        character(*), intent(in) :: lastName
        character(*), intent(in) :: firstName
        real,         intent(in) :: newPayRate
        type (Employee)          :: E    ! employee
        type (Manager )          :: M    ! manager constructed
          E = setDataE (lastName, firstName, newPayRate)
                                         ! use intrinsic constructor
          M = Manager(E, 0)              ! default to hourly
      end function Manager_

      function setDataM (lastName, firstName, newPayRate) result (M)
        character(*), intent(in) :: lastName
        character(*), intent(in) :: firstName
        real,         intent(in) :: newPayRate    ! hourly OR weekly
        type (Employee)          :: E             ! employee
        type (Manager )          :: M             ! manager constructed
          E = setDataE (lastName, firstName, newPayRate)
          M % Person = E ; M % isSalaried = 0      ! default to hourly
      end function setDataM

      subroutine setSalaried ( Who, salariedFlag ) ! 0=hourly, 1=weekly
        type (Manager), intent(inout) :: Who
        integer,        intent(in)    :: salariedFlag  ! 0 OR 1
          Who % isSalaried = salariedFlag ; end subroutine setSalaried

      function payM ( Human, hoursWorked ) result ( amount )
        type (Manager), intent(in) :: Human
        real,           intent(in) :: hoursWorked
        real                       :: amount, value
          value = getRate( getEmployee(Human) )
          if ( Human % isSalaried == 1 ) then
            amount = value               ! for weekly person
          else
            amount = value * hoursWorked ! for hourly person
          end if ; end function payM

      subroutine PrintPayManager ( Human, hoursWorked )
        type (Manager) :: Human
        real           :: hoursWorked
          print *, "Pay: ", payM ( Human , hoursworked )
      end subroutine
    end module class_Manager
```

Figure 6.15: A Better Private Access Form of a Manager Class

( ) when we create a function, module, or subroutine name that is based on a derived type data entity. Then we obtain

```
subroutine swap_chemical_element (x,y)
  implicit none
  type (chemical_element), intent (inout)::x,y
  type (chemical_element)                ::temp
        temp = x
        x    = y
        y    = temp
end subroutine swap_chemical_element
```

which yields a completely valid routine.

Unfortunately, text editors do not offer us such logic capabilities. However, as we have seen, high level programming languages like C++ and F90 do have those abilities. At this point you should be able to envision writing a `pre-processor` program that would accept a file of template routines, replace the template “wildcard” words with the desired generic forms to produce a module or `header file` containing the expanded source files that can then be brought into the desired program with an `include` or `use` statement. The C++ language includes a template pre-processor to expand template files as needed.

```
program main ! Final employee and manager classes
  use class_Manager ! and thus class_Employee
  implicit none

  type (Employee) empl   ;  type (Manager)  mgr

  ! Set up a hourly employee and print out his name and pay
    empl = setDataE ( "Burke", "John", 25.0 )

    print *, "Name: ", getName ( empl )
    call PrintPay ( empl, 40.0 )        ! polymorphic

  ! Set up a weekly manager and print out her name and pay
    mgr = setDataM ( "Kovacs", "Jan", 1200.0 )
    call setSalaried ( mgr, 1 )         ! rate is weekly

    print *, "Name: ", getName ( mgr )
    call PrintPay ( mgr, 40.0 )         ! polymorphic
end program                           ! Running produces;
! Name: John Burke
! Pay:    1000.
! Name: Jan Kovacs
! Pay:    1200.
```

Figure 6.16: Testing the Better Employee-Manager Forms

Some programmers criticize F90/95 for not offering this ability as part of the standard. A few C++ programmers criticize templates and advise against their use. Regardless of the merits of including template pre-processors in a language standard it should be clear that it is desirable to plan software for its efficient reuse.

With F90 if one wants to take advantage of the concepts of templates then the only choices are to carry out a little text editing or develop a pre-processor with the outlined capabilities. The former is clearly the simplest and for many projects may take less time than developing such a template pre-processor. However, if one makes the time investment to produce a template pre-processor one would have a tool that could be applied to basically any coding project.

6.3.2 Subtyping Objects (Dynamic Dispatching)

One polymorphic feature missing from the Fortran 90 standard (but expected in Fortran 2000) that is common to most object oriented languages is called run-time polymorphism or dynamic dispatching. In the C++ language this ability is introduced in the so-called "virtual function." To emulate this ability is quite straightforward in F90 but is not elegant since it usually requires a group of if-elseif statements or other selection processes. It is only tedious if the inheritance hierarchy contains many unmodified subroutines and functions. The importance of the lack of a standardized dynamic dispatching depends on the problem domain to which it must be applied. For several applications demonstrated in the literature the alternate use of subtyping has worked quite well and resulted in programs that have been shown to run several times faster than equivalent C++ versions.

We implement dynamic dispatching in F90 by a process often called subtyping. Two features must be constructed to do this. First, a pointer object, which can point to any subtype member in an inheritance hierarchy, must be developed. Second, an if-elseif or other selection method is developed to serve as a dispatch mechanism to select the unique appropriate procedure to be executed based on the actual class referenced in the controlling pointer object. This subtyping process is also referred to as implementing a polymorphic class. Of course, the details of the actual dispatching process can be hidden from the procedures that utilize the polymorphic class.

This process will be illustrated buy creating a specific polymorphic class, called Is_A_Member_Class, which has polymorphic procedures named new, assign, and display. They will construct a new instance of the object, assign it a value, and list its components. The minimum example of such a process requires two members and is easily extended to any number of member classes. We begin by defining each of the subtype classes of interest.

The first is a class, Member_1_Class, which has two real components and the encapsulated functionality to construct a new instance and another to accept a pointer to such a subtype and display related information. It is shown in Fig. 6.17. The next class, Member_2_Class, has three components: two reals and one of type Member_1. It has the same sort of functionality, but clearly must act on more

```
Module Member_1_Class
  implicit none
  type member_1
    real :: real_1, real_2
  end type member_1

contains

  subroutine new_member_1 (member, a, b)
    real, intent(in) :: a, b
    type (member_1)  :: member
      member%real_1 = a ; member%real_2 = b
  end subroutine new_member_1

  subroutine display_memb_1  (pt_to_memb_1, c)
    type (member_1), pointer :: pt_to_memb_1
    character(len=1),   intent(in) :: c
     print *, 'display_memb_1 ', c
  end subroutine display_memb_1

End Module Member_1_Class
```

Figure 6.17: Defining Subtype_1

```
Module Member_2_Class
 Use Member_1_class
  implicit none
  type member_2
    type (member_1)  :: r_1_2
    real :: real_3, real_4
  end type member_2

contains

  subroutine new_member_2 (member, a, b, c, d)
    real, intent(in) :: a, b, c, d
    type (member_2)  :: member
      call new_member_1 (member%r_1_2, a, b)
      member%real_3 = c ; member%real_4 = d
  end subroutine new_member_2

  subroutine display_memb_2  (pt_to_memb_2, c)
    type (member_2), pointer :: pt_to_memb_2
    character(len=1),   intent(in) :: c
      print *, 'display_memb_2 ', c
  end subroutine display_memb_2

End Module Member_2_Class
```

Figure 6.18: Defining Subtype_2

components. It has also inherited the functionally from the Member_1_Class; as displayed in Fig. 6.18.

The polymorphic class is called the Is_A_Member_Class and is shown in Fig. 6.19. It includes all of the encapsulated data and function's of the above two subtypes by including their use statements. The necessary pointer object is defined as an Is_A_Member type that has a unique pointer for each subtype member (two in this case). It also defines a polymorphic interface to each of the common procedures to be applied to the various subtype objects. In the polymorphic function assign the dispatching is done very simply. First, all pointers to the family of subtypes are nullified, and then the unique pointer component to the subtype of interest is set to point to the desired member. The dispatching process for the display procedure is different. It requires an if-elseif construct that contains calls to all of the possible subtype members (two here) and a failsafe default state to abort the process or undertake the necessary exception handling. Since all but one of the subtype pointer objects have been nullified it employs the associated intrinsic function to select the one, and only, procedure to call and passes the pointer object on to that procedure. The validation of this dynamic dispatching through a polymorphic class is shown in Fig. 6.20. There a target is declared for reach possible subtype and then each of them is constructed and sent on to the other polymorphic functions. The results clearly show that different display procedures were used depending on the class of object supplied as an argument. It is expected that the new Fortran 2000 standard will allow such dynamic dispatching in a much simpler fashion.

```
Module Is_A_Member_Class
Use Member_1_Class ; Use Member_2_Class
  implicit none

  type Is_A_Member
    private
    type (member_1), pointer :: pt_to_memb_1
    type (member_2), pointer :: pt_to_memb_2
  end type Is_A_Member

  interface new
    module procedure new_member_1
    module procedure new_member_2
  end interface

  interface assign
    module procedure assign_memb_1
    module procedure assign_memb_2
  end interface

  interface display
    module procedure display_memb_1
    module procedure display_memb_2
  end interface

contains

  subroutine assign_memb_1 (Family, member)
   type (member_1), target, intent(in)  :: member
   type (Is_A_Member),      intent(out) :: Family
     call nullify_Is_A_Member (Family)
     Family%pt_to_memb_1 => member
  end subroutine assign_memb_1

  subroutine assign_memb_2 (Family, member)
   type (member_2), target, intent(in)  :: member
   type (Is_A_Member),      intent(out) :: Family
     call nullify_Is_A_Member (Family)
     Family%pt_to_memb_2 => member
  end subroutine assign_memb_2

  subroutine nullify_Is_A_Member (Family)
    type (Is_A_Member), intent(inout) :: Family
      nullify (Family%pt_to_memb_1)
      nullify (Family%pt_to_memb_2)
  end subroutine nullify_Is_A_Member

  subroutine display_members (A_Member, c)
    type (Is_A_Member), intent(in) :: A_Member
    character(len=1),   intent(in) :: c

  ! select the proper member
      if     ( associated (A_Member%pt_to_memb_1) ) then
             call display (A_Member%pt_to_memb_1, c)
      else if ( associated (A_Member%pt_to_memb_2) ) then
             call display (A_Member%pt_to_memb_2, c)
      else ! default case
        stop 'Error, no member defined in Is_A_Member_Class'
      end if
  end subroutine display_members
End Module Is_A_Member_Class
```

Figure 6.19: Combining Subtypes in an Is_A Class

```
program main
use Is_A_Member_Class
  implicit none

  type (Is_A_Member)      :: generic_member
  type (member_1), target :: pt_to_memb_1
  type (member_2), target :: pt_to_memb_2
  character(len=1) :: c

    c = 'A'
    call new (pt_to_memb_1, 1.0, 2.0)
    call assign (generic_member, pt_to_memb_1)
    call display_members (generic_member, c)

    c = 'B'
    call new (pt_to_memb_2, 1.0, 2.0, 3.0, 4.0)
    call assign (generic_member, pt_to_memb_2)
    call display_members (generic_member, c)

end program main
! running gives
! display_memb_1 A
! display_memb_2 B
```

Figure 6.20: Testing the Is_A Subtypes

6.4 Exercises

1. Write a main program that will use the Class_X and Class_Y, given below, to invoke each of the f(v) routines and assign a value of 66 to the integer component in X, and 44 to the integer component in Y. (Solution given.)

```
module class_X
  public :: f
  type X_; integer a; end type X_
contains ! functionality
  subroutine f(v); type (X_), intent(in) :: v
    print *,"X_ f() executing"; end subroutine
end module class_X

module class_Y
  use class_X, X_f => f  ! renamed
  public :: f
  type Y_; integer a; end type Y_ ! dominates X_ a
contains         ! functionality, overrides X_ f()
  subroutine f(v);  type (Y_), intent(in) :: v
    print *,"Y_ f() executing"; end subroutine
end module class_Y
```

2. Create the generic interface that would allow a single constructor name, `Position_Angle_`, to be used for all the constructors given in the previous chapter for the class `Position_Angle`. Note that this is possible because they all had unique argument signatures. Also provide a new `main` program to test this polymorphic version.

3. Modify the last `Manager` class by deleting the member `setDataM` and replace its appearance in the last `main` with an existing constructor (but not used) in that class. Also provide a generic `setData` interface in the class `Employee` as a nicer name and to allow for other employees, like executives, that may have different kinds of attributes that may need to be set in the future. Explain why we could not use `setDataM` in the generic `setData`.

4. The final member `setDataE` in `Employee` is actually a constructor and the name is misleading since it does not just set data values, it also builds the name. Rename `setDataE` to the constructor notation `Employee_` and provide a new member in `Employee` called `setRateE` that only sets the employee pay rate.

Chapter 7

OO Data Structures

7.1 Data Structures

We have seen that F90 has a very strong intrinsic base for supporting the use of subscripted arrays. Fortran arrays can contain intrinsic data types as well as user defined types (i.e., ADT's). One can not directly have an array of pointers but you are allowed to have an array contain defined types that are pointers or that have components that are pointers. Arrays offer an efficient way to contain information and to insert and extract information. However, there are many times when creating an efficient algorithm dictates that we use some specialized storage method, or *container*, and a set of operations to act with that storage mode. The storage representation and the set of operations that are allowed for it are known as a *data structure*. How you store and retrieve an item from a container is often independent of the nature of the item itself. Thus, different instances of a data structure may produce containers for different types of objects. Data structures have the potential for a large amount of code reuse, which is a basic goal of OOP methods. In the following sections we will consider some of the more commonly used containers.

7.2 Stacks

A stack is a data structure where access is restricted to the last inserted object. It is referred to as a *last-in first-out* (LIFO) container. In other words, a stack is a container to which elements may only be inserted or removed at one end of the container, called the *top* of the stack. It behaves much like a pile of dinner plates. You can place a new element on the pile (widely known as a *push*), remove the top element from the pile (widely known as a *pop*), and identify the element on the top of the pile. You can also have the general concept of an empty pile, and possibly a full pile if it is associated with some type of restrictive container. Since at this point we only know about using arrays as containers we will construct a stack container by using an array.

Assume that we have defined the attributes of the "Object" that is to use our container by building a module called `object_type`. Then we could declare the array implementation of a stack type to be:

```
module stack_type
  use object_type ! to define objects in the stack
  implicit none

  integer, parameter :: limit = 999 ! stack size limit

  type stack
    private
      integer       :: size         ! size of array
      integer       :: top          ! top of stack
      type (Object) :: a(limit)     ! stack items array
  end type stack
end module stack_type
```

The interface contract to develop one such stack support system (or ADT) is given as:

```
module stack_of_objects
implicit none
  public :: stack, push_on_Stack, pop_from_Stack, &
            is_Stack_Empty, is_Stack_Full

interface  ! for a class_Stack contract

  function make_Stack (n) result (s)   ! constructor
    use stack_type                     ! to define stack structure
    integer, optional :: n             ! size of stack
    type (stack)      :: s             ! the new stack
  end function make_Stack

  subroutine push_on_Stack (s, item)    ! push item on top of stack
    use stack_type                      ! for stack structure
    type (stack),  intent(inout) :: s
    type (Object), intent(in)    :: item
  end subroutine push_on_Stack

  function pop_from_Stack (s) result (item) ! pop item from top
    use stack_type                          ! for stack structure
    type (stack), intent(inout) :: s
    type (Object)               :: item
  end function pop_from_Stack

  function is_Stack_Empty (s) result (b)  ! test stack
    use stack_type                        ! for stack structure
    type (stack), intent(in) :: s
    logical                  :: b
  end function is_Stack_Empty

  function is_Stack_Full (s) result (b)  ! test stack
    use stack_type                       ! for stack structure
    type (stack), intent(in) :: s
    logical                  :: b
  end function is_Stack_Full

end interface
end module stack_of_objects
```

In the interface we see that some of the member services (`is_Stack_Empty` and `is_Stack_Full`) are independent of the contained objects. Others (`pop_from_Stack` and `push_on_Stack`) explicitly depend on the Object utilizing the container. Of course, the constructor (here `make_Stack`) always indirectly relates to the Object being contained in the array. The full details of a `Stack` class are given in Fig. 7.1.

For a specific implementation test we will simply utilize objects that have a single integer attribute. That is, we define the object of interest by a code segment like:

```
module object_type
  type Object
    integer :: data  ; end type  ! one integer attribute
end module object_type
```

Obviously, there are many other types of objects that one may want to create and place in a container like a stack. At the present one would have to edit the above segment to define all the attributes of the object. (Begin to think about how you might seek to automate such a process.) The new `Stack` class is tested in Fig. 7.2, while a history of the example stack is sketched in Fig. 7.3. The only part of that code that depends on a specific object is in line 7 where the (public) intrinsic constructor, `Object`, was utilized rather that some more general constructor, say `Object_`.

In Fig. 7.1 note that we have used an alternate syntax and specified the type of function result (logical, Object, or stack) as a prefix to the function name (lines 16, 28, 36, 40). The author thinks that the form used in the interface contract is easier to read and understand since it requires an extra line of code, however some programmers prefer the condensed style of Fig. 7.1. Later we will examine an alternate implementation of a stack by using a linked list.

The stack implementation shown here is not complete. For example, some programmers like to include a member, say `show_Stack_top`, to display the top element on the container without removing it from the stack. Also we need to be concerned about *pre-conditions* that need to be satisfied for a member and may require that we throw an exception message. You can not pop an item off of an empty stack, nor can you push an item onto the top of a full stack. Only the member `pop_from_Stack` does such pre-condition checking in the sample code. Note that members `is_Stack_Empty` and `is_Stack_Full` are called *accessors*, as would be `show_Stack_top`, since they query the container but do not change it.

```
 module class_Stack
 implicit none
   use exceptions  ! to warn of errors
   use object_type
   public :: stack, push_on_Stack, pop_from_Stack, &
             is_Stack_Empty, is_Stack_Full
   integer, parameter :: limit = 999 ! stack size limit

 type stack
   private
     integer       :: size         ! size of array
     integer       :: top          ! top of stack
     type (Object) :: a(limit)     ! stack items array
  end type
contains ! encapsulated functionality

 type (stack) function make_Stack (n) result (s)     ! constructor
   integer, optional :: n ! size of stack
     s%size = limit ; if ( present (n) ) s%size = n
     s%top = 0      ! object array not initialized
 end function make_Stack

 subroutine push_on_Stack (s, item) ! push item on top of stack
   type (stack),  intent(inout) :: s
   type (Object), intent(in)    :: item
     s%top = s%top + 1 ; s%a(s%top) = item
 end subroutine push_on_Stack

 type (Object) function pop_from_Stack (s) result (item) ! off top
   type (stack), intent(inout) :: s
     if ( s%top < 1 ) then
       call exception ("pop_from_Stack","stack is empty")
     else
       item = s%a(s%top) ; s%top = s%top - 1
     end if ; end function pop_from_Stack

 logical function is_Stack_Empty (s) result (b)
   type (stack), intent(in) :: s
     b = ( s%top == 0 ) ; end function is_Stack_Empty

 logical function is_Stack_Full (s) result (b)
   type (stack), intent(in) :: s
     b = ( s%top == s%size ) ; end function is_Stack_Full

 end module class_Stack
```

Figure 7.1: A Typical Stack Class

```
[ 1]  include 'class_Stack.f'      ! previous figure
[ 2]  program main
[ 3]  use class_Stack
[ 4]  implicit none
[ 5]   type (stack)  :: b
[ 6]   type (object) :: value, four, five, six
[ 7]
[ 8]     four = Object(4) ; five = Object(5) ; six = Object(6)  ! initialize
[ 9]
[10]     b = make_Stack(3)                              ! private constructor
[11]     print *, is_Stack_Empty(b), is_Stack_Full(b) ! b = [], empty
[12]
[13]     call  push_on_Stack (b, four)                ! b = [4]
[14]     call  push_on_Stack (b, five)                ! b = [5,4]
[15]     call  push_on_Stack (b, six )                ! b = [6,5,4], full
[16]     print *, is_Stack_Empty(b), is_Stack_Full(b) ! F T
[17]
[18]     value = pop_from_Stack (b) ; print *, value   ! b = [5,4]
[19]     print *, is_Stack_Empty(b), is_Stack_Full(b) ! F F
[20]
[21]     value = pop_from_Stack (b) ; print *, value   ! b = [4]
[22]     print *, is_Stack_Empty(b), is_Stack_Full(b) ! F F
[23]
[24]     value = pop_from_Stack (b) ; print *, value   ! b = [], empty
[25]     print *, is_Stack_Empty(b), is_Stack_Full(b) ! T F
[26]
[27]     value = pop_from_Stack (b)                    ! nothing to pop
[28]   end program main ! running gives:
[29]   ! T F  ! F T
[30]   ! 6    ! F F
[31]   ! 5    ! F F
[32]   ! 4    ! T F
[33]   ! Exception occurred in subprogram pop_from_Stack
[34]   ! With message: stack is empty
```

Figure 7.2: Testing a Stack of Objects

```
Full  ?   F     F     F     T     F     F     F     F
Empty ?   T     F     F     F     F     F     T     T
Error ?   N     N     N     N     N     N     N     Y

Stack:   | |   |4|   |5|   |6|   |5|   |4|   | |   | |
         | |   | |   |4|   |5|   |4|   | |   | |   | |
         | |   | |   | |   |4|   | |   | |   | |   | |
         ---   ---   ---   ---   ---   ---   ---   ---

(Line)    9     12    13    14    17    20    23    26
```

Figure 7.3: Steps in the Stack Testing

```
     E <-----> Top
    |D|
    |C|                              ---------
    |B|                Front <---- A B C D E <---- Rear
    |A|                              ---------
    ---
 a) Stack                            b) Queue
```

Figure 7.4: Simple Containers

7.3 Queues

A comparison of a stack and another simple container, a *queue*, is given in Fig. 7.4. Its name queue comes from the British word which means waiting in a line for service. A queue is a container into which elements may be inserted at one end, called the *rear*, and leave only from the other end, called the *front*. The first element in the queue expects to be the first serviced and, thus, be the first out of line. A queue is a *first-in first-out* (FIFO) container system. In planning our first queue container we will again make use of an array of objects. Doing so one quickly finds that you are much less likely to encounter a full queue if it is stored as a so-called fixed circular array with a total of `Q_Size_Limit` storage slots. At this point we define the structure of our queue to be:

```
module Queue_type
!  A queue stored as a so-called fixed circular array with a total
!  of Q_Size_Limit storage slots; requires remainder function, mod.
!     (version 1, i.e., without allocatable arrays and pointers)
  use object_type  ! to define objects in the Container
  implicit none

  integer, parameter :: Q_Size_Limit = 999

  type Queue
    private
      integer       :: head                  ! index of first element
      integer       :: tail                  ! index of last element
      integer       :: length                ! size of used storage
      type (Object) :: store (Q_Size_Limit) ! a circular array
  end type Queue
end module Queue_type
```

An interface contract that will allow us to build a typical queue is:

```
module Queue_of_Objects
implicit none
  public :: Queue, Add_to_Q, Create_Q, Get_Front_of_Q, Is_Q_Empty,&
            Is_Q_Full, Get_Length_of_Q, Remove_from_Q

interface  ! for a class_Queue contract

 subroutine Add_to_Q (Q, item)          ! add to tail of queue
   use Queue_type                        ! for Queue structure
   type (Queue),  intent(inout) :: Q
   type (Object), intent(in)    :: item ; end Subroutine Add_to_Q

 function Create_Q (N) result (Q)   ! manual constructor
   use Queue_type                   ! for Queue structure
   integer, intent(in) :: N         ! size of the new array
   type (Queue)        :: Q ;       end function Create_Q

 function Get_Capacity_of_Q (Q) result (item)
   use Queue_type                       ! for Queue structure
   type (Queue), intent(in) :: Q
   type (Object)            :: item ; end function Get_Capacity_of_Q

 function Get_Front_of_Q (Q) result (item)
   use Queue_type                     ! for Queue structure
  type (Queue), intent(in) :: Q
  type (Object)            :: item ; end function Get_Front_of_Q

 function Is_Q_Empty (Q) result(B)
   use Queue_type                  ! for Queue structure
   type (Queue), intent(in) :: Q
   logical                  :: B ; end function Is_Q_Empty

 function Is_Q_Full (Q) result(B)
   use Queue_type                  ! for Queue structure
   type (Queue), intent(in) :: Q
   logical                  :: B ; end function Is_Q_Full

 function Get_Length_of_Q (Q) result (N)
   use Queue_type                  ! for Queue structure
   type (Queue), intent(in) :: Q
         integer                  :: N ; end function Get_Length_of_Q

 subroutine Remove_from_Q (Q)       ! remove from head of queue
   use Queue_type                   ! for Queue structure
   type (Queue), intent(inout) :: Q; end subroutine Remove_from_Q

 end interface
end module Queue_of_Objects
```

For a specific version we provide full details for objects containing an integer in Fig. 7.5, and test and display the validity of the implementation in Fig. 7.6, where again the objects are taken to be integers (lines 15, 19, 20).

```
module class_Queue                          ! file: class_Queue.f90

!  A queue stored as a so-called fixed circular array with a total of
!  Q_Size_Limit storage slots; requires remainder function, mod.
!     (i.e., without allocatable arrays and pointers)

 use exceptions                          ! inherit exception handler
 implicit none

 public :: Queue, Add_to_Q, Create_Q, Get_Front_of_Q
            Is_Q_Full, Get_Length_of_Q, Remove_from

  integer, parameter :: Q_Size_Limit = 3

  type Queue
    private
      integer :: head                  ! index of first element
      integer :: tail                  ! index of last element
      integer :: length                ! size of used storage
      integer :: store (Q_Size_Limit) ! a circular array of elements
  end type Queue

contains                               ! member functionality

 Subroutine Add_to_Q (Q, item)          ! add to tail of queue
   type (Queue), intent(inout) :: Q
   integer,      intent(in)    :: item

     if ( Is_Q_Full(Q) ) call exception ("Add_to_Q","full Q")
     Q%store (Q%tail) = item
     Q%tail           = 1 + mod (Q%tail, Q_Size_Limit)
     Q%length         = Q%length + 1 ; end Subroutine Add_to_Q

 type (Queue) function Create_Q (N) result (Q)   ! manual constructor
   integer, intent(in) :: N  ! size of the new array
   integer             :: k  ! implied loop

     if (N > Q_Size_Limit) call exception("Create_Q","increase size")
     Q = Queue (1, 1, 0, (/ (0, k=1,N) /))    ! intrinsic constructor
 end function Create_Q

 integer function Get_Capacity_of_Q (Q) result (item)
   type (Queue), intent(in) :: Q

     item = Q_size_Limit - Q%length ; end function Get_Capacity_

 integer function Get_Front_of_Q (Q) result (item)
  type (Queue), intent(in) :: Q

    if (Is_Q_Empty(Q)) call exception("Get_Front_of_Q","em
    item = Q%store (Q%head) ; end function Get_Front_of_Q

 logical function Is_Q_Empty (Q) result(B)
  type (Queue), intent(in) :: Q

    B = (Q%length == 0) ; end function Is_Q_Empty

 logical function Is_Q_Full (Q) result(B)
   type (Queue), intent(in) :: Q

     B = (Q%length == Q_Size_Limit) ; end function Is_Q_Full

 integer function Get_Length_of_Q (Q) result (N)
   type (Queue), intent(in) :: Q
     N = Q%length ; end function Get_Length_of_Q

 subroutine Remove_from_Q (Q)           ! remove from head of queue
   type (Queue), intent(inout) :: Q

     if (Is_Q_Empty(Q)) call exception("Remove_from_Q","empty Q"
     Q%head   = 1 + mod (Q%head, Q_Size_Limit)
     Q%length = Q%length - 1 ; end subroutine Remove_from_Q

end module class_Queue             ! file: class_Queue.f
```

Figure 7.5: A Typical Queue Class

```
program main
 use class_Queue  ! inherit its methods & class global constants
 implicit none

 type (Queue) :: C, B              ! not used, used
 integer :: value, limit = 3       ! work items

   C = Create_Q (limit)          ! private constructor
   print *, "Length of C = ",   Get_Length_of_Q (C)
   print *, "Capacity of C = ", Get_Capacity_of_Q (C)
   print *, "C empty? full? ",  is_Q_Empty (C), is_Q_Full (C)  !

   B = Create_Q (3)              ! private constructor
   print *, "B empty? full? ",  is_Q_Empty (B), is_Q_Full (B)  !

   call Add_to_Q (B, 4);         print *, "B = [4]"
   print *, "Length of B = ",   Get_Length_of_Q (B)
   print *, "B empty? full? ",  is_Q_Empty (B), is_Q_Full (B)  !

   call Add_to_Q (B, 5);         print *, " B = [4,5]"
   call Add_to_Q (B, 6);         print *, " B = [4,5,6], full"
   print *, "Length of B = ",   Get_Length_of_Q (B)
   print *, "B empty? full? ",  is_Q_Empty (B), is_Q_Full (B)  !
   print *, "Capacity of B = ", Get_Capacity_of_Q (B)

   value = Get_Front_of_Q (B);  print *, "Front Q value = ", value

   call Remove_from_Q (B);      print *, "Removing from B"
   print *, "Length of B = ",   Get_Length_of_Q (B)
   print *, "B empty? full? ",  is_Q_Empty (B), is_Q_Full (B) !
   value = Get_Front_of_Q (B);  print *, "Front Q value = ", value

   call Remove_from_Q (B);      print *, "Removing from B"
   print *, "Length of B = ",   Get_Length_of_Q (B)
   print *, "B empty? full? ",  is_Q_Empty (B), is_Q_Full (B) !

   call Remove_from_Q (B);      print *, "Removing from B"
   print *, "Length of B = ",   Get_Length_of_Q (B)
   print *, "B empty? full? ",  is_Q_Empty (B), is_Q_Full (B) !

   print *, "Removing from B";  call Remove_from_Q (B)
   call exception_status
end program main          ! running gives:
! Length of C = 0       ! Capacity of C = 3    ! C empty? full? T,  F
! B empty? full? T,  F
! B = [4]               ! Length of B = 1      ! B empty? full? F,  F
! B = [4,5]
! B = [4,5,6], full     ! Length of B = 3      ! B empty? full? F,  T
! Capacity of B = 0     ! Front Q value = 4    ! Removing from B
! Length of B = 2       ! B empty? full? F,  F ! Front Q value = 5
! Removing from B       ! Length of B = 1      ! B empty? full? F,  F
! Removing from B       ! Length of B = 0      ! B empty? full? T,  F
! Removing from B
! Exception Status Thrown
!   Program :Remove_from_Q
!   Message :empty Q
!   Level   : 5
!
! Exception Summary:
!   Exception count =  1
!   Highest level   =  5
```

Figure 7.6: Testing of the Queue Class

7.4 Linked Lists

From our limited discussion of stacks and queues it should be easy to see that to try to insert or remove an object at the middle of a stack or queue is not an efficient process. *Linked lists* are containers which make it easy to perform the operations of insertion and deletion. A linked list of objects can be thought of as a group of boxes, usually called *nodes*, each containing an object to stored and a *pointer*, or reference, to the box containing the next object in the list. In most of our applications a list is referenced by a special box, called the *header* or *root* node, which does not store an object but serves mainly to point to the first linkable box, and thereby produces a condition where the list is never truly empty. This simplifies the insertion scheme by removing an algorithmic special case. We will begin our introduction of these topics with a *singly linked list*, also known as a simple list. It is capable of being traversed in only one direction, from the beginning of the list to the end, or vice versa.

As we have seen, arrays of data objects work well so long as we know, or can compute, in advance the amount of data to be stored. The data structures (linked lists and trees) to be considered here employ *pointers* to store and change data objects when we do not know the required amount of storage in advance. During program execution linked lists and trees allow separate memory allocations for each individual data object. However, they do not permit direct access to an arbitrary object in the container. Instead some searching must be performed and thus they incur an execution time penalty for such an access operation. That penalty is smaller in tree structures than in linked lists (but is smallest of all in arrays).

Linked lists and trees must use pointer (reference) variables. Fortran pointers can simply be thought of as an alias for other variables of the same type. We are beginning to see that pointers give a programmer more power. However, that includes more power to "shoot yourself in the foot"; they make it hard to find some errors; and can lead to new types of errors such as the so called *memory leaks*. Recall that each pointer must be in one of three states: undefined, null, or associated. As dummy arguments within routines pointer variables cannot be assigned the INTENT attribute. That means they have a greater potential for undesired *side effects*. To avoid accidentally changing a pointer it is good programming practice to clearly state in comments the INTENT of all dummy pointer arguments and to immediately copy those with an INTENT IN attribute. Thereafter working with the copied pointer guarantees that an error or later modification of the routine can not produce a side effect on the pointer. We also want to avoid a *dangling pointer* which is caused by a deallocation that leaves its target object forever inaccessible. A related problem is a memory leak or *unreferenced storage* such as the program segment:

```
real, pointer :: X_ptr (:)
  allocate ( X_ptr(Big_number) )
  . . . ! use X_ptr
  nullify ( X_ptr ) ! dangling pointer
```

because now there is no way to release memory for X_ptr. To avoid this we need to free the memory before the pointer is nullified, so the segment becomes:

```
real, pointer :: X_ptr (:)
  allocate ( X_ptr(Big_number) )
  . . . ! use X_ptr
  deallocate ( X_ptr ) ! memory released
  nullify ( X_ptr )
```

Remember that in F95 the memory is automatically deallocated at the end of the scope of the variable, unless one retains the variable with a SAVE statement (and formally deallocates it elsewhere).

7.4.1 Singly Linked Lists

We begin the study of the singly linked list by showing the notations employed in Fig. 7.7. From experienced we have chosen to have a dummy first node, called `first`, to simplify our algorithms so that a list is never truly empty. Also as we scan through a list we will use one pointer, called `current`, to point to the current object in the list and a companion, called `previous`, to point to the directly preceding object (if any). If no objects have been placed in the list then both of these simply point to the `first` node. The end of the list is denoted by the `next` pointer attribute taking on the `null` value. To insert or delete objects one must be able to rank two objects. This means that in order to have a generic linked list one must overload the relational operators, (< and ==) when the object to be placed in the container is defined. Since most objects have different types of attributes the overloading process is clearly application

```
                                -----------
Type (Singly_Linked_Node) ::   | Object    |  An Object instance attribute
                               |           |  and one pointer attribute.
                               | instance  |
                               |-----------|
                               | Next      |
                               |       ---+---->
                               | pointer   |
                                -----------

                        a) Singly linked node


-----------
| First    |<--- Singly_Linked_List % First  (An empty object instance)
-----------     -----------
| Next  --+---->| Obj_1  |<--- Previous_pointer
-----------     -----------      -----------
                | Next  --+---->| Obj_m   |<--- Current_pointer
                -----------      -----------      -----------
                                 | Next  --+---->| Obj_n   |
                                 -----------      -----------
                                                 | Next  --+----> Null
                                                  -----------     -----
                                                                   ---
                                                                    -
                      b) List of singly linked nodes

                        -----------
                        |         |<--- Singly_Linked_List % First
                        | First   |<--- Previous_pointer
                        |         |<--- Current_pointer
                        -----------
                        | Next  --+-----> Null
                        -----------       -----
                                           ---
                                            -

                c) An ‘‘empty’’ (one node) singly linked list
```

Figure 7.7: Singly linked list terminology

dependent. The process for inserting an object is sketched in Fig. 7.8 while that for deleting an object is in Fig. 7.9.

The `Singly_Linked_List` class is given in Fig. 7.10. It starts with the definition of a singly linked node (lines 4-8) that has an object attribute and a pointer attribute to locate the next node. Then a list is begun (lines 10–13) by creating the dummy first node that is consider to represent an empty list. The object deletion member must employ an overloaded operator (line 28), as must the insertion member (line 52). Observe that a list never gets “full”, unless the system runs out of memory. The empty list test member (line 62) depends on the pointer status, but is independent of the objects stored. The constructor for a list (line 68) simply creates the first node and nullifies it. The printing member (line 74) is called an `iterator` since it runs through all objects in the list. The testing program for this container type and its output results are given in Fig. 7.11. In order to test such a container it is necessary to have an object type defined. Here an object with a single integer value was selected, and thus it was easy to overload the relational operators with a clear meaning as shown in Fig. 7.12.

INSERT

Figure 7.8: Inserting an Object in a Singly Linked List

DELETE

Figure 7.9: Deleting an Object from a Singly Linked List

```
module singly_linked_list
 use class_Object
 implicit none

  type S_L_node                            ! Singly Linked Node
    private
    type (Object)             :: value       ! Object attribute
    type (S_L_node), pointer :: next        ! Pointer to next node
  end type S_L_node

  type S_L_list                      ! Singly Linked List of Nodes
    private
    type (S_L_node), pointer :: first ! Dummy first object in list
  end type S_L_list

contains
  subroutine S_L_delete (links, Obj, found)
    type (S_L_list), intent (inout) :: links
    type (Object),   intent (in)     :: Obj
    logical,         intent (out)    :: found
    type (S_L_node), pointer        :: previous, current

    ! find location of Obj
      previous => links%first        ! begin at top of list
      current  => previous%next      ! begin at top of list
      found = .false.                 ! initialize
      do
        if ( found .or. (.not. associated (current))) return ! list end
          if ( Obj == current%value ) then ! *** OVERLOADED ***
            found = .true. ; exit ! this location search
          else ! move the next node in list
            previous => previous%next
            current  => current%next
          end if
      end do ! to find location of node with Obj
    ! delete if found
      if ( found )  then
        previous%next => current%next ! redirect pointer
        deallocate ( current )        ! free space for node
      end if
  end subroutine S_L_delete

```

Fig. 8.5, A Typical Singly Linked List Class of Objects (continued)

```
   subroutine S_L_insert (links, Obj )
     type (S_L_list), intent (inout) :: links
     type (Object),   intent(in)     :: Obj
     type (S_L_node), pointer        :: previous, current

   !  Find location to insert a new object
       previous => links%first                  ! initialize
       current  => previous%next                ! initialize
       do
         if ( .not. associated (current) ) exit ! insert at end
           if ( Obj < current%value ) exit      ! *** OVERLOADED ***
             previous => current                ! inserbefor current
             current  => current%next           ! move to next node
       end do ! to locate insert node
   !  Insert before current (duplicates allowed)
       allocate ( previous%next )      ! get new node space
       previous%next%value = Obj       ! new object inserted
       previous%next%next => current   ! new next pointer
    end subroutine S_L_insert

    function is_S_L_empty (links) result (t_or_f)
      type (S_L_list), intent (in) :: links
      logical                      :: t_or_f
        t_or_f = .not. associated ( links%first%next )
     end function is_S_L_empty

     function S_L_new () result (new_list)
       type (S_L_list) :: new_list
         allocate ( new_list%first )         ! get memory for the object
         nullify  ( new_list%first%next )    ! begin with empty list
     end function S_L_new

     subroutine print_S_L_list (links)
       type (S_L_list), intent (in) :: links
       type ( S_L_node), pointer    :: current
       integer                      :: counter
         current => links%first%next
         counter = 0 ; print *,'Link    Object Value'
         do
           if ( .not. associated (current) ) exit ! list end
             counter = counter + 1
             print *, counter, '     ', current%value
             current => current%next
         end do
     end subroutine print_S_L_list
 end module singly_linked_list
```

Figure 7.10: A Typical Singly Linked List Class of Objects

```fortran
program main   ! test a singly linked object list
use singly_linked_list
implicit none
  type (S_L_list) :: container
  type (Object)    :: Obj_1, Obj_2, Obj_3, Obj_4
  logical          :: delete_ok

    Obj_1 = Object(15) ; Obj_2 = Object(25) ! constructor
    Obj_3 = Object(35) ; Obj_4 = Object(45) ! constructor
    container = S_L_new()
    print *, 'Empty status is ', is_S_L_empty (container)
    call S_L_insert (container, Obj_4) ! insert object
    call S_L_insert (container, Obj_2) ! insert object
    call S_L_insert (container, Obj_1) ! insert object
    call print_S_L_list (container)

    call S_L_delete (container, obj_2, delete_ok)
    print *, 'Object: ', Obj_2, '  deleted status is ', delete_ok
    call print_S_L_list (container)
    print *, 'Empty status is ', is_S_L_empty (container)

    call S_L_insert (container, Obj_3) ! insert object
    call print_S_L_list (container)
    call S_L_delete (container, obj_1, delete_ok)
    print *, 'Object: ', Obj_1, '  deleted status is ', delete_ok
    call S_L_delete (container, obj_4, delete_ok)
    print *, 'Object: ', Obj_4, '  deleted status is ', delete_ok
    call print_S_L_list (container)
    print *, 'Empty status is ', is_S_L_empty (container)

    call S_L_delete (container, obj_3, delete_ok)
    print *, 'Object: ', Obj_3, '  deleted status is ', delete_ok
    print *, 'Empty status is ', is_S_L_empty (container)
    call print_S_L_list (container)
end program           ! running yields
! Empty status is  T
! Link    Object Value
! 1       15
! 2       25
! 3       45
! Object:  25  deleted status is  T
! Link    Object Value
! 1       15
! 2       45
! Empty status is  F
! Link    Object Value
! 1       15
! 2       35
! 3       45
! Object:  15  deleted status is  T
! Object:  45  deleted status is  T
! Link    Object Value
! 1       35
! Empty status is  F
! Object:  35  deleted status is  T
! Empty status is  T
! Link    Object Value
```

Figure 7.11: Testing the singly linked list with integers

```fortran
module class_Object
implicit none
  type Object           ! An integer object for testing lists
    integer :: data ; end type Object

  interface operator (<)          ! for sorting or insert
    module procedure less_than_Object ; end interface
  interface operator (==)          ! for sorting or delete
    module procedure equal_to_Object ; end interface

contains                           ! overload definitions only
  function less_than_Object (Obj_1, Obj_2) result (Boolean)
    type (Object), intent(in) :: Obj_1, Obj_2
    logical                   :: Boolean
      Boolean = Obj_1%data < Obj_2%data   ! standard (<) here
  end function less_than_Object
  function equal_to_Object (Obj_1, Obj_2) result (Boolean)
    type (Object), intent(in) :: Obj_1, Obj_2
    logical                   :: Boolean
      Boolean = Obj_1%data == Obj_2%data  ! standard (==) here
  end function equal_to_Object
end module class_Object
```

Figure 7.12: Typical object definition to test a singly linked list

```
                           --------------------------------
                           |\  |                       |   |
Doubly_Linked_List =>      | \ |    Header             | | |
                           |  \|                       | | |
                           ----------------------------|---
                            /|\                        |
                             |                        \|/
                           --|-----------------------------
                           | | |                       |   |
Trailing_pointer --->      | | |    Object_1           | | |
                           |   |                       | | |
                           ----------------------------|---
                            /|\                        |
                             | Previous_pointer       \|/
                           --|-----------------------------
                           | | |                       |   |
Current_pointer ---->      | | |    Object             | | |
                           |   |                       | | |
                           ----------------------------|---
                            /|\                        | Next_pointer
                             |                        \|/
                           --|-----------------------------
                           | | |                       |   |
                           | | |    Object_m           | | |
                           |   |                       | | |
                           ----------------------------|---
                            /|\                        |
                             |                        \|/
                           --|-----------------------------
                           | | |                       |\  |
                           | | |    Object_n           | \ | Null_pointer
                           |   |                       |  \|
                           --------------------------------
```

Figure 7.13: Notations for a Doubly Linked List

7.4.1.1 Example: A List of Sparse Vectors

In this example we want to create a linked list to hold sparse vectors (singly subscripted arrays) where the length of each vector is specified. We will do simple operations on all the vectors like input them, normalize them, add them (if their sizes are the same), etc. In doing this we will make use of some of the efficiencies that F90 provides for arrays, such as using the subscript array triplet to avoid serial loops, and operating on arrays by name alone. This is an example where a similar C++ implementation would be much longer in length because of the need to provide all the serial loops.

7.4.2 Doubly Linked Lists

The notations of the doubly linked list are shown in Fig. 7.13. Again we have chosen to have a dummy first node, called `header`, to simplify our algorithms so that a list is never truly empty. Also as we scan through a list we will use one pointer, called `current`, to point to the current object in the list and a companion, called `previous`, to point to the directly preceding object (if any). If no objects have been placed in the list then both of these simply point to the `header` node. The end of the list is denoted by the `next` pointer attribute taking on the `null` value. To insert or delete objects one must be able to rank two objects. This means that in order to have a generic linked list one must again overload the relational operators, (< and ==) when the object to be placed in the container is defined.

An incomplete, but illustrative `Doubly_Linked_List` class is given in Fig. 7.14. It starts with the definition of a doubly linked node (lines 4-8) that has an object attribute and a pair of pointer attributes to locate the nodes on either side of the object. Then a list is begun (lines 10-13) by creating the dummy first node that is consider to represent an empty list. The object insertion member must employ an overloaded operator (line 53), as before. Observe that a list never gets "full", unless the system runs out of memory. The constructor for a list (line 17) simply creates the first node and nullifies its pointers. A corresponding destructor (line 24) has been provided to delete every thing associated with the list when we are done

```
[  1]  module doubly_linked_list
[  2]  use class_Object
[  3]  implicit none
[  4]    type D_L_node
[  5]      private
[  6]         type (Object)            :: Obj
[  7]         type (D_L_node), pointer :: previous
[  8]         type (D_L_node), pointer :: next
[  9]    end type D_L_node
[ 10]
[ 11]    type D_L_list
[ 12]      private
[ 13]         type (D_L_node), pointer :: header
[ 14]    end type D_L_list
[ 15]
[ 16]  contains
[ 17]
[ 18]  function D_L_new () result (new_list)       ! constructor
[ 19]    type (D_L_list) :: new_list
[ 20]      allocate (new_list % header)
[ 21]      nullify  (new_list % header % previous)
[ 22]      nullify  (new_list % header % next)
[ 23]  end function D_L_new
[ 24]
[ 25]  subroutine destroy_D_L_List (links)          ! destructor
[ 26]    type (D_L_list), intent (in) :: links
[ 27]    type (D_L_node), pointer     :: current
[ 28]      do
[ 29]        current => links % header % next
[ 30]        if ( .not. associated ( current ) ) exit
[ 31]          current % previous % next => current % next
[ 32]          if ( associated ( current % next ) ) then
[ 33]             current % next % previous => current % previous
[ 34]          end if
[ 35]          nullify ( current % previous )
[ 36]          nullify ( current % next )
[ 37]          print *, 'Destroying object ', current % Obj
[ 38]          deallocate ( current )
[ 39]      end do
[ 40]      deallocate ( links % header )
[ 41]      print *,'D_L_List destroyed'
[ 42]  end subroutine destroy_D_L_List
[ 43]
```

Fig. 7.14, A Typical Doubly Linked List Class of Objects (continued)

with it. The printing member (line 90) is called an `iterator` since it runs through all objects in the list. The testing program for this container type and its output results are given in Fig. 7.15. Here an object with a single integer value was selected, and thus it was easy to overload the relational operators with a clear meaning as shown in Fig. 7.12.

7.5 Direct (Random) Access Files

Often it may not be necessary to create special object data structures such as those outlined above. From its beginning Fortran has had the ability to create a sophisticated random access data structure where the implementation details are hidden from its user. This was necessary originally since the language was utilized on computers with memory sizes that are considered tiny by today's standard (e.g., 16 Kb), but it was still necessary to efficiently create and modify large amounts of data. The standard left the actual implementation details to the compiler writers. That data structure is known as a "direct access file". It behaves like a single subscript array in that the object at any position can be read, modified, or written at random so long as the user keeps up with the position of interest. The user simply supplies the position, known as the record number, as additional information in the read and write statements. With today's hardware, if the file is stored on a virtual disk (stored in random access memory) there is practically no difference in access times for arrays and direct files.

It should be noted here that since pointers are addresses in memory they can not be written to any type of file. That, of course, means that no object having a pointer as an attribute can be written either. Thus in some cases one must employ the other types of data structures illustrated earlier in the chapter.

To illustrate the basic concepts of a randon access file consider the program called random_access_file which is given in Fig. 7.16. In this case the object is simply a character string, as

```
subroutine D_L_insert_before (links, values)
  type (D_L_list), intent (in) :: links
  type (Object),   intent (in)  :: values
  type (D_L_node), pointer     :: current     ! Temp traversal pointer
  type (D_L_node), pointer     :: trailing    ! Preceding node pointer
!  Find location to insert new node, in ascending order
    trailing => links % header                ! initialize
    current  => trailing % next               ! initialize
    do
      if (.not. associated (current)) exit    ! insert at end
        if (values < current % Obj ) exit     ! insert before current
          trailing => current                 ! move to next node
          current  => current % next          ! move to next node
    end do
!  Insert before current (duplicates allowed)
    allocate (trailing % next)                 ! get new node space
    trailing % next % Obj  = values            ! new object inserted
!  Insert the new pointers
    if (.not. associated (current)) then       ! End of list (special)
      nullify (trailing % next % next)
      trailing % next % previous => trailing
    else                                      ! Not the end of the list
      trailing % next % next => current
      trailing % next % previous => trailing
      current % previous => trailing % next
    end if
end subroutine D_L_insert_before

function Get_Obj_at_Ptr  (ptr_to_Obj)  result ( values)
  type (D_L_node), intent (in)  :: ptr_to_Obj
  type (Object)                 :: values   ! intent out
    values = ptr_to_Obj % Obj
end function Get_Obj_at_Ptr

function Get_Ptr_to_Obj (links, values) result (ptr_to_Obj)
  type (D_L_list), intent (in) :: links      ! D_L_list header
  type (Object),   intent (in)  :: values     ! Node identifier Object
  type (D_L_node), pointer     :: ptr_to_Obj ! Pointer to the Object
  type (D_L_node), pointer     :: current    ! list traversal pointer
    current => links % header % next
    do ! Search list, WARNING: runs forever if values not in list
      if (current % Obj ==  values) exit     ! *** OVERLOADED ***
        current => current % next
    end do
    ptr_to_Obj => current                     ! Return pointer to node
end function Get_Ptr_to_Obj

subroutine print_D_L_list ( links )
  type (D_L_list), intent (in) :: links
  type (D_L_node), pointer     :: current ! Node traversal pointer
  integer                      :: counter ! Link position
!  Traverse the list and print its contents to standard output
    current => links % header % next
    counter = 0 ; print *,'Link    Object Value'
    do
      if (.not. associated (current)) exit
        counter = counter + 1
        print *, counter, '     ', current % Obj
        current => current % next
    end do
end subroutine print_D_L_list
end module doubly_linked_list
```

Figure 7.14: A Typical Doubly Linked List Class of Objects

defined in line 4. The hardware transportability of this code is assured by establishing the required constant record with the intrinsic given in line 10. It is then used in opening the file, which is designated as a direct file in line 12. Lines 16–24 create the object record numbers in a sequential fashion. They also define the new object to be stored with each record. In lines 27–32 the records are accessed in a backwards order, but could have been accessed in any random or partial order. In line 35 a random object is given a new value. Finally, the changes are output in a sequential order in lines 37–42. Sample input data and program outputs are included as comments at the end of the program.

```
program main
use doubly_linked_list
implicit none
  type (D_L_list)          :: container
  type (Object)            :: Obj_1, Obj_2, Obj_3, Obj_4
  type (Object)            :: value_at_pointer
  type (D_L_node), pointer :: point_to_Obj_3

  Obj_1 = Object(15) ; Obj_2 = Object(25)
  Obj_3 = Object(35) ; Obj_4 = Object(45)
  container = D_L_new()
  ! print *, 'Empty status is ', is_D_L_empty (container)
  call D_L_insert_before (container, Obj_4)
  call D_L_insert_before (container, Obj_2)
  call D_L_insert_before (container, Obj_1)
  call D_L_insert_before (container, Obj_3)
  call print_D_L_list (container)

  ! find and get Obj_3
  point_to_Obj_3 = Get_Ptr_to_Obj (container, Obj_L
  value_at_pointer = Get_Obj_at_Ptr (point_to_
  print *, 'Object: ', Obj_3, '  has a value of ', value_at_pointer
  call destroy_D_L_List (container)
end program main                        ! Running gives:
! Link    Object Value
! 1       15
! 2       25
! 3       35
! 4       45
! Object:  35   has a value of  35
! Destroying object  15
! Destroying object  25
! Destroying object  35
! Destroying object  45
! D_L_List destroyed
```

Figure 7.15: Testing a Partial Doubly Linked List

```
program random_access_file
! create a file and access or modify it randomly
implicit none
  character(len=10) :: name
  integer :: j, rec_len, no_name, no_open
  integer :: names = 0, unit = 1

! find the hardware dependent record length of the object
! to be stored and modified. Then open a binary file.
    inquire (iolength = rec_len) name
    open (unit, file = "random_list", status = "replace",
          access = "direct", recl = rec_len,
          form = "unformatted", iostat = no_open)
    if ( no_open > 0 ) stop 'open failed for random_list'

! read and store the names sequentially
    print *, ' '; print *, 'Original order'
    do ! forever from standard input
      read (*, '(a)', iostat = no_name)  name
      if ( no_name < 0 ) exit ! the read loop
        names = names + 1               ! record number
        write (unit, rec = names) name  ! save record
        print *, name                   ! echo
    end do
    if ( names == 0 ) stop 'no records read'

! list names in reverse order
    print *, ' '; print *, 'Reverse order'
    do j = names, 1, -1
      read (unit, rec = j) name
      print *, name
    end do ! of random read

! change the middle name in random file
    write (unit, rec = (names + 1)/2) 'New_Name'

! list names in original order
    print *, ' '; print *, 'Modified data'
    do j = 1, names
      read (unit, rec = j) name
      print *, name
    end do ! of random read

    close (unit) ! replace previous records and save
end program random_access_file
! Running with input of:    Name_1
!                           B_name
!                           3_name
!                           name_4
!                           Fifth
! Yields:
! Original order  Reverse order  Modified data
!  Name_1          Fifth          Name_1
!  B_name          name_4          B_name
!  3_name          3_name          New_Name
!  name_4          B_name          name_4
!  Fifth          Name_1          Fifth
```

Figure 7.16: Utilizing a Random Access File as a Data Structure

7.6 Exercises

Chapter 8

Arrays and Matrices

8.1 Subscripted Variables: Arrays

It is common in engineering and mathematics to employ a notation where one or more subscripts are appended to a variable which is a member of some larger set. Such a variable may be a member of a list of scalars, or it may represent an element in a vector, matrix, or Cartesian tensor.† In engineering computation, we usually refer to subscripted variables as *arrays*. Since programming languages do not have a convenient way to append the subscripts, we actually denote them by placing them in parentheses or square brackets. Thus, an element usually written as A_{jk} becomes `A(j,k)` in Fortran and MATLAB, and `A[j][k]` in C++.

Arrays have properties that need to be understood in order to utilize them correctly in any programming language. The primary feature of an array is that it must have at least one subscript. The "rank" of an array is the number of subscripts, or dimensions, it has. Fortran allows an array to have up to seven subscripts, C++ allows four, and MATLAB allows only two since it deals only with matrices. An array with two subscripts is called a rank-two array, one with a single subscript is called a rank-one array, or a vector. Matrices are rank-two arrays that obey special mathematical operations. A scalar variable has no subscripts and is sometimes called a rank zero array. Rank-one arrays with an extent of one are also viewed as a scalar.

The "extent" of a subscript or dimension is the number of elements allowed for that subscript. That is, the extent is an integer that ranges from the lower bound of the subscript to its upper bound. The lower bound of a subscript is zero in C++, and it defaults to unity in Fortran. However, Fortran allows the programmer to assign any integer value to the lower and upper bounds of a subscript.

The "size" of an array is the number of elements in it. That is, the size is the product of the extents of all of its subscripts. Most languages require the extend of each subscript be provided in order to allocate memory storage for the array.

The "shape" of an array is defined by its rank and extents. The shape is a rank-one array where each of its elements is the extent of the corresponding subscript of the array whose shape is being determined. Both Fortran and MATLAB have statements that return the shape and size of an array as well as statements for defining a new array by re-shaping an existing array.

It is also important to know which of two "storage mode" options a language employs to store and access array elements. This knowledge is especially useful when reading or writing full arrays. Arrays are stored by either varying their leftmost subscript first or by varying the rightmost subscript first. These are referred to as "column-wise" and "row-wise" access, respectively. Clearly, they are the same for rank-one arrays and differ for arrays of higher rank. Column-wise storage is used by Fortran and C++, while MATLAB uses row-wise storage.

Matrices are arrays that usually have only two subscripts: the first represents the row number, and the second the column number where the element is located. Matrix algebra places certain restrictions on the subscripts of two matrices when they are added or multiplied, etc. The fundamentals of matrices are covered in detail in this chapter.

† An n-th order tensor has n subscripts and transforms to different coordinate systems by a special law. The most common uses are scalars $(n = 0)$ and vectors $(n = 1)$.

Action	C++[a]	F90	F77	MATLAB
Pre-allocate Initialize	`integer A[100]` `for j=0,99` `    A[j]=12` `end`	`INTEGER A(100)` `A=12`	`INTEGER A(100)` `do 5 J=1,100` `    A(J)=12` `5  continue`	`A(100)=0` `for j=1:100` `    A(j)=12` `end`

[a]Arrays in C++ have a starting index of zero.

Table 8.1: Typical Vector Initialization

Purpose	F90	MATLAB
Form subscripts	( )	( )
Separates subscripts & elements	,	,
Generates elements & subscripts	:	:
Separate commands	;	;
Forms arrays	(/ /)	[ ]
Continue to new line	&	. . .
Indicate comment	!	%
Suppress printing	default	;

Table 8.2: Special Array Characters

Both Fortran and C++ require you to specify the maximum range of each subscript of an array before the array or its elements are used. MATLAB does not have this as a requirement, but pre-allocating the array space can drastically improve the speed of MATLAB, as well as making much more efficient use of the available memory. If you do not pre-allocate MATLAB arrays, then the interpreter must check at each step to see if a position larger than the current maximum has been reached. If so, the maximum value is increased and memory is found to store the new element. Thus, failure to pre-allocate MATLAB arrays is permissible but inefficient.

For example, assume we want to set a vector `A` having 100 elements, to an initial value of 12. The procedures are compared in Table 8.1. This example could have also been done efficiently in F90 and MATLAB by using the colon operator: `A(1:100) = 12`. The programmer should be alert for the chance to replace loops with the colon operator: it's more concise while retaining readability and executes more quickly. The joys of the colon operator are described more fully in §8.1.3 (page 159).

Array operations often use special characters and operators. Fortran has "implied" `DO` loops associated with its array operations (see §4.3.2, page 60). Similar features in MATLAB and F90 are listed in Table 8.2.

Fortran has always had efficient array handling features, but until the release of F90 it was not easy to dynamically create and release the memory space needed to store arrays. That is a useful feature for arrays that require large amounts of space but are not needed for the entire life of the program. F90 has several types of arrays, with the most recent types being added to allow the use of array operations, and intrinsic functions similar to those in MATLAB. Without getting into the details of the F90 standards and terminology we will introduce the most common array usages in a historical order:

```
F77: Constant Arrays, Dummy Dimension Arrays, Variable Rank Arrays
F90: Automatic Arrays, Allocatable Arrays.
```

These different approaches all have the common feature that memory space needed for an array must be set aside (allocated) before any element in the array is utilized.

The new F90 array features include the so-called automatic arrays. An automatic array is one that appears in a subroutine, or function and has its size, but *not* its name, provided in the argument list of the subprogram. For example,

```
subroutine auto_A_B (M, N, Other_arguments)
  implicit none
  integer :: M, N
```

```
   real    :: A(M, N), B(M)   ! Automatic arrays
   ! Create arrays A & B and use them for some purpose
     ...
 end subroutine auto_A_B
```

would automatically allocate space for the `M` rows and `N` columns of the array `A` and for the `M` rows of array `B`. When the purpose of the subroutine is finished and it "returns" to the calling program the array space is automatically released, and the arrays `A` and `B` cease to exist. This is a useful feature, especially in Object Oriented programs. If the system does not have enough space available to allocate for the array the program stops and gives an error message to that effect. With today's large memory computers that is unlikely to occur except for the common user error where the dimension argument is undefined.

An extension of this concept that allows more flexibility and control is the allocatable array. An allocatable array is one that has a known rank (number of subscripts), but an initially unknown extent (range over each subscript). It can appear in any program, function, or subroutine. For example,

```
program  make_A_B     ! Allocatable arrays
 implicit none
 real, allocatable :: A(:,:), B(:)   ! Declares rank of each
 integer           :: M, N           ! Row and column sizes
 integer           :: A_B_Status     ! Optional status check
   print *,"Enter the number of rows and columns: "
   read  *, M, N  ! Now know the (default) extent of each subscript
     allocate ( A(M, N), B(M), stat = A_B_Status ) ! dynamic storage
!  Verify that the dynamic memory was available
     if ( A_B_Status /= 0 ) stop "Memory not available in make_A_B"
! Create arrays A & B and use them for some purpose
     ...
     deallocate (A, B) ! free the memory space
! Do other things
     ...
end program  make_A_B
```

would specifically allocate space for the M rows and N columns of the array A and for the M rows of array B, and optionally verify that the space was available. When the purpose of the arrays are finished the space is specifically released, and the arrays A and B cease to exist. The optional status checking feature is useful in the unlikely event that the array is so large that the system does not have that much dynamic space available. Then the user has the option of closing down the program in some desirable way, or simply stopping on the spot.

The old F77 standard often encouraged the use of dummy dimension arrays. The dummy dimension array is one that appears in a subroutine, or function and has its size *and* its name provided in the argument list of the subprogram. For example,

```
 subroutine dummy_A_B (M, N, A, B, Other_things)
   implicit none
   integer :: M, N
   real    :: A(M, N), B(M)   ! dummy arrays
  !  Create arrays A & B and use them for some purpose
     ...
 end subroutine dummy_A_B
```

would imply that *existing* space for the `M` rows and `N` columns of the array `A` and for the `M` rows of array `B` (*or more*) was declared or allocated in the calling program. When the purpose of the subroutine is finished and it "returns" to the calling program the space in the calling program for the arrays `A` and `B` continues to exist until the declaring program unit terminates.

Of course the use of constant dimensioned arrays is always allowed. The constant dimension array is one that appears in any program unit and has integer constants, or integer *parameter* variables (preferred) as given extents for each subscript of an array. For example,

```
program  main
 implicit none
 integer, parameter :: M_max=20, N_max=40 ! Maximum expected
 integer            :: Days_per_Month(12) ! Constant array
 integer            :: M, N              ! User sizes
 real :: A(M_max, N_max), B(M_max)        ! Constant arrays
   print *,"Enter the number of rows and columns: "
   read  *, M, N                ! The user extent of each subscript

!  Verify that the constant memory is available
   if ( M > M_max ) stop "Row size exceeded in main"
   if ( N > N_max ) stop "Column size exceeded in main"
! Create arrays A & B and use them for some purpose
   call  dummy_A_B (M, N, A, B, Other_things)  ! dummy arrays
```

Action	F90	MATLAB
Define size[a] Enter rows	`integer :: A (2, 3)` `A(1,:)=(/1,7,-2/)` `A(2,:)=(/3,4,6/)`	`A(2,3)=0;` `A=[1,7,-2;` `3,4,6];`

[a]Optional in MATLAB, but improves efficiency.

Table 8.3: Example Array Definitions

F90	MATLAB	Result
`data = (/(k, k=1,6)/)` `M = reshape(data,(/3,2/))`	`data = [1 : 6]` `M = reshape(data,3,2)`	$M = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$
`N = reshape(data,(/2,3/))`	`N = reshape(data,2,3)`	$N = \begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix}$

Table 8.4: Array Reshape Intrinsics

```
    ...
 end program main

  subroutine dummy_A_B (M, N, A, B, Other_things)  ! dummy arrays
    implicit none
    integer :: M, N
    real    :: A(M, N), B(M)
   !  Create arrays A & B and use them for some purpose
      ...
  end subroutine  main
```

In general it is considered *very bad style* to use integer constants, like 12, in a dimension, or in a `DO` loop control, except for the unusual case where its meaning is obvious, and where you never expect to have to change the number. In the example declaration:

```
integer :: Days_per_Month(12) ! Constant array
```

It is obvious that we are thinking about 12 months per year and that we do not expect the number of months per year to ever change in other potential applications of this program.

8.1.1 Initializing Array Elements

Explicit lists of the initial elements in an array are allowed by C++, Fortran, and MATLAB. MATLAB is oriented to enter element values in the way that we read, that is, row by row. Fortran and C also allow array input by rows, but the default procedure is to accept values by ranging over its subscripts from left to right. That is, both F90 and C++ read by columns as their default mode. For example, consider the 2×3 array

$$A = \begin{bmatrix} 1 & 7 & -2 \\ 3 & 4 & 6 \end{bmatrix} .$$

This array could be typed as explicit input with the commands shown in Table 8.3. An alternative for F90 and MATLAB is to define the full array by column order as a vector that is then reshaped into a matrix with a specified number of rows and columns. The use of the `RESHAPE` operator is shown in Table 8.4.

Returning to the previous example, we see that the matrix `A` could have also been defined as

F90	`A = reshape((/1,3,7,4, -2,6/), (/2,3/))` `A = reshape((/1,3,7,4, -2,6/),shape(A))`
MATLAB	`A = reshape([1,3,7,4, -2,6], 2,3)`

To initialize the elements of an array to zero or unity, F90 and MATLAB have special constructs or functions that fill the bill. For example, for A to be zero and B to have unity elements, we could use the following commands.

Action	F90	MATLAB
Define size	`integer :: A (2, 3)` `integer :: B (3)`	`A(2,3)=0;` `B(3)=0;`
Zero `A`	`A=0`	`A=zeros(2,3);`
Initialize `B`	`B=1`	`B=ones(3);`

If we want to create a new array `B` with the first three even numbers, we would use *implied loops*.

Action	F90	MATLAB
Even set	`B=(/(2*k,k=1,3)/)` `B=(/(k,k=2,6,2)/)`	`B=2*[1:1:3];` `B=[2:2:6];`

Arrays can also be initialized by reading their element values from a stored data file. The two most common types of files are ASCII (standard characters) and binary (machine language) files. ASCII files are easy to read and edit, but binary files make more efficient use of storage, and are read or written much faster than ASCII files. ASCII files are often denoted by the name extension of "dat". Binary files are denoted by the name extension "mat" in MATLAB, while in Fortran the extension "bin" is commonly employed.

For example, assume that the above `A(2,3)` array is to be initialized by reading its values from an ASCII file created by a text editor and given the name of `A.dat`. Further, assume that we wish to multiply all elements by 3 and store it as a new ASCII file. Then we could use `read` procedures like those in Table 8.5 where the last MATLAB command associated a file name and a file type with the desired input/output (I/O) action. Fortran requires an `OPEN` statement to do this if the default I/O files (unit 5 to read and unit 6 to write) are not used in the read or write.

8.1.2 Intrinsic Array Functions

Note that MATLAB has intrinsic functions `ones` and `zeros` to carry out a task that F90 does with an operator. Often the reverse is true. MATLAB has several operators that in Fortran correspond to an intrinsic function or a `CALL`ed function. A comparison of the similar F90 and MATLAB array mathematical operators are given in Table 8.5. They generally only differ slightly in syntax. For example, to transpose the matrix `A`, the F90 construct is `transpose(A)` while in MATLAB it's simply `A'`.[†] In F90, the `*` operator means, for matrices, term by term multiplication: when `A`=$\begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix}$ and `B`=$\begin{bmatrix} 1 & 2 & 4 \\ 3 & 5 & 6 \end{bmatrix}$, `A*B` yields $\begin{bmatrix} 1 & 6 & 20 \\ 6 & 20 & 36 \end{bmatrix}$. In MATLAB, the same operation is expressed as `A.*B`. To multiply the matrices `A` and `B`, Fortran requires the use of the intrinsic function `matmul` (i.e., `matmul(A,B)`) while MATLAB uses the `*` operator (`A*B`).

Another group of commonly used functions that operate on arrays in Fortran90 and MATLAB are briefly described in Table 8.6. Both languages have several other functions of a more specialized nature, but those in Table 8.6 are probably the most commonly used in programs.

Often one needs to truncate a real number in some special fashion. Table 8.7 illustrates how to do that using some of the functions common to the languages of interest. That table also implies how one can convert reals to integers and vice versa.

8.1.3 Colon Operations on Arrays (Subscript Triplet)

The syntax of the colon operator, which is available in MATLAB and F90, is detailed in Table 4.6. What the colon operator concisely expresses is a sequence of numbers in an arithmetic progression. As shown in the table, the MATLAB expression `B:I:E` expresses the sequence `B, B+I, B+2*I, ..., B+`$\lfloor \frac{E-B}{I} \rfloor$`I`. The complicated expression for the sequence's last term simply means that the last value of the sequence does not exceed (in magnitude) the end value `E`.

[†] In MATLAB, `A'` actually means conjugate transpose. If `A` is real, this operator performs the transpose as desired. If `A` is complex and we want its transpose, the MATLAB construct is `A.'`.

Description	*Equation*	*Fortran90 Operator*	*Matlab Operator*	*Original Sizes*	*Result Size*
Scalar plus scalar	$c = a \pm b$	$c = a \pm b$	$c = a \pm b;$	$1, 1$	$1, 1$
Element plus scalar	$c_{jk} = a_{jk} \pm b$	$c = a \pm b$	$c = a \pm b;$	m, n and $1, 1$	m, n
Element plus element	$c_{jk} = a_{jk} \pm b_{jk}$	$c = a \pm b$	$c = a \pm b;$	m, n and m, n	m, n
Scalar times scalar	$c = a \times b$	$c = a * b$	$c = a * b;$	$1, 1$	$1, 1$
Element times scalar	$c_{jk} = a_{jk} \times b$	$c = a * b$	$c = a * b;$	m, n and $1, 1$	m, n
Element times element	$c_{jk} = a_{jk} \times b_{jk}$	$c = a * b$	$c = a. * b;$	m, n and m, n	m, n
Scalar divide scalar	$c = a/b$	$c = a/b$	$c = a/b;$	$1, 1$	$1, 1$
Scalar divide element	$c_{jk} = a_{jk}/b$	$c = a/b$	$c = a/b;$	m, n and $1, 1$	m, n
Element divide element	$c_{jk} = a_{jk}/b_{jk}$	$c = a/b$	$c = a./b;$	m, n and m, n	m, n
Scalar power scalar	$c = a^b$	$c = a{*}{*}b$	$c = a \wedge b;$	$1, 1$	$1, 1$
Element power scalar	$c_{jk} = a_{jk}^b$	$c = a{*}{*}b$	$c = a \wedge b;$	m, n and $1, 1$	m, n
Element power element	$c_{jk} = a_{jk}^{b_{jk}}$	$c = a{*}{*}b$	$c = a. \wedge b;$	m, n and m, n	m, n
Matrix transpose	$C_{kj} = A_{jk}$	$C = \text{transpose } (A)$	$C = A';$	m, n	n, m
Matrix times matrix	$C_{ij} = \sum_k A_{ik} B_{kj}$	$C = \text{matmul}(A, B)$	$C = A * B;$	m, r and r, n	m, n
Vector dot vector	$c = \sum_k A_k B_k$	$c = \text{sum}(A * B)$	$c = \text{sum}(A. * B);$	$m, 1$ and $m, 1$	$1, 1$
		$c = \text{dot\_product}(A, B)$	$c = A * B';$	$m, 1$ and $m, 1$	$1, 1$

Table 8.5: Array Operations in Programming Constructs. Lower case letters denote scalars or scalar elements of arrays. Matlab arrays are allowed a maximum of two subscripts while Fortran allows seven. Upper case letters denote matrices or scalar elements of matrices.

You can also use the colon operator to extract smaller arrays from larger ones. If we wanted to extract the second row and third column of the array, $A = \begin{bmatrix} 1 & 7 & -2 \\ 3 & 4 & 6 \end{bmatrix}$, to get, respectively,

$$G = [3\ 4\ 6], \quad C = \left\{ \begin{array}{c} -2 \\ 6 \end{array} \right\},$$

we could use the colon operator as follows.

Action	F90	MATLAB
Define size	`integer :: B (3)` `integer :: C (2)`	`B(3)=0;` `C(2)=0;`
Extract row	`B=A(2,:)`	`B=A(2,:);`
Extract columns	`C=A(:,3)`	`C=A(:,3);`

Table 8.6: Equivalent Fortran90 and MATLAB Intrinsic Functions. The following KEY symbols are utilized to denote the TYPE of the intrinsic function, or subroutine, and its arguments: A-complex, integer, or real; I-integer; L-logical; M-mask (logical); R-real; X-real; Y-real; V-vector (rank 1 array); and Z-complex. Optional arguments are not shown. Fortran90 and MATLAB also have very similar array operations and colon operators.

Type	Fortran90	MATLAB	Brief Description
A	ABS(A)	abs(a)	Absolute value of A.
R	ACOS(X)	acos(x)	Arc cosine function of real X.
R	AIMAG(Z)	imag(z)	Imaginary part of complex number.
R	AINT(X)	real(fix(x))	Truncate X to a real whole number.
L	ALL(M)	all(m)	True if all mask elements, M, are true.
R	ANINT(X)	real(round(x))	Real whole number nearest to X.
L	ANY(M)	any(m)	True if any mask element, M, is true.
R	ASIN(X)	asin(x)	Arcsine function of real X.
R	ATAN(X)	atan(x)	Arctangent function of real X.
R	ATAN2(Y,X)	atan2(y,x)	Arctangent for complex number(X, Y).
I	CEILING(X)	ceil(x)	Least integer >= real X.
Z	CMPLX(X,Y)	(x+yi)	Convert real(s) to complex type.
Z	CONJG(Z)	conj(z)	Conjugate of complex number Z.
R	COS(R_Z)	cos(r_z)	Cosine of real or complex argument.
R	COSH(X)	cosh(x)	Hyperbolic cosine function of real X.
I	COUNT(M)	sum(m==1)	Number of true mask, M, elements.
R,L	DOT_PRODUCT(X,Y)	x'⋆y	Dot product of vectors X and Y.
R	EPSILON(X)	eps	Number, like X, $\ll 1$.
R,Z	EXP(R_Z)	exp(r_z)	Exponential of real or complex number.
I	FLOOR(X)	floor	Greatest integer $\leq$ X.
R	HUGE(X)	realmax	Largest number like X.
I	INT(A)	fix(a)	Convert A to integer type.
R	LOG(R_Z)	log(r_z)	Logarithm of real or complex number.
R	LOG10(X)	log10(x)	Base 10 logarithm function of real X.
R	MATMUL(X,Y)	x⋆y	Conformable matrix multiplication, X*Y.
I,V	I=MAXLOC(X)	[y,i]=max(x)	Location(s) of maximum array element.
R	Y=MAXVAL(X)	y=max(x)	Value of maximum array element.
I,V	I=MINLOC(X)	[y,i]=min(x)	Location(s) of minimum array element.
R	Y=MINVAL(X)	y=min(x)	Value of minimum array element.

(continued)

Type	Fortran90	MATLAB	Brief Description
I	NINT(X)	round(x)	Integer nearest to real X.
A	PRODUCT(A)	prod(a)	Product of array elements.
call	RANDOM_NUMBER(X)	x=rand	Pseudo-random numbers in $(0, 1)$.
call	RANDOM_SEED	rand('seed')	Initialize random number generator.
R	REAL (A)	real(a)	Convert A to real type.
R	RESHAPE(X, (/ I, I2 /))	reshape(x, i, i2)	Reshape array X into I×I2 array.
I,V	SHAPE(X)	size(x)	Array (or scalar) shape vector.
R	SIGN(X,Y)		Absolute value of X times sign of Y.
R	SIGN(0.5,X)-SIGN(0.5,-X)	sign(x)	Signum, normalized sign, –1, 0, or 1.
R,Z	SIN(R_Z)	sin(r_z)	Sine of real or complex number.
R	SINH(X)	sinh(x)	Hyperbolic sine function of real X.
I	SIZE(X)	length(x)	Total number of elements in array X.
R,Z	SQRT(R_Z)	sqrt(r_z)	Square root, of real or complex number.
R	SUM(X)	sum(x)	Sum of array elements.
R	TAN(X)	tan(x)	Tangent function of real X.
R	TANH(X)	tanh(x)	Hyperbolic tangent function of real X.
R	TINY(X)	realmin	Smallest positive number like X.
R	TRANSPOSE(X)	x'	Matrix transpose of any type matrix.
R	X=1	x=ones(length(x))	Set all elements to 1.
R	X=0	x=zero(length(x))	Set all elements to 0.

For more detailed descriptions and example uses of these intrinsic functions see Adams, J.C., *et al.*, *Fortran 90 Handbook*, McGraw-Hill, New York, 1992, ISBN 0–07–000406–4.

C++ F90 MATLAB	– `aint` `real` (fix)	`int` `int` `fix`	– `anint` `real` (round)	– `nint` `round`	`floor` `floor` `floor`	`ceil` `ceiling` `ceil`
Argument	**Value of Result**					
–2.000	–2.0	–2	–2.0	–2	–2	–2
–1.999	–1.0	–1	–2.0	–2	–2	–1
–1.500	–1.0	–1	–2.0	–2	–2	–1
–1.499	–1.0	–1	–1.0	–1	–2	–1
–1.000	–1.0	–1	–1.0	–1	–1	–1
–0.999	0.0	0	–1.0	–1	–1	0
–0.500	0.0	0	–1.0	–1	–1	0
–0.499	0.0	0	0.0	0	–1	0
0.000	0.0	0	0.0	0	0	0
0.499	0.0	0	0.0	0	0	1
0.500	0.0	0	1.0	1	0	1
0.999	0.0	0	1.0	1	0	1
1.000	1.0	1	1.0	1	1	1
1.499	1.0	1	1.0	1	1	2
1.500	1.0	1	2.0	2	1	2
1.999	1.0	1	2.0	2	1	2
2.000	2.0	2	2.0	2	2	2

Table 8.7: Truncating Numbers

`WHERE (logical_array_expression)` `   true_array_assignments` `ELSEWHERE` `   false_array_assignments` `END WHERE`
`WHERE (logical_array_expression)` `true_array_assignment`

Table 8.8: F90 `WHERE` Constructs

One can often use colon operators to avoid loops acting on arrays to define new arrays. For example, consider a square matrix

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} .$$

We can flip it left to right to create a new matrix (in F90 syntax)

$$\texttt{B=A(:, n:1:-1)} = \begin{bmatrix} 3 & 2 & 1 \\ 6 & 5 & 4 \\ 9 & 8 & 7 \end{bmatrix}$$

or flip it up to down

$$\texttt{C=A(n:1:-1, :)} = \begin{bmatrix} 7 & 8 & 9 \\ 4 & 5 & 6 \\ 1 & 2 & 3 \end{bmatrix}$$

or flip it up to down, then left to right

$$\texttt{D = A (n:1:-1, n:1:-1)} = \begin{bmatrix} 9 & 8 & 7 \\ 6 & 5 & 4 \\ 3 & 2 & 1 \end{bmatrix} ,$$

where $n = 3$ is the number of rows in the matrix A. In the MATLAB syntax, the second and third numbers would be interchanged in the colon operator. Actually, MATLAB has intrinsic operators to flip the matrices so that one could simply write

```
B = fliplr(A); C = flipud(A); D = rot90(A);
```

8.1.4 Array Logical Mask Operators

By default most MATLAB commands are designed to operate on arrays. Fortran77 and C++ have no built in array operations and it is necessary to program each loop. The Fortran90 standard has many of the MATLAB array commands and often with the identical syntax as shown in Table 8.5 and 8.6. Often the F90 versions of these functions have optional features (arguments) that give the user more control than MATLAB does by including a logical control mask to be defined shortly.

To emphasize that an `IF` type of relational operator is to act on all elements of an array, Fortran90 also includes an array `WHERE` block or statement control (that is, an `IF` statement acting on all array elements) which is outlined in Table 8.8.

Note that the necessary loops are implied and need not be written. As an example, if

$$A = \begin{bmatrix} 0 & 3 & 5 \\ 7 & 4 & 8 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix}$$

Function	*Description*	*Opt*	*Example*
`all`	Find if all values are true, for a fixed dimension.	d	`all(B = A, DIM = 1)` (true, false, false)
`any`	Find if any value is true, for a fixed dimension.	d	`any (B > 2, DIM = 1)` (false, true, true)
`count`	Count number of true elements for a fixed dimension.	d	`count(A = B, DIM = 2)` (1, 2)
`maxloc`	Locate first element with maximum value given by mask.	m	`maxloc(A, A < 9)` (2, 3)
`maxval`	Max element, for fixed dimension, given by mask.	b	`maxval (B, DIM=1, B > 0)` (2, 4, 6)
`merge`	Pick true array, A, or false array, B, according to mask, L.	–	`merge(A, B, L)` $\begin{bmatrix} 0 & 3 & 5 \\ 2 & 4 & 8 \end{bmatrix}$
`minloc`	Locate first element with minimum value given by mask.	m	`minloc(A, A > 3)` (2, 2)
`minval`	Min element, for fixed dimension, given by mask.	b	`minval(B, DIM = 2)` (1, 2)
`pack`	Pack array, A, into a vector under control of mask.	v	`pack(A, B < 4)` (0, 7, 3)
`product`	Product of all elements, for fixed dimension, controlled by mask.	b	`product(B)` ; (720) `product(B, DIM = 1, T)` (2, 12, 30)
`sum`	Sum all elements, for fixed dimension, controlled by mask.	b	`sum(B)` ;(21) `sum(B, DIM = 2, T)` (9, 12)
`unpack`	Replace the true locations in array B controlled by mask L with elements from the vector U.	–	`unpack(U, L, B)` $\begin{bmatrix} 7 & 3 & 8 \\ 2 & 4 & 9 \end{bmatrix}$

$$A = \begin{bmatrix} 0 & 3 & 5 \\ 7 & 4 & 8 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix}, \quad L = \begin{bmatrix} T & F & T \\ F & F & T \end{bmatrix}, \quad U = (7, 8, 9)$$

Table 8.9: F90 Array Operators with Logic Mask Control. T and F denote true and false, respectively. Optional arguments: `b -- DIM & MASK`, `d -- DIM`, `m -- MASK`, `v -- VECTOR` and `DIM = 1` implies for any rows, `DIM = 2` for any columns, and `DIM = 3` for any plane.

then, `WHERE (A > B) B = A` gives a new $B = \begin{bmatrix} 1 & 3 & 5 \\ 7 & 4 & 8 \end{bmatrix}$. By default, MATLAB always acts on matrices and considers scalars a special case. Thus, it would employ the standard syntax, `if A > B,B=A`, to do the same task.

A more sophisticated way to selectively pick subscripts of an array is to use a *mask* array. A mask array is the same size and shape as the array on which it will act. It is a Boolean array: All its elements have either true or false values. When associated with an operator, the operator will only act on those elements in the original array whose corresponding mask location is true (i.e., `.true.` in Fortran, `true` in C++ and `1` in MATLAB and C). Fortran90 has several operations that allow or require masks (Table 8.9). MATLAB functions with the same name exist in some cases, as seen in Table 8.6. Usually, they correspond to the F90 operator where the mask is true everywhere.

ALL	ANY	COUNT
CSHIFT	DOT_PRODUCT	EOSHIFT
MATMUL	MAXLOC	MAXVAL
MINLOC	MINVAL	PACK
PRODUCT	REPEAT	RESHAPE
SPREAD	SUM	TRANSFER
TRANSPOSE	TRIM	UNPACK

Table 8.10: Intrinsic Functions Allowing Logical Mask Control

A general Fortran principle underlies the fact that the array mentioned in the `WHERE` mask may be changed within the `WHERE` construct. When an array appears in the `WHERE` statement mask, the logical test is executed **first** and the host system retains the result independent of whatever happens later inside the `WHERE` construct. Thus, in the program fragment

```
integer, parameter :: n = 5
real :: x (n) = (/ (k, k = 1, n) /)
  where (x > 0.0)
           x = -x
  end where
```

the sign is reversed for all elements of `x` because they all pass the initial logical mask. It is as if a classic `DO` sequence had been programmed

```
do i = 1, n, 1
    if (x(i) > 0.0) x(i) = -x(i)
end do
```

instead of the `WHERE` construct.

A more ominous and subtle issue surrounds the use of other transformational intrinsic functions listed in Table 8.10. The danger is that when these intrinsics appear inside the body of a `WHERE` construct, the `WHERE` statement's initial mask may no longer apply. Hence, in the following example the transformational intrinsic function `SUM` operates over all five elements of `X` rather than just the two elements of `X` that exceed six.

```
integer, parameter :: n = 5
real :: x(n) = (/ 2, 4, 6, 8, 10 /)
  where (x > 6.0)
           x = x / sum(x)
  end where
```

Thus, the new values for `x` are $\{ 2, 4, 6, 8/30, 10/30 \}$ rather than $\{2, 4, 6, 8/18, 10/18\}$. This standard-conforming, but otherwise "unexpected", result should raise a caution for the programmer. If one did not want the above illustrated result, then it would be necessary to use the same mask of the `WHERE` as an optional argument to `SUM`: `sum(x, mask = x > 6.0)`. A lot of care needs to be taken to assure that transformational intrinsics that appear in a `WHERE` construct use exactly the same mask.

8.1.5 User Defined Operators

In addition to the many intrinsic operators and functions we have seen so far, the F90 user can also define new operators or extend existing ones. User defined operators can employ intrinsic data types and/or user defined data types. The user defined operators, or extensions, can be unary or binary (i.e., have one or two arguments). The operator symbol must be included between two periods, such as '`.op.`'. As an example, consider a program to be used to create a shorthand notation to replace the standard F90 matrix transpose and matrix multiplication functions so that we could write

	`B = .t.  A`
	`C = B .x.  D`
or	`C = (.t.A) .x.  D`
instead of	`B = TRANSPOSE(A)`
	`C = MATMUL (B, D)`
or	`C = MATMUL(TRANSPOSE (A), D)`

Operator	*Action*	*Use*	*Algebra*
`.t.`	transpose	`.t.A`	A^T
`.x.`	multiplication	`A.x.B`	AB
`.i.`	inverse of matrix	`.i.A`	A^{-1}
`.ix.`	solution	`A.ix.B`	$A^{-1}B$
`.tx.`	transpose times matrix	`A.tx.B`	A^TB
`.xt.`	matrix times transpose	`A.xt.B`	AB^T
`.eye.`	identity matrix	`.eye.N`	I, $N \times N$

Table 8.11: Definitions in Matrix Operators.

To do this, one must have a `MODULE PROCEDURE` to define the operator actions for all envisioned (and incorrect) inputs and an `INTERFACE OPERATOR` that informs F90 what your operation symbol is.

Fig. 8.1 illustrates the code that would partially define the operator '`.t.`'. Note that while `TRANSPOSE` accepts any type of matrix of any rank, our operator works only for real or integer rectangular arrays (of rank 2). It would not transpose `LOGICAL` arrays or vectors. That oversight can be extended by adding more functions to the interface.

If one works with matrices often, then one may want to define your own library of matrix operators. Such operators are not standard in F90 as they are in MATLAB, but can be easily added. To provide a foundation for such a library, we provide a `Matrix_Operators` module with the operators defined in Table 8.11. The reader is encouraged to expand the initial support provided in that module.

8.1.6 Connectivity Lists and Vector Subscripts

When using an array with constant increments in its subscripts, we usually provide its subscript in the form of a colon operator or a control variable in a `DO` or `FOR` loop. In either case, the array subscripts are integers. There are several practical programming applications where the required subscripts are not known in advance. Typically, this occurs when we are dealing with an assemblage of components that can be connected together in an arbitrary fashion by the user (e.g., electric circuits, truss structures, volume elements in a solid model). To get the subscripts necessary to build the assemblage we must read an integer data file that lists the junction numbers to which each component is attached. We call those data a *connectivity file*. If we assume each component has the same number of junction points, then the list can be input as a two-dimensional array. One subscript will range over the number of components and the other will range over the number of possible junctions per component. For ease of typing these data, we usually assume that the $\mathrm{k^{th}}$ row of the array contains the integer junction, or connection, points of that component. Such a row of connectivity data is often used in two related operations: `gather` and `scatter`. A `gather` operation uses the lists of connections to gather or collect information from the assembly necessary to describe the component or its action. The `scatter` operation has the reverse effect. It takes information about the component and sends it back to the assembly. Usually, values from the component are added into corresponding junction points of the assembly.

The main point of this discussion is that another way to define a non-sequential set of subscripts is to use an integer vector array that contains the set. Then one can use the array name as a way to range over the subscripts. This is a compact way to avoid an additional `FOR` or `DO` loop. The connectivity list for a component is often employed to select the subscripts needed for that component.

To illustrate the concept of vector subscripts, we will repeat the array flip example shown in §8.1.3 via the colon operators. Here we will define an integer vector called `Reverse` that has constant increments to be used in operating on the original array `A`. By using the vector name as a subscript, it automatically invokes an implied loop over the contents of that vector. As shown in Figure 8.2, this has the same effect as employing the colon operator directly.

The real power of the vector subscripts comes in the case where it has integers in a random, or user input, order rather than in an order that has a uniform increment. For example, if we repeat the above example using a vector `Random=[3 1 2]`, then both MATLAB and F90 would give the result

```
MODULE Ops_Example   ! User defined matrix transpose example

IMPLICIT NONE
INTERFACE OPERATOR (.t.)              ! transpose operator
   MODULE PROCEDURE Trans_R, Trans_I ! for real or integer matrix
   ! Remember to add logicals and vectors later
END INTERFACE                        ! defining .t.

CONTAINS  ! the actual operator actions for argument types

FUNCTION  Trans_R ( A ) ! defines .t. for real rank 2 matrix
   REAL, DIMENSION(:,:), INTENT(IN)      :: A
   REAL, DIMENSION(SIZE(A,2), SIZE(A,1)) :: Trans_R
   Trans_R = TRANSPOSE (A)
END FUNCTION  Trans_R  ! for real rank 2 transpose via .t.

FUNCTION  Trans_I ( A ) ! defines .t. for integer rank 2 matrix
   INTEGER, DIMENSION(:,:), INTENT(IN)      :: A
   INTEGER, DIMENSION(SIZE(A,2), SIZE(A,1)) :: Trans_I
   Trans_I = TRANSPOSE (A)
END FUNCTION  Trans_I  ! for integer rank 2 transpose via .t.

END MODULE Ops_Example   ! User defined matrix transpose example

PROGRAM Demo_Trans      ! illustrate the .t. operator
  USE Ops_Example       ! module with user definitions
  IMPLICIT NONE
  INTEGER, PARAMETER   :: M = 3, N = 2  ! rows, columns
  REAL, DIMENSION(M,N) :: A ; REAL, DIMENSION(N,M) :: B

  ! define A, test operator, print results
  A = RESHAPE ( (/ ((I*J , I=1,M), J=1,N) /), SHAPE(A) )
  B = .t. A
  PRINT *, 'MATRIX A' ;  CALL M_print (A, M, N)
  PRINT *, 'MATRIX B' ;  CALL M_print (B, N, M)
  !                Produces the result:
  !  MATRIX A
  !  RC     1          2
  !  1   1.000      2.000
  !  2   2.000      4.000
  !  3   3.000      6.000
  !
  !  MATRIX B
  !  RC     1          2          3
  !  1   1.000      2.000      3.000
  !  2   2.000      4.000      6.000
END PROGRAM Demo_Trans
```

Figure 8.1: Creating and applying user defined operators

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}, \quad \text{Reverse} = [321]$$

Flip left to right:

$$\texttt{B=A(: , Reverse)} = \begin{bmatrix} 3 & 2 & 1 \\ 6 & 5 & 4 \\ 9 & 8 & 7 \end{bmatrix}$$

Flip up to down:

$$\texttt{C = A(Reverse, :)} = \begin{bmatrix} 7 & 8 & 9 \\ 4 & 5 & 6 \\ 1 & 2 & 3 \end{bmatrix}$$

Flip up to down, left to right:

$$\texttt{D = A (Reverse,Reverse)} = \begin{bmatrix} 9 & 8 & 7 \\ 6 & 5 & 4 \\ 3 & 2 & 1 \end{bmatrix}$$

Figure 8.2: F90 and MATLAB Vector Subscripts and Array Shifts.

```
five  =  (/  1  2  3  4  5  /)
! without a pad
three =  eoshift(five,2) ! = (/  3  4  5  0  0  /)
three =  eoshift(five,-2) ! = (/  0  0  1  2  3  /)
! with a pad
pad = eoshift(five,2,9) ! = (/  3  4  5  9  9  /)
pad = eoshift(five,-2,9) ! = (/  9  9  1  2  3  /)
```

Figure 8.3: F90 end-off shift (`eoshift`) intrinsic.

```
five = (/  1  2  3  4  5  /)
left_3 = cshift(five,3) ! = (/  3  4  5  1  2  /)
right_3 = cshift(five,-3) ! = (/  4  5  1  2  3  /)
```

Figure 8.4: F90 Circular shift (`cshift`) intrinsic.

$$\texttt{E = A (:, Random)} = \begin{bmatrix} 3 & 1 & 2 \\ 6 & 4 & 5 \\ 9 & 7 & 8 \end{bmatrix}.$$

While the `reshape` option of F90 and MATLAB allows the array elements to change from one rectangular storage mode to another, one can also move elements around in the fixed shape array by utilizing the colon operators, or by the use of "shift operators." The latter accept an integer to specify how many locations to move or shift an element. A positive number moves an element up a column, a negative value moves it down the column, and a zero leaves it unchanged. The elements that are moved out of the array either move from the head of the queue to the tail of the queue (called a "circular shift") or are replaced by a user specified "pad" value (called an "end off shift"). If no pad is given, its value defaults to zero. These concepts are illustrated for F90 in Figures 8.3 and 8.4.

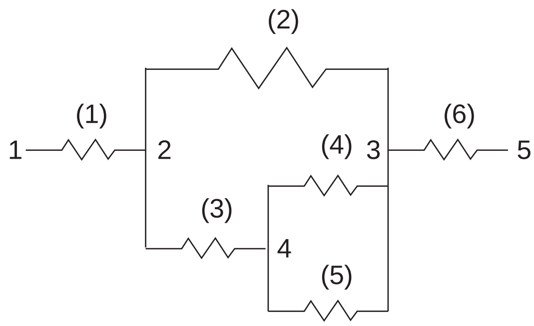
8.1.7 Component Gather and Scatter

Often the equations governing a system balance principle are assembled from the relative contributions of each component. When the answers for a complete system have been obtained, it is then possible to recover the response of each component. The automation of these processes has six basic requirements:

1. a component balance principle written in matrix form,
2. a joint connectivity data list that defines where a given component type connects into the system,
3. a definition of a `scatter` operator that scatters the coefficients of the component matrices into corresponding locations in the governing system equations,
4. an efficient system equation solver,
5. a `gather` operator to gather the answers from the system for those joints connected to a component, and
6. a recovery of the internal results in the component.

The first of these is discipline-dependent. We are primarily interested in the gather-scatter operations. These are opposites that both depend on the component connectivity list, which is often utilized as a vector subscript. The number of rows in the component equations is less than the number of rows in the assembled system, except for the special case where the system has only a single component. Thus, it is the purpose of the gather-scatter operators to define the relation between a system row number and a particular component row number. That is, they define the relation that defines the subset of component unknowns, say $\mathbf{V}^e$ for component e, in terms of all the system unknowns, say $\mathbf{V}$: $\mathbf{V}^e \subset_e \mathbf{V}$. Here the containment $\subset$ is defined by the component's connection list and the number of unknowns per joint. If there is only one unknown per joint, then the subset involves only the connection list. The above process gathers the subset of component unknowns from the full set of system unknowns.

Let the list of joints or nodes connected to the component be called $\mathbf{L}^e$. The k^{th} member in this list contains the corresponding system node number, `K`: i.e. `K = L_e(k)`. Thus, for a single unknown per



Component	Nodes	Property
(1)	1, 2	1
(2)	2, 3	2
(3)	2, 4	1
(4)	4, 3	3
(5)	4, 3	4
(6)	3, 5	1

Figure 8.5: Example Circuit or Axial Spring System

joint, one simply has $\mathbf{V}^e = \mathbf{V}(\mathbf{L}^e) \subset_e \mathbf{V}$. Written in full loop form, the component gather operation would be

```
DO  k = 1,  size(L_e)
  V_e (k) = V(L_e (k))
END DO  !  OVER LOCAL JOINTS
```

while in F90 or MATLAB vector subscript form, it is simply `V_e = V(L_e)`, for a single unknown per joint. When there is more than one unknown per joint, the relation can be written in two ways.

We pick the one that counts (assigns equation numbers to) all unknowns at a joint before going on to the next joint. Let the number of unknowns per joint be N. Then by deduction, one finds that the equation number for the j-th unknown at the K^{th} system node is

$$E(K, j) = N * (K - 1) + j, \quad 1 \leq j \leq N.$$

But to find which equation numbers go with a particular component, we must use the connection list `L_e`. For the k^{th} local node, `K = L_e (k)` and

$$E(k, j) = N * (L\_e(k) - 1) + j \ , \quad 1 \leq j \leq N \ .$$

If we loop over all nodes on a component, we can build an index list, say `I_e`, that tells which equations relate to the component.

```
INTEGER, ALLOCATABLE :: I_e(:), V_e(:)
ALLOCATE(I_e(N * SIZE (L_e)), V_e (N*SIZE(L_e)))
DO  k = 1, SIZE(L_e) ! component nodes
  DO  j = 1, N  !  unknowns per node
    LOCAL  = N *(k-1) + j
    SYSTEM = N *(L_e (k) - 1) + j
    I_e (LOCAL) = SYSTEM
  END DO  !  on unknowns
END DO  !  on local nodes.
```

Therefore, the generalization of the component gather process is

```
DO  m = 1, SIZE(I_e)
  V_e (m) = V(I_e (m))
END DO  !  over local unknowns
```

or in vector subscript form `V_e = V(I_e)` for an arbitrary number of unknowns per joint.

To illustrate the scatter concept, consider a system shown in Figure 8.5, which has six components and five nodes. If there is only one unknown at each joint (like voltage or axial displacement), then the system equations will have five rows. Since each component is connected to two nodes, each will contribute to (scatter to) two of the system equation rows. Which two rows? That is determined by the connection list shown in the figure. For example, component (4) is joined to nodes 4 and 3. Thus, the coefficients in the first row of the local component balance low would scatter into (be added to) the fourth row of the system, while the second row of the component would scatter to the third system equation row. If the component balance law is symmetric, then the columns locations scatter in the same fashion.

8.2 Matrices

Matrices are very commonly used in many areas of applied mathematics and engineering. While they can be considered a special case of the subscripted arrays given above they have their on special algebra and calculus notations that are useful to know. In the following sections we will describe matrices and the intrinsic operations on them that are included in F90 and MATLAB. Neither C nor C++ have such useful intrinsics, but require the programmer to develop them or extract them from a special library.

A *matrix* is defined as a rectangular array of quantities arranged in rows and columns. The array is enclosed in brackets, and thus if there are m rows and n columns, the matrix can be represented by

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1j} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2j} & \cdots & a_{2n} \\ \vdots & & & & & & \vdots \\ a_{i1} & a_{i2} & a_{i3} & \cdots & a_{ij} & \cdots & a_{in} \\ \vdots & & & & & & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mj} & \cdots & a_{mn} \end{bmatrix} = [\mathbf{A}] \tag{8.1}$$

where the typical element a_{ij} has two subscripts, of which the first denotes the row (i^{th}) and where the second denotes the column (j^{th}) which the element occupies in the matrix. A matrix with m rows and n columns is defined as a matrix of order $m \times n$, or simply an $m \times n$ matrix. The number of rows is always specified first. In Equation 8.1, the symbol $\mathbf{A}$ stands for the matrix of m rows and n columns, and it is usually printed in **boldface** type. If $m = n = 1$, then the matrix is equivalent to a scalar. If $m = 1$, the matrix $\mathbf{A}$ reduces to the single row

$$\mathbf{A} = [\ a_{11} \quad a_{12} \quad a_{13} \quad \cdots \quad a_{1j} \quad \cdots \quad a_{1n}\ ] = (\mathbf{A})$$

which is called a *row matrix*. Similarly, if $n = 1$, the matrix $\mathbf{A}$ reduces to the single column

$$\mathbf{A} = \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{bmatrix} = \text{col}[\ a_{11} \quad a_{21} \quad \cdots \quad a_{m1}\ ] = \{\mathbf{A}\}$$

which is called a *column matrix*, or vector. When all the elements of matrix are equal to zero, the matrix is called *null* or *zero* and is indicated by **0**. A null matrix serves the same function as zero does in ordinary algebra. To set all the elements of $\mathbf{A}$ to zero, one writes $A = 0$ in F90, and $A = \text{zeros}\,[m,\, n]$ in MATLAB.

If $m = n$, the matrix is said to be *square*.

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

Before considering some of the matrix algebra implied by the above equation, a few other matrix types need definition. A *diagonal matrix* is a square matrix which has zero elements outside the principal diagonal. It follows, therefore, that for a diagonal matrix $a_{ij} = 0$ when $i \neq j$, and not all a_{ii} are zero. A typical diagonal matrix may be represented by

$$\mathbf{A} = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix},$$

or more concisely as $\mathbf{A} = \text{diag}[a_{11} a_{22} \cdots a_{nn}]$.

A *unit* or *identity* matrix is a diagonal matrix whose elements are equal to 0 except those located on its main diagonal, which are equal to 1. That is, $a_{ij} = 1$ if $i = j$, and $a_{ij} = 0$ if $i \neq j$. The unit matrix will be given the symbol **I** throughout these notes. An example of a 3×3 unit matrix is

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \mathrm{diag}[1\ 1\ 1]\ .$$

A *Toeplitz* matrix has constant-valued diagonals. An identity matrix is Toeplitz as is the following matrix.

$$\mathbf{A} = \begin{bmatrix} 1 & -2 & 3 & 5 \\ 4 & 1 & -2 & 3 \\ -1 & 4 & 1 & -2 \\ 10 & -1 & 4 & 1 \end{bmatrix}$$

Note how the values of a Toeplitz matrix's elements are determined by the first row and the first column. MATLABuses the Toeplitz function to create this unusual matrix.

A *symmetric matrix* is a square matrix whose elements $a_{ij} = a_{ji}$ for all i, j. For example,

$$\mathbf{A} = \begin{bmatrix} 12 & 2 & -1 \\ 2 & 33 & 0 \\ -1 & 0 & 15 \end{bmatrix}$$

is symmetric: The first row equals the first column, the second row the second column, etc.

An *antisymmetric* or *skew symmetric* matrix is a square matrix whose elements $a_{ij} = -a_{ji}$ for all i, j. Note that this condition means that the diagonal values of an antisymmetric matrix must equal zero. An example of such a matrix is

$$\mathbf{A} = \begin{bmatrix} 0 & 2 & -1 \\ -2 & 0 & 10 \\ 1 & -10 & 0 \end{bmatrix}$$

The *transpose* of a matrix **A**, denoted by $\mathbf{A}^{\mathrm{T}}$, is obtained by interchanging the rows and columns. Thus, the transpose of an $m \times n$ matrix is an $n \times m$ matrix. For example,

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 3 & 5 \\ 0 & 1 \end{bmatrix} \qquad \mathbf{A}^{\mathrm{T}} = \begin{bmatrix} 2 & 3 & 0 \\ 1 & 5 & 1 \end{bmatrix}\ .$$

In MATLAB an appended prime is used to denote the transpose of any matrix, such as $\mathbf{B} = \mathbf{A}'$, whereas in F90 we employ the intrinsic function $\mathbf{B} = \mathrm{transpose}\,(\mathbf{A})$, or a user defined operator like $\mathbf{B} =$ `.t.`**A** which we defined earlier.

If all the elements on one side of the diagonal of a square matrix are zero, the matrix is called a *triangular* matrix. There are two types of triangular matrices: (1) an upper triangular **U**, whose elements below the diagonal are all zero, and (2) a lower triangular **L**, whose elements above the diagonal are all zero. An example of a lower triangular matrix is

$$\mathbf{L} = \begin{bmatrix} 10 & 0 & 0 \\ 1 & 3 & 0 \\ 5 & 1 & 2 \end{bmatrix}\ .$$

A matrix may be divided into smaller arrays by horizontal and vertical lines. Such a matrix is then referred to as a *partitioned matrix*, and the smaller arrays are called *submatrices*. For example, we can partition a 3×3 matrix into four submatrices as shown:

$$\mathbf{A} = \left[\begin{array}{cc|c} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ \hline a_{31} & a_{32} & a_{33} \end{array}\right] = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} = \left[\begin{array}{cc|c} 2 & 1 & 3 \\ 10 & 5 & 0 \\ \hline 4 & 6 & 10 \end{array}\right]$$

where, in the F90 and MATLABcolon notation;

$$
\begin{aligned}
\mathbf{A}_{11} &= \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} 2 & 1 \\ 10 & 5 \end{bmatrix} = \mathbf{A}(1:2,\, 1:2) \\
\mathbf{A}_{12} &= \begin{bmatrix} a_{13} \\ a_{23} \end{bmatrix} = \begin{bmatrix} 3 \\ 0 \end{bmatrix} = \mathbf{A}(1:2,\, 3) \\
\mathbf{A}_{21} &= \begin{bmatrix} a_{31} & a_{32} \end{bmatrix} = \begin{bmatrix} 4 & 6 \end{bmatrix} = \mathbf{A}(3,\, 1:2) \\
\mathbf{A}_{22} &= [a_{33}] = [10] = \mathbf{A}(3,\, 3)
\end{aligned}
$$

It should be noted that the elements of a partitioned matrix must be so ordered that they are compatible with the whole matrix $\mathbf{A}$ and with each other. That is, $\mathbf{A}_{11}$ and $\mathbf{A}_{12}$ must have an equal number of rows. Likewise, $\mathbf{A}_{21}$ and $\mathbf{A}_{22}$ must have an equal number of rows. Matrices $\mathbf{A}_{11}$ and $\mathbf{A}_{21}$ must have an equal number of columns. Likewise, for $\mathbf{A}_{12}$ and $\mathbf{A}_{22}$. Note that $\mathbf{A}_{22}$ is a matrix even though it consists of only one element. Provided the general rules for matrix algebra are observed, the submatrices can be treated as if they were ordinary matrix elements.

8.2.1 Matrix Algebra

To define what addition and multiplication means for matrices, we need to define an *algebra* for arrays of numbers so that they become useful to us. Without an algebra, all we have is a sequence of definitions without the ability to manipulate what they mean!

Addition of two matrices of the same order is accomplished by adding corresponding elements of each matrix. The matrix addition $\mathbf{C} = \mathbf{A} + \mathbf{B}$ (as we write it in F90 and MATLAB), where $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are matrices of the *same* order $m \times n$ can be indicated by the equation

$$c_{ij} = a_{ij} + b_{ij}, \;\; 1 \le i \le m, \; 1 \le j \le n$$

where c_{ij}, a_{ij}, and b_{ij} are typical elements of the $\mathbf{C}$, $\mathbf{A}$, and $\mathbf{B}$ matrices, respectively. An example of matrix addition is

$$\begin{bmatrix} 3 & 0 & 1 \\ 2 & -1 & 2 \\ 1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} -1 & 1 & -1 \\ 2 & 5 & 6 \\ -3 & 4 & 9 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 0 \\ 4 & -4 & 8 \\ -2 & 5 & 10 \end{bmatrix} .$$

Matrix subtraction, $\mathbf{C} = \mathbf{A} - \mathbf{B}$, is performed in a similar manner.

Matrix addition and subtraction are *associative* and *commutative*. That is, with the previous definitions for matrix addition and subtraction, grouping and ordering with respect to these operations does not affect the result.

$$\mathbf{A} \pm (\mathbf{B} \pm \mathbf{C}) = (\mathbf{A} \pm \mathbf{B}) \pm \mathbf{C} \quad \text{and} \quad \mathbf{C} \pm \mathbf{B} \pm \mathbf{A}$$

Multiplication of the matrix $\mathbf{A}$ by a scalar c is defined as the multiplication of every element of the matrix by the scalar c. Thus, the elements of the product $\mathbf{B} = c\mathbf{A}$ are given by $b_{ij} = ca_{ij}$, and is written as $\mathbf{B} = C * \mathbf{A}$ in both F90 and MATLAB. Clearly, scalar multiplication distributes over matrix addition.

We could define special multiplication in the somewhat boring way as the term by term product of two identical sized matrices: $\mathbf{C} = \mathbf{AB} \Longrightarrow c_{ij} = a_{ij} b_{ij}$. This feature is allowed in both F90 and MATLAB where it is written as $\mathbf{C} = \mathbf{A}{*}\mathbf{B}$, and $\mathbf{C} = \mathbf{A}\,.{*}\mathbf{B}$, respectively. Although this definition might be useful in some applications, this choice for what multiplication means in our algebra does not give us much power. Instead, we define the matrix product $\mathbf{C} = \mathbf{AB}$ to mean

$$c_{ij} = \sum_{k=1}^{p} a_{ik} b_{kj}, \; 1 \le i \le m, 1 \le j \le n \; .$$

$\mathbf{A}$ and $\mathbf{B}$ can be multiplied together as *only* when the number of columns in $\mathbf{A}, p$, equals the number of rows in $\mathbf{B}$. When this condition is fulfilled, the matrices $\mathbf{A}$ and $\mathbf{B}$ are said to be *conformable* for multiplication. Otherwise, matrix multiplication of two matrices cannot be defined. The product of two conformable matrices $\mathbf{A}$ and $\mathbf{B}$ having orders $m \times p$ and $p \times n$, respectively, yields an $m \times n$ matrix $\mathbf{C}$. In MATLAB this is simply written as $\mathbf{C} = \mathbf{A}{*}\mathbf{B}$, where as in F90 one would use the intrinsic function $\mathbf{C} = \mathrm{matmul}\,(\mathbf{A}, \mathbf{B})$, or a user defined operator such as $\mathbf{C} = \mathbf{A}\,.\mathtt{x}.\,\mathbf{B}$ which we defined earlier.

The reason why this definition for matrix multiplication was chosen so that we can concisely represent a system of linear equations. The verbose form explicitly lists the equations.

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n &= c_1 \\
a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n &= c_2 \\
a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \cdots + a_{3n}x_n &= c_3 \\
\vdots \qquad\qquad & \quad \vdots \\
a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n &= c_n
\end{aligned}
$$

where the a_{ij}'s and c_i's usually represent known coefficients and the x_i's unknowns. To express these equations more precisely, we define matrices for each of these arrays of numbers and lay them out as a matrix-vector product equaling a vector.

$$
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\
a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\
a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\
 & & \vdots & & \\
a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn}
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}
=
\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix}
$$

We thus obtain the more compact matrix form $\mathbf{AX} = \mathbf{C}$. $\mathbf{A}$ represents the square matrix of coefficients, $\mathbf{X}$ the vector (column matrix) of unknowns, and $\mathbf{C}$ the vector of known quantities.

Matrix multiplication is associative and distributive. For example,

$$
\begin{aligned}
(\mathbf{AB})\mathbf{C} &= \mathbf{A}(\mathbf{BC}) \\
\mathbf{A}(\mathbf{B} + \mathbf{C}) &= \mathbf{AB} + \mathbf{AC}
\end{aligned}
$$

However, matrix multiplication is *not* commutative. In general, $\mathbf{AB} \neq \mathbf{BA}$. Consequently, the order in which matrix multiplication is specified is by no means arbitrary. Clearly, if the two matrices are not conformable, attempting to commute the product makes no sense (the matrix multiplication $\mathbf{BA}$ is not defined). In addition, when the matrices are conformable so that either product makes sense (the matrices are both square and have the same dimensions, for example), the product cannot be guaranteed to commute. You should try finding a simple example that illustrates this point. When two matrices $\mathbf{A}$ and $\mathbf{B}$ are multiplied, the product $\mathbf{AB}$ is referred to either as $\mathbf{B}$ *premultiplied* by $\mathbf{A}$, or as $\mathbf{A}$ *postmultiplied* by $\mathbf{B}$. When $\mathbf{AB} = \mathbf{BA}$, the matrices $\mathbf{A}$ and $\mathbf{B}$ are then said to be *commutable*. For example, the unit matrix $\mathbf{I}$ commutes with any square matrix of the same order: $\mathbf{AI} = \mathbf{IA} = \mathbf{A}$.[†]

The process of matrix multiplication can also be extended to partitioned matrices, provided the individual products of submatrices are conformable for multiplication. For example, the multiplication

$$
\mathbf{AB} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}
\begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix}
= \begin{bmatrix} \mathbf{A}_{11}\mathbf{B}_{11} + \mathbf{A}_{12}\mathbf{B}_{21} & \mathbf{A}_{11}\mathbf{B}_{12} + \mathbf{A}_{12}\mathbf{B}_{22} \\ \mathbf{A}_{21}\mathbf{B}_{11} + \mathbf{A}_{22}\mathbf{B}_{21} & \mathbf{A}_{21}\mathbf{B}_{12} + \mathbf{A}_{22}\mathbf{B}_{22} \end{bmatrix}
$$

is possible provided the products $\mathbf{A}_{11}\mathbf{B}_{11}$, $\mathbf{A}_{12}\mathbf{B}_{21}$, etc. are conformable. For this condition to be fulfilled, it is only necessary for the vertical partitions in $\mathbf{A}$ to include a number of columns equal to the number of rows in the corresponding horizontal partitions in $\mathbf{B}$.

The transpose of a product of matrices equals $(\mathbf{AB}\cdots\mathbf{YZ})^{\mathrm{T}} = \mathbf{Z}^{\mathrm{T}}\mathbf{Y}^{\mathrm{T}}\cdots\mathbf{B}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}$. As an example of matrix multiplication, let $\mathbf{B} = \begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix}$ and $\mathbf{A} = \left[\begin{smallmatrix} 2 & 1 & 0 \\ 1 & 0 & 1 \end{smallmatrix}\right]$; then

$$
\mathbf{AB} = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 7 \\ 6 \end{bmatrix}
$$

[†]This result is why $\mathbf{I}$ is called the identity matrix: It is the identity element with respect to matrix multiplication.

$$\mathbf{B}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}} = \left[\begin{array}{ccc} 3 & 1 & 2 \end{array}\right] \left[\begin{array}{cc} 2 & 1 \\ 1 & 0 \\ 0 & 1 \end{array}\right] = \left[\begin{array}{cc} 7 & 6 \end{array}\right]$$

8.2.2 Inversion

Every (non-singular) square matrix $\mathbf{A}$ has an *inverse*, indicated by $\mathbf{A}^{-1}$, such that by definition the product $\mathbf{A}\mathbf{A}^{-1}$ is a unit matrix $\mathbf{I}$. The reverse is also true: $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$. Inverse matrices are very useful in the solution of simultaneous equations $\mathbf{AX} = \mathbf{C}$ such as above where $\mathbf{A}$ and $\mathbf{C}$ are known and $\mathbf{X}$ is unknown. If the inverse of $\mathbf{A}$ is known, the unknowns of the $\mathbf{X}$ matrix can be (symbolically) found by premultiplying both sides of the equation by the inverse $\mathbf{A}^{-1}\mathbf{AX} = \mathbf{A}^{-1}\mathbf{C}$ so that

$$\mathbf{X} = \mathbf{A}^{-1}\mathbf{C}\ .$$

In this way, in theory we have "solved" our system of linear equations. To employ this approach, we must find the inverse of the matrix $\mathbf{A}$, which is not any easy task. Despite this computational difficulty, using matrix algebra to concisely express complicated linear combinations of quantities often provides much insight into a problem and its solution techniques.

Various methods can be used to determine the inverse of a given matrix. For very large systems of equations it is probably more practical to avoid the calculation of the inverse and solve the equations by a procedure called *factorization*. Various procedures for computing an inverse matrix can be found in texts on numerical analysis. The inverse of 2×2 or 3×3 matrices can easily be written in closed form by using *Cramer's rule*. For a 2×2 matrix, we have the classic formula, which *no* engineering student should forget.

$$\boxed{\left[\begin{array}{cc} a & b \\ c & d \end{array}\right]^{-1} = \frac{\left[\begin{array}{cc} d & -b \\ -c & a \end{array}\right]}{ad - bc}}$$

However, finding the inverse of larger arrays using Cramer's rule is very inefficient computationally. In MATLAB an inverse matrix of A is computed as `inv(A)`, but this is only practical for matrices of a small size, say < 100. F90 does not have an intrinsic matrix inversion function but we provide such a function, named `inv`, in our operator library.

8.2.3 Factorizations

We have indicated that we will frequently employ matrices to solve linear equation systems like $A*x = b$, where $\mathbf{A}$ is a known square matrix, $\mathbf{B}$ is a known vector, and $\mathbf{X}$ is an unknown vector. While in theory the solution is simply the inverse of $\mathbf{A}$ times the vector $\mathbf{B}$, $x = \mathbf{A}^{(-1)} * b$, that is computationally the least efficient way to find the vector $\mathbf{X}$. In practice, one usually uses some form of factorization of the matrix $\mathbf{A}$. A very common method is to define $\mathbf{A}$ to be the product of two triangular matrices, defined above, say $L * U = A$, where $\mathbf{L}$ is a square lower triangular matrix and $\mathbf{U}$ is a square upper triangular matrix. Skipping the details of this "$\mathbf{LU}$-factorization" we could rewrite the original matrix system as $L * U * x = b$, which can be viewed as two matrix identities:

$$L * h = b$$
$$U * x = h,$$

where h is a new temporary vector, and where both $\mathbf{L}$ and $\mathbf{U}$ are much cheaper to compute than the inverse of $\mathbf{A}$. We do not need the inverse of $\mathbf{L}$ or $\mathbf{U}$ since, as triangular matrices, their first or last row contains only one non-zero term. That allows us to find one term in the unknown vector from one scalar equation. The processes of recovering the vectors from these two identities is called substitution.

We illustrate this process with a example set of four equations with $\mathbf{A}$ and b given as:

$$\mathbf{A} = \left[\begin{array}{rrrr} 1800 & 600 & -360 & 900 \\ 0 & 4500 & -2700 & 2250 \\ 0 & -2700 & 2700 & -1890 \\ 6300 & 5250 & -1890 & 3795 \end{array}\right]$$

$$\mathbf{b}^T = [\,6300 \quad -2250 \quad 1890 \quad 21405\,]\,.$$

The $\mathbf{LU}$-factorization process mentioned above gives the first of two lower triangular systems; $L{*}h = b$:

$$\left[\begin{array}{rrrr} 60 & 0 & 0 & 0 \\ 0 & 150 & 0 & 0 \\ 0 & -90 & 36 & 0 \\ 210 & 105 & 42 & -10 \end{array}\right] \left\{\begin{array}{c} h_1 \\ h_2 \\ h_3 \\ h_4 \end{array}\right\} = \left\{\begin{array}{r} 6300 \\ -2250 \\ 1890 \\ 21405 \end{array}\right\}.$$

Observe that the significant difference from $A * x = b$ is that the first row of this identity has one equation and one unknown:

$$60 * h_1 = 6300$$

which yields $h_1 = 105$. This process continues through all the rows solving for one unknown, h_k in row k, because all the above h values are known. For example, the next row gives $0 * 105 + 150 * h_2 = -2250$, which yields $h_2 = -15$. This process is known as "forward substitution." When completed the substitution yields the intermediate answer:

$$h^T = [\,105 \quad -15 \quad 15 \quad -30\,]\,.$$

Now that h is known we can write the upper triangular identity, $U * x = h$, as:

$$\left[\begin{array}{rrrr} 30 & 10 & -6 & 15 \\ 0 & 30 & -18 & 15 \\ 0 & 0 & 30 & -15 \\ 0 & 0 & 0 & 30 \end{array}\right] \left\{\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \end{array}\right\} = \left\{\begin{array}{r} 105 \\ -15 \\ 15 \\ -30 \end{array}\right\}.$$

This time the bottom row has only one unknown, $30 * x_4 = -30$, so the last unknown is $x_4 = -1$. Working backward up to the next row again there is only one unknown:

$$30 * x_3 + -15 * (-1) = 15$$

so that $x_3 = 0$. Proceeding back up through the remaining rows to get all the unknowns is called "back substitution." It yields

$$x^T = [\,4 \quad 0 \quad 0 \quad -1\,]\,.$$

By inspection you can verify that this satisfies the original system of linear equations, $A * x = b$. With a little more work one can employ matrix multiplication to verify that $L * U = A$. While we have not given the simple algorithm for computing $\mathbf{L}$ and $\mathbf{U}$ from $\mathbf{A}$, it is widely known as the "$\mathbf{LU}$ Factorization," and is in many texts on numerical analysis. Other common factorizations are the "QR Factorization," the "Cholesky Factorization" for a symmetric positive definite $\mathbf{A}$, and the "SVD Factorization" for the case where $\mathbf{A}$ is rectangular, or ill-conditioned and one is seeking a best approximation to $\mathbf{X}$.

The factorization process is relatively expensive to compute but is much less expensive that an inversion. The forward and backward substitutions are very fast and cheap. In problems where you have many different b vectors (and corresponding x vectors, such as time dependent problems), one carries out the expensive factorization process only once and the executes the cheap forward and back substitution for each b vector supplied.

8.2.4 Determinant of a Matrix

Every square matrix, say $\mathbf{A}$, has a single scalar quantity associated with it. That scalar is called the determinant, $|\mathbf{A}|$, of the matrix. The determinant is important in solving equations and inverting matrices. A very important result is that the inverse $\mathbf{A}^{-1}$ exists if and only if $|\mathbf{A}| \neq 0$. If the determinant is zero, the matrix $\mathbf{A}$ (and the equivalent set of equations) is said to be *singular*. Simple conditions on a matrix's structure can be used to infer the determinant or its properties.

- If two rows or columns are equal, the determinant is zero.

- Interchanging two rows, or two columns, changes the sign of the determinant.
- The determinant is unchanged if any row, or column, is modified by adding to it a linear combination of any of the other rows, or columns.
- A singular square matrix may have nonsingular square partitions.

The last two items will become significant when we consider how to apply boundary conditions and how to solve a system of equations.

8.2.5 Matrix Calculus

At times you might find it necessary to differentiate or integrate matrices. These operations are simply carried out on each and every element of the matrix. Let the elements a_{ij} of $\mathbf{A}$ be a function of a parameter t. Then, the derivative and integral of a matrix simply equals term-by-term differentiation and integration, respectively.

$$\begin{aligned}\mathbf{B} &= \frac{d\mathbf{A}}{dt} \longleftrightarrow b_{ij} = \frac{da_{ij}}{dt},\ 1 \le i \le m, 1 \le j \le n \\ \mathbf{C} &= \int \mathbf{A}\, dt \longleftrightarrow c_{ij} = \int a_{ij}\, dt,\ 1 \le i \le m, 1 \le j \le n\end{aligned}$$

When dealing with functional relations the concept of rate of change is often very important. If we have a function $f(\cdot)$ of a single independent variable, say x, then we call the rate of change the derivative with respect to x, which is written as df/dx. Generalizing this notion to functions of more than two variables, say $z = f(x, y)$, we may define two distinct rates of change. One is the function's rate of change with respect to one variable with the other held constant. We thus define *partial derivatives*. When x is allowed to vary, the derivative is called the *partial derivative with respect to* x, and is denoted by $\partial f/\partial x$. By analogy with the usual definition of derivative, this partial derivative is mathemtically defined as

$$f_x = \frac{\partial f}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x} .$$

A similar definition describes the partial derivative with respect to y, denoted by $\partial f/\partial y$. The second notion of rate-of-change is the *total* derivative, which is expressed as df.

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy$$

These definitions can be extended to include a function of any number of independent variables.

Often one encounters a scalar u defined by a symmetric square $n \times n$ matrix, $\mathbf{A}$, a column vector $\mathbf{B}$, and a column vector $\mathbf{X}$ of n parameters. The combination we have in mind has the form

$$u = \frac{1}{2}\mathbf{X}^{\mathrm{T}}\mathbf{A}\mathbf{X} + \mathbf{X}^{\mathrm{T}}\mathbf{B} + \mathbf{C} \tag{8.2}$$

If we calculate the derivative of the scalar u with respect to each x_i, the result is the column vector

$$\frac{\partial u}{\partial \mathbf{X}} = \mathbf{A}\mathbf{X} + \mathbf{B} ,$$

a result that can be verified by expanding Equation 8.2, differentiating with respect to every x_i in $\mathbf{X}$, and rewriting the result as a matrix product.

8.2.6 Computation with Matrices

Clearly, matrices are useful in representing systems of linear equations and expressing the solution. As said earlier, we need to be able to express linear equations in terms of matrix notation so that analytic manipulations become easy. Furthermore, calculations with linear equations become easy if we can *directly* express our matrix formulas in terms of programs. This section describes programming constructs for the simple matrix expressions and manipulations covered in this chapter.

	MATLAB	C++	F90
Pre-allocate linear array	`A(100)=0`	`int A[100];`[a]	`integer A(100)`
Initialize to a constant value of 12	`for j=1:100 % slow` `  A(j)=12` `  end` `% better way` `A=12*ones(1,100)`	`for (j=0; j<100; j++)` `  A[j]=12;`	`A=12`
Pre-allocate two-dimensional array	`A=ones(10,10)`	`int A[10][10];`	`integer A(10,10)`

[a]C++ has a starting subscript of 0, but the argument in the allocation statement is the array's size.

Table 8.12: Array initialization constructs.

Action	MATLAB	C++	F90
Define size	`A=zeros(2,3)`[a]	`int A[2][3];`	`integer, dimension (2,3)::A`
Enter rows	`A=[1,7,-2;` `  3, 4, 6];`	`int A[2][3]={` `  {1,7,2},` `  {3,4,6}` `};`	`A(1,:)=(/1,7,-2/)` `A(2,:)=(/3,4,6/)`

[a]Optional in MATLAB, but improves efficiency.

Table 8.13: Array initialization constructs

In most languages, we must express the fact that a variable is an ordered array of numbers—a matrix—rather than a scalar (or some other kind of variable). Such *declaration* statements usually occur at the beginning of the program or function. Table 8.12 shows the declaration of an integer array for our suite of programming languages. Both Fortran and C++ require you to specify the maximum range of each subscript of an array before the array or its elements are used. Such range specification is not *required* by MATLAB, but pre-allocating the array space can drastically improve the speed of MATLAB, as well as making much more efficient use of the available memory. If you do not pre-allocate MATLAB arrays, the interpreter must check at each step if a position in a row or column is larger than the current maximum. If so, the maximum value is increased and the memory found to store the new element. Thus, failure to pre-allocate MATLAB arrays is permissible but inefficient.

Array initialization is concisely expressed in both Fortran and MATLAB; in C++, you must write a small program to initialize an array to a nonzero value.[†] If an array contains a variety of different numbers, we can concisely express the initialization; again, in C++, we must explicitly write statements for each array element.

An Aside: Matrix Storage

Most computer languages do not make evident how matrices are stored. More frequently than you might think, it becomes necessary to know how an array is actually stored in the computer's memory and retrieved. The procedure both Fortran and MATLAB use to store the elements of an array is known as *column major order*: all the elements of the first column are stored sequentially, then all of the second, etc. Another way of saying this is that the first (left most) subscript ranges over all its values before the second is incremented. After the second subscript has been incremented then the first again ranges over all its values. In C++, *row major order* is used: The first row of an array is stored sequentially, then the second, etc. Clearly, translating programs from Fortran to C++ or vice versa must be done with care.

However, the above knowledge can be used to execute some operations more efficiently. For example, the matrix addition procedure could be written as $c_k = a_k + b_k$, $1 \le k \le m \times n$. One circumstance

[†]Global arrays—those declared outside of any function definition—are initialized to zero in many versions of C++. Array declared within the scope of a function have no predefined values.

	MATLAB	C++	F90
Addition $\mathbf{C} = \mathbf{A} + \mathbf{B}$	`C=A+B`	`for (i=0; i<n; i++){` `  for (j=0; j<n; j++){` `    C[i][j]=A[i][j]+B[i][j];` `    }` `  }`	`C=A+B`
Multiplication $\mathbf{C} = \mathbf{AB}$	`C=A*B`	`for (i=0; i<n; i++){` `  for (j=0; j<n; j++){` `    C[i][j] = 0;` `    for (k=0; k<n; k++){` `      C[i][j] += A[i][k]*B[k][j];` `      }` `    }` `  }`	`C=matmul(A,B)`
Scalar multiplication $\mathbf{C} = a\mathbf{B}$	`C=a*B`	`for (i=0; i<n; i++){` `  for (j=0; j<n; j++){` `    C[i][j] = a*B[i][j];` `    }` `  }`	`C=a*B`
Matrix inverse $\mathbf{B} = \mathbf{A}^{-1}$	`B=inv(A)`	[a]	`B=inv(A)`[a]

[a]Neither C++ nor F90 have matrix inverse functions as part of their language definitions nor as part of standard collections of mathematical functions (like those listed in Table 4.7). Instead, a special function, usually drawn from a library of numerical functions, or a user defined operation, must be used.

Table 8.14: Elementary matrix computational routines (for $n \times n$ matrices)

where knowing the storage format becomes crucial is extracting submatrices in partitioned arrays. Such a Fortran subroutine would have to `dimension` the arrays with a single subscript.

Expressing the addition, subtraction, or multiplication of arrays in Fortran or MATLAB is concise and natural. Explicit programs must be written in C++ to accomplish these calculations. Table 8.14 displays what these constructs are for the special case of square matrices with n rows.

8.3 Exercises

1. Often it is necessary to check computer programs that invert matrices. One approach is use test matrices for which the inverse is known analytically. Few such matrices are known, but one is the following $n \times n$ matrix.

$$\begin{bmatrix} \frac{n+2}{2n+2} & -\frac{1}{2} & 0 & 0 & \cdots & 0 & \frac{1}{2n+2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \cdots & -\frac{1}{2} & 1 & -\frac{1}{2} \\ \frac{1}{2n+2} & 0 & \cdots & \cdots & 0 & -\frac{1}{2} & \frac{n+2}{2n+2} \end{bmatrix}^{-1} = \begin{bmatrix} n & n-1 & n-2 & \cdots & 2 & 1 \\ n-1 & n & n-1 & \cdots & 3 & 2 \\ n-2 & n-1 & n & \cdots & 4 & 3 \\ \vdots & & & & & \vdots \\ 2 & 3 & 4 & \cdots & n & n-1 \\ 1 & 2 & 3 & \cdots & n-1 & n \end{bmatrix}$$

Develop two routines that will create each of these two matrices for a given `n` value, and test them with a main program that uses `matmul` to compute their matrix product. The result should be the identity matrix.

2. The numerical accuracy in calculating an inverse is always an issue: To what extent can you believe the accuracy of the numbers that computer programs calculate. Because of the finite precision used to represent floating point numbers, floating point calculations can only rarely yield exact answers. We want to empirically compute the difference between the inverse of the first matrix in the previous exercise by using a library inversion routine and compare its result with the exact answer. Because the error varies throughout the matrix, we need to summarize the error with a single quantity. Two measures are routinely used: the peak absolute error $\max_{i,j} |a_{ij} - b_{ij}|$ and the root-mean-squared (rms) error $\sqrt{\frac{1}{n^2} \sum_{i,j} (a_{ij} - b_{ij})^2}$.[†] The first captures the biggest difference between the elements of two matrices, and the second summarizes the error throughout the entire difference. Clearly, the peak absolute error is always larger than the rms error. Comparing these two error measures provides some insight into the distribution of error: If the two are comparable, the errors have about the same size; if not, the errors deviate greatly throughout the matrix.

3. Combine the intrinsic array features of F90 with the concepts of OO classes to create a Vector Class that is built around a type that has attributes consisting of the integer length of a vector and an array of its real components. Provide members to construct vectors, delete the arrays, real vectors, list vectors, and carry out basic mathematics operations. Overload the operators +, -, *, =, and ==. Avoid writing any serial loops.

4. Extend the above Vector Class concepts to a Sparse Vector Class where it is assumed that most of the values in the vector are zero and for efficiency only the non-zero entries are to be stored. This clearly exceeds the intrinsic array features of F90 and begins to show the usefulness of OOP. The defined type must be extended to include an integer array that contains the location (row number) of the non-zero values. In addition to changing the input and output routines to utilize the extra integer position list, all the mathematical member functions such as addition will have to be changed so that the resulting vector has non-zero terms in locations that are a union of the two given location sets (unless the operation creates new zero values). Use the concept of logical array masks in computing the dot product. Avoid writing any serial loops.

[†] The $1/n^2$ term occurs in this expression because that equals the number of terms in the sum. The rms error is used frequently in the practice to measure error; you average the squared error across the dataset and evaluate the square-root of the result.

Chapter 9

Advanced Topics

9.1 Templates

One of our goals has been to develop software that can be reused for other applications. There are some algorithms that are effectively independent of the object type on which they operate. For example, in a sorting algorithm one often needs to interchange, or swap, two objects. A short routine for that purpose follows:

```
subroutine swap_integers (x, y)
implicit none
  integer, intent(inout) :: x, y
  integer                :: temp
    temp = x
    x    = y
    y    = temp
end subroutine swap_integers
```

Observe that in this form it appears necessary to have one version for integer arguments and another for real arguments. Indeed we might need a different version of the routine for each type of argument that you may need to swap. A slightly different approach would be to write our swap algorithm as:

```
subroutine swap_objects (x, y)
implicit none
  type (Object), intent(inout) :: x, y
  type (Object)                :: temp
    temp = x
    x    = y
    y    = temp
end subroutine swap_objects
```

which would be a single routine that would work for any Object, but it has the disadvantage that one find a way to redefine the Object type for each application of the routine. That would not be an easy task. (While we will continue with this example with the algorithm in the above forms it should be noted that the above approaches would not be efficient if x and y were very large arrays or derived type objects. In that case we would modify the algorithm slightly to employ pointers to the large data items and simply swap the pointers for a significant increase in efficiency.)

Consider ways that we might be able to generalize the above routines so that they could accept and swap any specific type of arguments. For example, the first two versions could be re-written in a so called template form as:

```
subroutine swap_Template$ (x, y)
implicit none
  Template$, intent(inout) :: x, y
  Template$                :: temp
    temp = x
    x    = y
    y    = temp
end subroutine swap_Template$
```

In the above template the dollar sign ($) was includes in the "wild card" because while it is a valid member of the F90 character set it is not a valid character for inclusion in the name of a variable, derived type, function, module, or subroutine. In other words, a template in the illustrated form would not compile, but such a name could serve as a reminder that its purpose is to produce a code that can be compiled after the "wild card" substitutions have been made.

With this type of template it would be very easy to use a modern text editor to do a global substitution of any one of the intrinsic types `character, complex, double precision, integer, logical,` or `real` for the "wild card" keyword `Template$` to produce a source code to swap any or all of the intrinsic data types. There would be no need to keep up with all the different routine names if we placed all of them in a single module and also created a generic `interface` to them such as:

```
module swap_library
implicit none
  interface swap    ! the generic name
    module procedure swap_character, swap_complex
    module procedure swap_double precision, swap_integer
    module procedure swap_logical, swap_real
  end interface
contains
  subroutine swap_characters (x, y)
   . . .
  end subroutine swap_characters
  subroutine swap_ . . .
   . . .
end module swap_library
```

The use of a text editor to make such substitutions is not very elegant and we expect that there may be a better way to pursue the concept of developing a re-useable software template. The concept of a text editor substitution also fails when we go to the next logical step and try to use a derived type argument instead of any of the intrinsic data types. For example, if we were to replace the "wild card" with our previous `type (chemical_element)` that would create:

```
subroutine swap_type (chemical_element) (x,y)
implicit none
  type (chemical_element), intent (inout)::x,y
  type (chemical_element)                ::temp
        temp = x
        x    = y
        y    = temp
end subroutine swap_type (chemical_element)
```

This would fail to compile because it violates the syntax for a valid function or subroutine name, as well as the end function or end subroutine syntax. Except for the first and last line syntax errors this would be a valid code. To correct the problem we simply need to add a little logic and omit the characters `type ( )` when we create a function, module, or subroutine name that is based on a derived type data entity. Then we obtain

```
subroutine swap_chemical_element (x,y)
implicit none
  type (chemical_element), intent (inout)::x,y
  type (chemical_element)                ::temp
        temp = x
        x    = y
        y    = temp
end subroutine swap_chemical_element
```

which yields a completely valid routine.

Unfortunately, text editors do not offer us such logic capabilities. However, as we have seen, high level programming languages like C++ and F90 do have those abilities. At this point you should be able to envision writing a `pre-processor` program that would accept a file of template routines, replace the template "wildcard" words with the desired generic forms to produce a module or `header file` containing the expanded source files that can then be brought into the desired program with an `include` or `use` statement. The C++ language includes a template pre-processor to expand template files as needed. Some programmers criticize F90/95 for not offering this ability as part of the standard. A few C++ programmers criticize templates and advise against their use. Regardless of the merits of including template pre-processors in a language standard it should be clear that it is desirable to plan software for its efficient reuse.

With F90 if one wants to take advantage of the concepts of templates then the only choices are to carry out a little text editing or develop a pre-processor with the outlined capabilities. The former is clearly the simplest and for many projects may take less time than developing such a template pre-processor. However, if one makes the time investment to produce a template pre-processor one would have a tool that could be applied to basically any coding project. In the following sections we will give one example of an F90 template pre-processor and demonstrate its application. Reviewing this approach you will probably notice alternate ways to solve the same problem.

9.2 Subtyping Objects (Dynamic Dispatching)

One polymorphic feature missing from the Fortran 90 standard that is common to most object oriented languages is called run-time polymorphism or *dynamic dispatching*. (This feature is expected in Fortran 200X as an "extensible" function.) In the C++ language this ability is introduced in the so-called " virtual function". To emulate this ability is quite straightforward in F90 but is not elegant since it usually requires a group of if-elseif statements or other selection processes. It is only tedious if the inheritance hierarchy contains many unmodified subroutines and functions. The importance of the lack of a standardized dynamic dispatching depends on the problem domain to which it must be applied. For several applications demonstrated in the literature the alternate use of subtyping has worked quite well and resulted in programs that have been shown to run several times faster than equivalent C++ versions.

We implement dynamic dispatching in F90 by a process often called subtyping. Two features must be constructed to do this. First, a pointer object, which can point to any subtype member in an inheritance hierarchy, must be developed. Remember that F90 uses the operator '=>' to assign pointers to objects, and any object to be pointed at must have the TARGET attribute. Second, we must construct a (dynamic) dispatching mechanism to select the single appropriate procedure to execute at any time during the dynamic execution of the program. This step is done by checking which of the pointers actually points to an object and then passing that (unique) pointer to the corresponding appropriate procedure. In F90 the necessary checking can be carried out by using the ASSOCIATED intrinsic. Here, an if-elseif or other selection method is developed to serve as a dispatch mechanism to select the unique appropriate procedure to be executed based on the actual class referenced in the controlling pointer object. This subtyping process is also referred to as implementing a *polymorphic class*. Of course, the details of the actual dispatching process can be hidden from the procedures that utilize the polymorphic class. The polymorphic class knows only about the interfaces and data types defined in the hierarchy and nothing about how those procedures are implemented.

This process will be illustrated buy creating a specific polymorphic class, in this case called `Is_A_Member_Class`, which has polymorphic procedures named `new, assign`, and `display`. They will construct a new instance of the object, assign it a value, and list its components. The minimum example of such a process requires two members and is easily extended to any number of member classes. We begin by illustrating a short dynamic dispatching program and then defining each of the subtype classes of interest. The validation of this dynamic dispatching through a polymorphic class is shown in Fig. 9.1. There a target is declared for reach possible subtype and then each of them is constructed and sent on to the other polymorphic functions. The results clearly show that different display procedures were used depending on the class of object supplied as an argument. It is expected that the new Fortran 200X standard will allow such dynamic dispatching in a much simpler fashion.

The first subtype is a class, `Member_1_Class`, which has two real components and the encapsulated functionality to construct a new instance and another to accept a pointer to such a subtype and display related information. It is shown in Fig. 9.2. The next subtype class, `Member_2_Class`, has three components: two reals and one of type `Member_1`. It has the same sort of functionality, but clearly must act on more components. It has also inherited the functionally from the `Member_1_Class`; as displayed in Fig. 9.3.

The polymorphic class, `Is_A_Member_Class`, is shown in Fig. 9.4. It includes all of the encapsulated data and function's of the above two subtypes by including their `use` statements. The necessary pointer object is defined as an `Is_A_Member` type that has a unique pointer for each subtype member (two in this case). That is, at any given time during execution it will associate only one of the pointers in this list with an actual pointer object, and the other pointers are nullified. That is why this dispatching is referred to as "dynamic". It also defines a polymorphic interface to each of the common procedures to be applied to the various subtype objects. In the polymorphic function assign the dispatching is done very simply. First, all pointers to the family of subtypes are nullified, and then the unique pointer component

```
program main
use Is_A_Member_Class
implicit none

  type (Is_A_Member)      :: generic_member
  type (member_1), target :: pt_to_memb_1
  type (member_2), target :: pt_to_memb_2
  character(len=1) :: c

    c = 'A'
    call new (pt_to_memb_1, 1.0, 2.0)
    call assign (generic_member, pt_to_memb_1)
    call display_members (generic_member, c)

    c = 'B'
    call new (pt_to_memb_2, 1.0, 2.0, 3.0, 4.0)
    call assign (generic_member, pt_to_memb_2)
    call display_members (generic_member, c)

end program main
! running gives
! display_memb_1 A
! display_memb_2 B
```

Figure 9.1: Test of Dynamic Dispatching

```
Module Member_1_Class
 implicit none
  type member_1
    real :: real_1, real_2
  end type member_1

contains

  subroutine new_member_1 (member, a, b)
    real, intent(in) :: a, b
    type (member_1)  :: member
      member%real_1 = a ; member%real_2 = b
  end subroutine new_member_1

  subroutine display_memb_1  (pt_to_memb_1, c)
    type (member_1), pointer :: pt_to_memb_1
    character(len=1),   intent(in) :: c
     print *, 'display_memb_1 ', c
  end subroutine display_memb_1

End Module Member_1_Class
```

Figure 9.2: The First Subtype Class Member

to the subtype of interest is set to point to the desired member. The dispatching process for the display procedure is different. It requires an if-elseif construct that contains calls to all of the possible subtype members (two here) and a failsafe default state to abort the process or undertake the necessary exception handling. Since all but one of the subtype pointer objects have been nullified it employs the ASSOCIATED intrinsic function to select the one, and only, procedure to call and passes the pointer object on to that procedure. In F90 a pointer can be nullified by using the NULLIFY statement, while F95 allows the alternative of pointing at the intrinsic NULL function with returns a disassociated pointer. The NULL function can also be used to define the initial association status of a pointer at the point it is declared. That is a better programming style.

The are other approaches for implementing the dynamic dispatching concepts. Several examples are give in the publications by the group Decyk, Norton, and Szymanski (1995, 1997, 1999) and on Prof. Szymanski's Web site.

9.3 Non-standard Features

Elsewhere in this work only features of Fortran included in the 1995 standard have been utilized. It is common for compiler developers to provide addition enhancements, that are hardware or environment specific, and for the most useful of those features to appear in the next standard release. Compiler releases by Cray © Digitial © and Silicon Graphics © computers are examples of versions with extensive enhancements. Some compilers, like the Digitial © Visual Fortran © are designed to develop applications

```
Module Member_2_Class
 Use Member_1_class
  implicit none
  type member_2
    type (member_1)  :: r_1_2
    real :: real_3, real_4
  end type member_2

contains

  subroutine new_member_2 (member, a, b, c, d)
    real, intent(in) :: a, b, c, d
    type (member_2)  :: member
      call new_member_1 (member%r_1_2, a, b)
      member%real_3 = c ; member%real_4 = d
  end subroutine new_member_2

  subroutine display_memb_2  (pt_to_memb_2, c)
    type (member_2), pointer :: pt_to_memb_2
    character(len=1),   intent(in) :: c
      print *, 'display_memb_2 ', c
  end subroutine display_memb_2

End Module Member_2_Class
```

Figure 9.3: The Second Subtype Class Member

for the Microsoft © Windows © system and contain library modules for "standard" graphical displays via QuickWin © for dialog routines to the Graphical User Interface (GUI), for interfacing with multiple programming languages or the operation system, and for multiple "thread" operations. Threads are not currently in the F90 standard. They allow for response to the user interaction with any of a set of multiple buttons or dials in an active GUI.

Fortran 90 is a subset of the High Performance Fortran (HPF) standard that has been developed for use on massively parallel computers. We have not discussed those enhancements.

Even without these special enhancements the OOP abilities of F90 provide an important tool in engineering and scientific programming. In support of that position we close with a quote from computer scientist Professor Boleslaw K. Szymanski's Web page on High Performance Object-Oriented Programming in Fortran 90 where his group concludes: "All of our Fortran 90 programs execute more quickly than the equivalent C++ versions, yet the abstraction modeling capabilities that we needed were comparably powerful."

```
Module Is_A_Member_Class
Use Member_1_Class ; Use Member_2_Class
 implicit none

  type Is_A_Member
    private
    type (member_1), pointer :: pt_to_memb_1
    type (member_2), pointer :: pt_to_memb_2 ! etc for others
  end type Is_A_Member

  interface new
    module procedure new_member_1
    module procedure new_member_2 ! etc for others
  end interface

  interface assign
    module procedure assign_memb_1
    module procedure assign_memb_2 ! etc for others
  end interface

  interface display
    module procedure display_memb_1
    module procedure display_memb_2 ! etc for others
  end interface

contains

  subroutine assign_memb_1 (Family, member)
   type (member_1), target, intent(in)  :: member
   type (Is_A_Member),      intent(out) :: Family
     call nullify_Is_A_Member (Family) ! nullify all
     Family%pt_to_memb_1 => member
  end subroutine assign_memb_1

  subroutine assign_memb_2 (Family, member)
   type (member_2), target, intent(in)  :: member
   type (Is_A_Member),      intent(out) :: Family
     call nullify_Is_A_Member (Family) ! nullify all
     Family%pt_to_memb_2 => member
  end subroutine assign_memb_2 ! etc for others

  subroutine nullify_Is_A_Member (Family)
    type (Is_A_Member), intent(inout) :: Family
      nullify (Family%pt_to_memb_1)
      nullify (Family%pt_to_memb_2) ! etc for others
  end subroutine nullify_Is_A_Member

  subroutine display_members (A_Member, c)
    type (Is_A_Member), intent(in) :: A_Member
    character(len=1),   intent(in) :: c

  ! select the one proper member
      if     ( associated (A_Member%pt_to_memb_1) ) then
             call display (A_Member%pt_to_memb_1, c)
      else if ( associated (A_Member%pt_to_memb_2) ) then
             call display (A_Member%pt_to_memb_2, c) ! etc for others
      else ! default case
        stop 'Error, no member defined in Is_A_Member_Class'
      end if
  end subroutine display_members
End Module Is_A_Member_Class
```

Figure 9.4: The Polymorphic Class for Subtypes

Appendix A

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Appendix B

Fortran 90 Overview

This overview of Fortran 90 (F90) features is presented as a series of tables that illustrate the syntax and abilities of F90. Frequently comparisons are made to similar features in the C++ and F77 languages and to the Matlab environment.

These tables show that F90 has significant improvements over F77 and matches or exceeds newer software capabilities found in C++ and Matlab for dynamic memory management, user defined data structures, matrix operations, operator definition and overloading, intrinsics for vector and parallel processors and the basic requirements for object-oriented programming.

They are intended to serve as a condensed quick reference guide for programming in F90 and for understanding programs developed by others.

B.1 List of Language Tables

Language	Syntax	Location
MATLAB	`% comment (to end of line)`	anywhere
C	`/*comment*/`	anywhere
F90	`!  comment (to end of line)`	anywhere
F77	`* comment (to end of line)`	column 1

Table B.1: Comment syntax.

Storage	MATLAB[a]	C++	F90	F77
byte		`char`	`character::`	`character`
integer		`int`	`integer::`	`integer`
single precision		`float`	`real::`	`real`
double precision		`double`	`real*8::`	`double precision`
complex		[b]	`complex::`	`complex`
Boolean		`bool`	`logical::`	`logical`
argument			`parameter::`	`parameter`
pointer		`*`	`pointer::`	
structure		`struct`	`type::`	

[a] MATLAB4 requires no variable type declaration; the only two distinct types in MATLAB are strings and reals (which include complex). Booleans are just 0s and 1s treated as reals. MATLAB5 allows the user to select more types.

[b] There is no specific data type for a complex variable in C++; they must be created by the programmer.

Table B.2: Intrinsic data types of variables.

Description	MATLAB[a]	C++	Fortran[b]
addition	`+`	`+`	`+`
subtraction[c]	`-`	`-`	`-`
multiplication	`*` and `.*`	`*`	`*`
division	`/` and `./`	`/`	`/`
exponentiation	`^` and `.^`	pow[d]	`**`
remainder		`%`	
increment		`++`	
decrement		`--`	
parentheses (expression grouping)	`()`	`()`	`()`

[a] When doing arithmetic operations on matrices in MATLAB, a period ('`.`') must be put before the operator if scalar arithmetic is desired. Otherwise, MATLAB assumes matrix operations; figure out the difference between '`*`' and '`.*`'. Note that since matrix and scalar addition coincide, no '`.+`' operator exists (same holds for subtraction).

[b] Fortran 90 allows the user to change operators and to define new operator symbols.

[c] In all languages the minus sign is used for negation (i.e., changing sign).

[d] In C++ the exponentiation x^y is calculated by function *pow* (x, y).

Table B.3: Arithmetic operators.

<table>
<tr><th>Description</th><th>MATLAB</th><th>C++</th><th>F90</th><th>F77</th></tr>
<tr><td>Equal to</td><td>==</td><td>==</td><td>==</td><td>.EQ.</td></tr>
<tr><td>Not equal to</td><td>~=</td><td>!=</td><td>/=</td><td>.NE.</td></tr>
<tr><td>Less than</td><td><</td><td><</td><td><</td><td>.LT.</td></tr>
<tr><td>Less or equal</td><td><=</td><td><=</td><td><=</td><td>.LE.</td></tr>
<tr><td>Greater than</td><td>></td><td>></td><td>></td><td>.GT.</td></tr>
<tr><td>Greater or equal</td><td>>=</td><td>>=</td><td>>=</td><td>.GE.</td></tr>
<tr><td>Logical NOT</td><td>~</td><td>!</td><td>.NOT.</td><td>.NOT.</td></tr>
<tr><td>Logical AND</td><td>&</td><td>&&</td><td>.AND.</td><td>.AND.</td></tr>
<tr><td>Logical inclusive OR</td><td>!</td><td>||</td><td>.OR.</td><td>.OR.</td></tr>
<tr><td>Logical exclusive OR</td><td>xor</td><td></td><td>.XOR.</td><td>.XOR.</td></tr>
<tr><td>Logical equivalent</td><td>==</td><td>==</td><td>.EQV.</td><td>.EQV.</td></tr>
<tr><td>Logical not equivalent</td><td>~=</td><td>!=</td><td>.NEQV.</td><td>.NEQV.</td></tr>
</table>

Table B.4: Relational operators (arithmetic and logical).

<table>
<tr><th>MATLAB Operators</th><th>C++ Operators</th><th>F90 Operators[a]</th><th>F77 Operators</th></tr>
<tr><td>()</td><td>() [] -> .</td><td>()</td><td>()</td></tr>
<tr><td>+ -</td><td>! ++ -- +
- * & (type)
sizeof</td><td>**</td><td>**</td></tr>
<tr><td>* /</td><td>* / %</td><td>* /</td><td>* /</td></tr>
<tr><td>+ -[b]</td><td>+ -[b]</td><td>+ -[b]</td><td>+ -[b]</td></tr>
<tr><td>< <= > >=</td><td><< >></td><td>//</td><td>//</td></tr>
<tr><td>== ~=</td><td>< <= > =></td><td>== /= < <= >
>=</td><td>.EQ. .NE.
.LT. .LE.
.GT. .GE.</td></tr>
<tr><td>~</td><td>== !=</td><td>.NOT.</td><td>.NOT.</td></tr>
<tr><td>&</td><td>&&</td><td>.AND.</td><td>.AND.</td></tr>
<tr><td>|</td><td>||</td><td>.OR.</td><td>.OR.</td></tr>
<tr><td>=</td><td>|</td><td>.EQV. .NEQV.</td><td>.EQV. .NEQV.</td></tr>
<tr><td></td><td>?:</td><td></td><td></td></tr>
<tr><td></td><td>= += -= *= /=
%= &= ^= |=
<<= >>=</td><td></td><td></td></tr>
<tr><td></td><td>,</td><td></td><td></td></tr>
</table>

[a] User-defined unary (binary) operators have the highest (lowest) precedence in F90.
[b] These are binary operators representing addition and subtraction. Unary operators + and - have higher precedence.

Table B.5: Precedence pecking order.

B = Beginning, E = Ending, I = Increment

Syntax	F90	MATLAB
Default	B:E:I	B:I:E
$\geq$ B	B:	B:
$\leq$ E	:E	:E
Full range	:	:

Use	F90	MATLAB
Array subscript ranges	yes	yes
Character positions in a string	yes	yes
Loop control	no	yes
Array element generation	no	yes

Table B.6: Colon Operator Syntax and its Applications.

Description	MATLAB	C++	F90	F77
exponential	`exp(x)`	`exp(x)`	`exp(x)`	`exp(x)`
natural log	`log(x)`	`log(x)`	`log(x)`	`log(x)`
base 10 log	`log10(x)`	`log10(x)`	`log10(x)`	`log10(x)`
square root	`sqrt(x)`	`sqrt(x)`	`sqrt(x)`	`sqrt(x)`
raise to power (x^r)	`x.^r`	`pow(x,r)`	`x**r`	`x**r`
absolute value	`abs(x)`	`fabs(x)`	`abs(x)`	`abs(x)`
smallest integer>x	`ceil(x)`	`ceil(x)`	`ceiling(x)`	
largest integer<x	`floor(x)`	`floor(x)`	`floor(x)`	
division remainder	`rem(x,y)`	`fmod(x,y)`	`mod(x,y)`[a]	`mod(x,y)`
modulo			`modulo(x,y)`[a]	
complex conjugate	`conj(z)`		`conjg(z)`	`conjg(z)`
imaginary part	`imag(z)`		`imag(z)`	`aimag(z)`
drop fraction	`fix(x)`		`aint(x)`	`aint(x)`
round number	`round(x)`		`nint(x)`	`nint(x)`
cosine	`cos(x)`	`cos(x)`	`cos(x)`	`cos(x)`
sine	`sin(x)`	`sin(x)`	`sin(x)`	`sin(x)`
tangent	`tan(x)`	`tan(x)`	`tan(x)`	`tan(x)`
arc cosine	`acos(x)`	`acos(x)`	`acos(x)`	`acos(x)`
arc sine	`asin(x)`	`asin(x)`	`asin(x)`	`asin(x)`
arc tangent	`atan(x)`	`atan(x)`	`atan(x)`	`atan(x)`
arc tangent[b]	`atan2(x,y)`	`atan2(x,y)`	`atan2(x,y)`	`atan2(x,y)`
hyperbolic cosine	`cosh(x)`	`cosh(x)`	`cosh(x)`	`cosh(x)`
hyperbolic sine	`sinh(x)`	`sinh(x)`	`sinh(x)`	`sinh(x)`
hyperbolic tangent	`tanh(x)`	`tanh(x)`	`tanh(x)`	`tanh(x)`
hyperbolic arc cosine	`acosh(x)`			
hyperbolic arc sine	`asinh(x)`			
hyperbolic arctan	`atanh(x)`			

[a] Differ for $x < 0$.

[b] `atan2(x,y)` is used to calculate the arc tangent of x/y in the range $[-\pi, +\pi]$. The one-argument function `atan(x)` computes the arc tangent of x in the range $[-\pi/2, +\pi/2]$.

Table B.7: Mathematical functions.

Description	**C++**	**F90**	**F77**	**MATLAB**
Conditionally execute statements	`if` `{ }`	`if` `end if`	`if` `end if`	`if` `end`
Loop a specific number of times	`for k=1:n` `{ }`	`do k=1,n` `end do`	`do # k=1,n` `# continue`	`for k=1:n` `end`
Loop an indefinite number of times	`while` `{ }`	`do while` `end do`	— —	`while` `end`
Terminate and exit loop	`break`	`exit`	`go to`	`break`
Skip a cycle of loop	`continue`	`cycle`	`go to`	—
Display message and abort	`error()`	`stop`	`stop`	`error`
Return to invoking function	`return`	`return`	`return`	`return`
Conditional array action	—	`where`	—	`if`
Conditional alternate statements	`else` `else if`	`else` `elseif`	`else` `elseif`	`else` `elseif`
Conditional array alternatives	— —	`elsewhere` —	— —	`else` `elseif`
Conditional case selections	`switch { }`	`select case` `end select`	`if` `end if`	`if` `end`

Table B.8: Flow Control Statements.

Loop	**MATLAB**	**C++**	**Fortran**
Indexed loop	`for index=matrix` *`statements`* `end`	`for (init;test;inc)` `{` *`statements`* `}`	`do index=b,e,i` *`statements`* `end do`
Pre-test loop	`while test` *`statements`* `end`	`while (test) {` *`statements`* `}`	`do while (test)` *`statements`* `end do`
Post-test loop		`do {` *`statements`* `} while (test)`	`do` *`statements`* `if (test) exit` `end do`

Table B.9: Basic loop constructs.

MATLAB	Fortran	C++
if l_expression *true group* end	IF (l_expression) THEN *true group* END IF	if (l_expression) { *true group;* }
	IF (l_expression) *true statement*	if (l_expression) *true statement;*

Table B.10: IF Constructs. The quantity l_expression means a logical expression having a value that is either TRUE of FALSE. The term *true statement* or *true group* means that the statement or group of statements, respectively, are executed if the conditional in the if statement evaluates to TRUE.

MATLAB	Fortran	C++
if l_expression1 *true group A* if l_expression2 *true group B* end *true group C* end *statement group D*	IF (l_expression1) THEN *true group A* IF (l_expression2) THEN *true group B* END IF *true group C* END IF *statement group D*	if (l_expression1) { true group A if (l_expression2) { *true group B* } *true group C* } *statement group D*

Table B.11: Nested IF Constructs.

MATLAB	Fortran	C++
if l_expression *true group A* else *false group B* end	IF (l_expression) THEN *true group A* ELSE *false group B* END IF	if (l_expression) { *true group A* } else { *false group B* }

Table B.12: Logical IF-ELSE Constructs.

MATLAB	Fortran	C++
if l_expression1 *true group A* elseif l_expression2 *true group B* elseif l_expression3 *true group C* else *default group D* end	IF (l_expression1) THEN *true group A* ELSE IF (l_expression2) THEN *true group B* ELSE IF (l_expression3) THEN *true group C* ELSE *default group D* END IF	if (l_expression1) { *true group A* } else if (l_expression2) { *true group B* } else if (l_expression3) { *true group C* } else { *default group D* }

Table B.13: Logical IF-ELSE-IF Constructs.

F90	C++
`SELECT CASE (expression)` `  CASE (value 1)` `    group 1` `  CASE (value 2)` `    group 2` `      :` `      :` `  CASE (value n)` `    group n` `  CASE DEFAULT` `    default group` `END SELECT`	`switch (expression)` `  {` `    case value 1 :` `      group 1` `      break;` `    case value 2 :` `      group 2` `      break;` `        :` `        :` `    case value n :` `      group n` `      break;` `    default:` `      default group` `      break;` `  }`

Table B.14: Case Selection Constructs.

F90 Named `IF`	F90Named `SELECT`
`name: IF (logical_1) THEN` `  true group A` `ELSE IF (logical_2) THEN` `  true group B` `ELSE` `  default group C` `ENDIF name`	`name: SELECT CASE (expression)` `  CASE (value 1)` `    group 1` `  CASE (value 2)` `    group 2` `  CASE DEFAULT` `    default group` `  END SELECT name`

Table B.15: F90 Optional Logic Block Names.

Fortran	C++
`   DO 1 ...` `     DO 2 ...` `       ...` `       IF (disaster) THEN` `         GO TO 3` `       END IF` `       ...` ` 2  END DO` ` 1 END DO` ` 3 next statement`	`for (...) {` `  for (...) {` `    ...` `    if (disaster)` `      go to error` `    ...` `  }` `}` `error:`

Table B.16: `GO TO` Break-out of Nested Loops. This situation can be an exception to the general recommendation to avoid `GO TO` statements.

F77	F90	C++
`   DO 1 I = 1,N` `     ...` `     IF (skip condition) THEN` `       GO TO 1` `     ELSE` `       false group` `     END IF` ` 1 continue`	`DO I = 1,N` `  ...` `  IF (skip condition) THEN` `    CYCLE ! to next I` `  ELSE` `    false group` `  END IF` `END DO`	`for (i=1; i<n; i++)` `  {` `  if (skip condition)` `    continue; // to next` `  else if` `    false group` `  end` `  }`

Table B.17: Skip a Single Loop Cycle.

F77	F90	C++
DO 1 I = 1,N IF (exit condition) THEN GO TO 2 ELSE *false group* END IF 1 CONTINUE 2 *next statement*	DO I = 1,N IF (exit condition) THEN EXIT ! this do ELSE *false group* END IF END DO *next statement*	for (i=1; i<n; i++) { if (exit condition) break;// out of loop else if *false group* end } *next statement*

Table B.18: Abort a Single Loop.

```
main: DO ! forever
  test: DO k=1,k_max
    third: DO m=m_max,m_min,-1
      IF (test condition) THEN
        CYCLE test ! loop on k
      END IF
    END DO third ! loop on m
    fourth: DO n=n_min,n_max,2
      IF (main condition) THEN
        EXIT main ! forever loop
    END DO fourth ! on n
  END DO test ! over k
END DO main

next statement
```

Table B.19: F90 `DO`s Named for Control.

MATLAB	C++
initialize test while l_expression true group change test end	*initialize test* while (l_expression) { *true group* *change test* }

F77	F90
initialize test # continue IF (l_expression) THEN *true group* *change test* go to # END IF	initialize test do while (l_expression) *true group* *change test* end do

Table B.20: Looping While a Condition is True.

Function Type	MATLAB[a]	C++	Fortran
program	*statements* `[y1...yn]=f(a1,...,am)` `[end of file]`	`main(argc,char **argv)` `{` *statements* `y = f(a1,I,am);` `}`	`program main` `type y` `type a1,...,type am` *statements* `y = f(a1,...,am)` `call s(a1,...,am)` `end program`
subroutine		`void f` `(type a1,...,type am)` `{` *statements* `}`	`subroutine s(a1,...,am)` `type a1,...,type am` *statements* `end`
function	`function [r1...rn]` `=f(a1,...,am)` *statements*	type f (type a1,...,type am) { *statements* }	`function f(a1,...,am)` `type f` `type a1,...,type am` *statements* `end`

[a] Every function or program in MATLAB must be in separate files.

Table B.21: Function definitions. In each case, the function being defined is named `f` and is called with `m` arguments `a1,...,am`.

One-Input, One-Result Procedures	
MATLAB	`function out = name (in)`
F90	`function name (in) !  name = out`
	`function name (in) result (out)`
C++	`name (in, out)`

Multiple-Input, Multiple-Result Procedures	
MATLAB	`function [inout, out2] = name (in1, in2, inout)`
F90	`subroutine name (in1, in2, inout, out2)`
C++	`name(in1, in2, inout, out2)`

Table B.22: Arguments and return values of subprograms.

Global Variable Declaration	
MATLAB	`global` list of variables
F77	`common` /set_name/ list of variables
F90	`module` set_name `save` `type` (type_tag) :: list of variables `end module` set_name
C++	`extern` list of variables

Access to Global Variables	
MATLAB	`global` list of variables
F77	`common` /set_name/ list of variables
F90	`use` set_name, `only` subset of variables `use` set_name2 list of variables
C++	`extern` list of variables

Table B.23: Defining and referring to global variables.

Action	C++	F90
Bitwise AND	&	`iand`
Bitwise exclusive OR	∧	`ieor`
Bitwise exclusive OR	|	`ior`
Circular bit shift		`ishftc`
Clear bit		`ibclr`
Combination of bits		`mvbits`
Extract bit		`ibits`
Logical complement	∼	`not`
Number of bits in integer	`sizeof`	`bit_size`
Set bit		`ibset`
Shift bit left	≪	`ishft`
Shift bit right	≫	`ishft`
Test on or off		`btest`
Transfer bits to integer		`transfer`

Table B.24: Bit Function Intrinsics.

0	NUL	1	SOH	2	STX	3	ETX	4	EOT	5	ENQ	6	ACK	7	BEL
8	BS	9	HT	10	NL	11	VT	12	NP	13	CR	14	SO	15	SI
16	DLE	17	DC1	18	DC2	19	DC3	20	DC4	21	NAK	22	SYN	23	ETB
24	CAN	25	EM	26	SUB	27	ESC	28	FS	29	GS	30	RS	31	US
32	SP	33	!	34	"	35	#	36	$	37	%	38	&	39	’
40	(	41	)	42	*	43	+	44	,	45	-	46	.	47	/
48	0	49	1	50	2	51	3	52	4	53	5	54	6	55	7
56	8	57	9	58	:	59	;	60	<	61	=	62	>	63	?
64	@	65	A	66	B	67	C	68	D	69	E	70	F	71	G
72	H	73	I	74	J	75	K	76	L	77	M	78	N	79	O
80	P	81	Q	82	R	83	S	84	T	85	U	86	V	87	W
88	X	89	Y	90	Z	91	[	92	\	93	]	94	ˆ	95	_
96	‘	97	a	98	b	99	c	100	d	101	e	102	f	103	g
104	h	105	i	106	j	107	k	108	l	109	m	110	n	111	o
112	p	113	q	114	r	115	s	116	t	117	u	118	v	119	w
120	x	121	y	122	z	123	{	124	|	125	}	126	˜	127	DEL

Table B.25: The ACSII Character Set.

ACHAR (I)	Character number I in ASCII collating set
ADJUSTL (STRING)	Adjust left
ADJUSTR (STRING)	Adjust right
CHAR (I) *	Character I in processor collating set
IACHAR (C)	Position of C in ASCII collating set
ICHAR (C)	Position of C in processor collating set
INDEX (STRING, SUBSTRING)[a]	Starting position of a substring
LEN (STRING)	Length of a character entity
LEN_TRIM (STRING)	Length without trailing blanks
LGE (STRING_A, STRING_B)	Lexically greater than or equal
LGT (STRING_A, STRING_B)	Lexically greater than
LLE (STRING_A, STRING_B)	Lexically less than or equal
LLT (STRING_A, STRING_B)	Lexically less than
REPEAT (STRING, NCOPIES)	Repeated concatenation
SCAN (STRING, SET)[a]	Scan a string for a character in a set
TRIM (STRING)	Remove trailing blank characters
VERIFY (STRING, SET)[a]	Verify the set of characters in a string
STRING_A//STRING_B	Concatenate two strings

[a] Optional arguments not shown.

Table B.26: F90 Character Functions.

Action	*ASCII Character*	F90 *Input*[a]	*C++ Input*
Alert (Bell)	7	Ctrl-G	\a
Backspace	8	Ctrl-H	\b
Carriage Return	13	Ctrl-M	\r
End of Transmission	4	Ctrl-D	Ctrl-D
Form Feed	12	Ctrl-L	\f
Horizontal Tab	9	Ctrl-I	\t
New Line	10	Ctrl-J	\n
Vertical Tab	11	Ctrl-K	\v

[a] "Ctrl-" denotes control action. That is, simultaneous pressing of the CONTROL key *and* the letter following.

Table B.27: How to type non-printing characters.

C, C++	`Variable.component.sub_component`
F90	`Variable%component%sub_component`

Table B.28: Referencing Structure Components.

C, C++	<pre>struct data_tag { intrinsic_type_1 component_names; intrinsic_type_2 component_names; } ;</pre>
F90	<pre>type data_tag intrinsic_type_1 :: component_names; intrinsic_type_2 :: component_names; end type data_tag</pre>

Table B.29: Defining New Types of Data Structure.

C, C++	<pre>struct data_tag { intrinsic_type_1 component_names; struct tag_2 component_names; } ;</pre>
F90	<pre>type data_tag intrinsic_type :: component_names; type (tag_2) :: component_names; end type data_tag</pre>

Table B.30: Nested Data Structure Definitions.

C, C++	<pre>struct data_tag variable_list; /* Definition */ struct data_tag variable = {component_values}; /* Initialization */ variable.component.sub_component = value; /* Assignment */</pre>
F90	<pre>type (data_tag) :: variable_list ! Definition variable = data_tag (component_values) ! Initialization variable%component%sub_component = value ! Assignment</pre>

Table B.31: Declaring, initializing, and assigning components of user-defined datatypes.

```
INTEGER, PARAMETER ::  j_max = 6
TYPE meaning_demo
    INTEGER, PARAMETER ::  k_max = 9, word = 15
    CHARACTER (LEN = word) ::  name(k_max)
END TYPE meaning_demo
TYPE (meaning_demo) derived(j_max)
```

Construct	**Interpretation**
`derived`	All components of all `derived`'s elements
`derived(j)`	All components of j^{th} element of `derived`
`derived(j)%name`	All `k_max` components of `name` within j^{th} element of `derived`
`derived%name(k)`	Component `k` of the `name` array for all elements of `derived`
`derived(j)%name(k)`	Component `k` of the `name` array of j^{th} element of `derived`

Table B.32: F90 Derived Type Component Interpretation.

	C++	**F90**
Declaration	`type_tag *pointer_name;`	`type (type_tag), pointer :: pointer_name`
Target	`&target_name`	`type (type_tag), target :: target_name`
Examples	`char *cp, c;` `int *ip, i;` `float *fp, f;` `cp = & c;` `ip = & i;` `fp = & f;`	`character, pointer :: cp` `integer, pointer :: ip` `real, pointer :: fp` `cp => c` `ip => i` `fp => f`

Table B.33: Definition of pointers and accessing their targets.

C, C++	`pointer_name = NULL`
F90	`nullify (list_of_pointer_names)`
F95	`pointer_name = NULL()`

Table B.34: Nullifing a Pointer to Break Association with Target.

Purpose	**F90**	**MATLAB**
Form subscripts	( )	( )
Separates subscripts & elements	,	,
Generates elements & subscripts	:	:
Separate commands	;	;
Forms arrays	(/ /)	[ ]
Continue to new line	&	...
Indicate comment	!	%
Suppress printing	default	;

Table B.35: Special Array Characters.

Description	*Equation*	*Fortran90 Operator*	*Matlab Operator*	*Original Sizes*	*Result Size*
Scalar plus scalar	$c = a \pm b$	$c = a \pm b$	$c = a \pm b;$	$1, 1$	$1, 1$
Element plus scalar	$c_{jk} = a_{jk} \pm b$	$c = a \pm b$	$c = a \pm b;$	m, n and $1, 1$	m, n
Element plus element	$c_{jk} = a_{jk} \pm b_{jk}$	$c = a \pm b$	$c = a \pm b;$	m, n and m, n	m, n
Scalar times scalar	$c = a \times b$	$c = a * b$	$c = a * b;$	$1, 1$	$1, 1$
Element times scalar	$c_{jk} = a_{jk} \times b$	$c = a * b$	$c = a * b;$	m, n and $1, 1$	m, n
Element times element	$c_{jk} = a_{jk} \times b_{jk}$	$c = a * b$	$c = a. * b;$	m, n and m, n	m, n
Scalar divide scalar	$c = a/b$	$c = a/b$	$c = a/b;$	$1, 1$	$1, 1$
Scalar divide element	$c_{jk} = a_{jk}/b$	$c = a/b$	$c = a/b;$	m, n and $1, 1$	m, n
Element divide element	$c_{jk} = a_{jk}/b_{jk}$	$c = a/b$	$c = a./b;$	m, n and m, n	m, n
Scalar power scalar	$c = a^b$	$c = a{*}{*}b$	$c = a \wedge b;$	$1, 1$	$1, 1$
Element power scalar	$c_{jk} = a_{jk}^b$	$c = a{*}{*}b$	$c = a \wedge b;$	m, n and $1, 1$	m, n
Element power element	$c_{jk} = a_{jk}^{b_{jk}}$	$c = a{*}{*}b$	$c = a. \wedge b;$	m, n and m, n	m, n
Matrix transpose	$C_{kj} = A_{jk}$	$C = \mathrm{transpose}\ (A)$	$C = A';$	m, n	n, m
Matrix times matrix	$C_{ij} = \sum_k A_{ik} B_{kj}$	$C = \mathrm{matmul}(A, B)$	$C = A * B;$	m, r and r, n	m, n
Vector dot vector	$c = \sum_k A_k B_k$	$c = \mathrm{sum}(A * B)$	$c = \mathrm{sum}(A. * B);$	$m, 1$ and $m, 1$	$1, 1$
		$c = \mathrm{dot\_product}(A, B)$	$c = A * B';$	$m, 1$ and $m, 1$	$1, 1$

Table B.36: Array Operations in Programming Constructs. Lower case letters denote scalars or scalar elements of arrays. Matlab arrays are allowed a maximum of two subscripts while Fortran allows seven. Upper case letters denote matrices or scalar elements of matrices.

Table B.37: Equivalent Fortran90 and MATLAB Intrinsic Functions.
The following KEY symbols are utilized to denote the TYPE of the intrinsic function, or subroutine, and its arguments: A-complex, integer, or real; I-integer; L-logical; M-mask (logical); R-real; X-real; Y-real; V-vector (rank 1 array); and Z-complex. Optional arguments are not shown. Fortran 90 and MATLAB also have very similar array operations and colon operators.

Type	**Fortran90**	**MATLAB**	**Brief Description**
A	ABS(A)	abs(a)	Absolute value of A.
R	ACOS(X)	acos(x)	Arc cosine function of real X.
R	AIMAG(Z)	imag(z)	Imaginary part of complex number.
R	AINT(X)	real(fix(x))	Truncate X to a real whole number.
L	ALL(M)	all(m)	True if all mask elements, M, are true.
R	ANINT(X)	real(round(x))	Real whole number nearest to X.
L	ANY(M)	any(m)	True if any mask element, M, is true.
R	ASIN(X)	asin(x)	Arcsine function of real X.
R	ATAN(X)	atan(x)	Arctangent function of real X.
R	ATAN2(Y,X)	atan2(y,x)	Arctangent for complex number(X, Y).
I	CEILING(X)	ceil(x)	Least integer >= real X.
Z	CMPLX(X,Y)	(x+yi)	Convert real(s) to complex type.
Z	CONJG(Z)	conj(z)	Conjugate of complex number Z.
R	COS(R_Z)	cos(r_z)	Cosine of real or complex argument.
R	COSH(X)	cosh(x)	Hyperbolic cosine function of real X.
I	COUNT(M)	sum(m==1)	Number of true mask, M, elements.
R,L	DOT_PRODUCT(X,Y)	x'⋆y	Dot product of vectors X and Y.
R	EPSILON(X)	eps	Number, like X, $\ll 1$.
R,Z	EXP(R_Z)	exp(r_z)	Exponential of real or complex number.
I	FLOOR(X)	floor	Greatest integer $\leq$ X.
R	HUGE(X)	realmax	Largest number like X.
I	INT(A)	fix(a)	Convert A to integer type.
R	LOG(R_Z)	log(r_z)	Logarithm of real or complex number.
R	LOG10(X)	log10(x)	Base 10 logarithm function of real X.
R	MATMUL(X,Y)	x⋆y	Conformable matrix multiplication, X*Y.
I,V	I=MAXLOC(X)	[y,i]=max(x)	Location(s) of maximum array element.
R	Y=MAXVAL(X)	y=max(x)	Value of maximum array element.
I,V	I=MINLOC(X)	[y,i]=min(x)	Location(s) of minimum array element.
R	Y=MINVAL(X)	y=min(x)	Value of minimum array element.
I	NINT(X)	round(x)	Integer nearest to real X.
A	PRODUCT(A)	prod(a)	Product of array elements.
call	RANDOM_NUMBER(X)	x=rand	Pseudo-random numbers in $(0, 1)$.
call	RANDOM_SEED	rand('seed')	Initialize random number generator.
R	REAL (A)	real(a)	Convert A to real type.
R	RESHAPE(X, (/ I, I2 /))	reshape(x, i, i2)	Reshape array X into I×I2 array.
I,V	SHAPE(X)	size(x)	Array (or scalar) shape vector.
R	SIGN(X,Y)		Absolute value of X times sign of Y.
R	SIGN(0.5,X)-SIGN(0.5,-X)	sign(x)	Signum, normalized sign, –1, 0, or 1.
R,Z	SIN(R_Z)	sin(r_z)	Sine of real or complex number.
R	SINH(X)	sinh(x)	Hyperbolic sine function of real X.
I	SIZE(X)	length(x)	Total number of elements in array X.
R,Z	SQRT(R_Z)	sqrt(r_z)	Square root, of real or complex number.
R	SUM(X)	sum(x)	Sum of array elements.

(continued)

Type	Fortran90	MATLAB	Brief Description
R	TAN(X)	tan(x)	Tangent function of real X.
R	TANH(X)	tanh(x)	Hyperbolic tangent function of real X.
R	TINY(X)	realmin	Smallest positive number like X.
R	TRANSPOSE(X)	x’	Matrix transpose of any type matrix.
R	X=1	x=ones(length(x))	Set all elements to 1.
R	X=0	x=zero(length(x))	Set all elements to 0.

For more detailed descriptions and example uses of these intrinsic functions see Adams, J.C., *et al.*, *Fortran 90 Handbook*, McGraw-Hill, New York, 1992, ISBN 0–07–000406–4.

B.2 Alphabetical Table of Fortran 90 Intrinsic Routines

The following KEY symbols are utilized to denote the TYPE of the intrinsic function, or subroutine, and its arguments: A-complex, integer, or real; B-integer bit; C-character; D-dimension; I-integer; K-kind; L-logical; M-mask (logical); N-integer, or real; P-pointer; R-real; S-string; T-target; V-vector (rank one array); X-real; Y-real; Z-complex; and *-any type. For more detailed descriptions and example uses of these intrinsic functions see Adams, J.C., et al., *Fortran 90 Handbook*, McGraw-Hill, New York, 1992, ISBN 0–07–000406–4.

C++	–	int	–	–	floor	ceil
F90	aint	int	anint	nint	floor	ceiling
MATLAB	real (fix)	fix	real (round)	round	floor	ceil
Argument	**Value of Result**					
–2.000	–2.0	–2	–2.0	–2	–2	–2
–1.999	–1.0	–1	–2.0	–2	–2	–1
–1.500	–1.0	–1	–2.0	–2	–2	–1
–1.499	–1.0	–1	–1.0	–1	–2	–1
–1.000	–1.0	–1	–1.0	–1	–1	–1
–0.999	0.0	0	–1.0	–1	–1	0
–0.500	0.0	0	–1.0	–1	–1	0
–0.499	0.0	0	0.0	0	–1	0
0.000	0.0	0	0.0	0	0	0
0.499	0.0	0	0.0	0	0	1
0.500	0.0	0	1.0	1	0	1
0.999	0.0	0	1.0	1	0	1
1.000	1.0	1	1.0	1	1	1
1.499	1.0	1	1.0	1	1	2
1.500	1.0	1	2.0	2	1	2
1.999	1.0	1	2.0	2	1	2
2.000	2.0	2	2.0	2	2	2

Table B.38: Truncating Numbers.

```
WHERE (logical_array_expression)
    true_array_assignments
ELSEWHERE
    false_array_assignments
END WHERE
```

```
WHERE (logical_array_expression) true_array_assignment
```

Table B.39: F90 `WHERE` Constructs.

Function	*Description*	*Opt*	*Example*
`all`	Find if all values are true, for a fixed dimension.	d	`all(B = A, DIM = 1)` (true, false, false)
`any`	Find if any value is true, for a fixed dimension.	d	`any (B > 2, DIM = 1)` (false, true, true)
`count`	Count number of true elements for a fixed dimension.	d	`count(A = B, DIM = 2)` (1, 2)
`maxloc`	Locate first element with maximum value given by mask.	m	`maxloc(A, A < 9)` (2, 3)
`maxval`	Max element, for fixed dimension, given by mask.	b	`maxval (B, DIM=1, B > 0)` (2, 4, 6)
`merge`	Pick true array, A, or false array, B, according to mask, L.	–	`merge(A, B, L)` $\begin{bmatrix} 0 & 3 & 5 \\ 2 & 4 & 8 \end{bmatrix}$
`minloc`	Locate first element with minimum value given by mask.	m	`minloc(A, A > 3)` (2, 2)
`minval`	Min element, for fixed dimension, given by mask.	b	`minval(B, DIM = 2)` (1, 2)
`pack`	Pack array, A, into a vector under control of mask.	v	`pack(A, B < 4)` (0, 7, 3)
`product`	Product of all elements, for fixed dimension, controlled by mask.	b	`product(B)` ; (720) `product(B, DIM = 1, T)` (2, 12, 30)
`sum`	Sum all elements, for fixed dimension, controlled by mask.	b	`sum(B)` ;(21) `sum(B, DIM = 2, T)` (9, 12)
`unpack`	Replace the true locations in array B controlled by mask L with elements from the vector U.	–	`unpack(U, L, B)` $\begin{bmatrix} 7 & 3 & 8 \\ 2 & 4 & 9 \end{bmatrix}$

$$A = \begin{bmatrix} 0 & 3 & 5 \\ 7 & 4 & 8 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix}, \quad L = \begin{bmatrix} T & F & T \\ F & F & T \end{bmatrix}, \quad U = (7, 8, 9)$$

Table B.40: F90 Array Operators with Logic Mask Control. T and F denote true and false, respectively. Optional arguments: `b -- DIM & MASK`, `d -- DIM`, `m -- MASK`, `v -- VECTOR` and `DIM = 1` implies for any rows, `DIM = 2` for any columns, and `DIM = 3` for any plane.

Type	**Intrinsic**	**Description**
A	ABS (A)	Absolute value of A.
C	ACHAR (I)	Character in position I of ASCII collating sequence.
R	ACOS (X)	Arc cosine (inverse cosine) function of real X.
C	ADJUSTL (S)	Adjust S left, move leading blanks to trailing blanks.
C	ADJUSTR (S)	Adjust S right, move trailing blanks to leading blanks.
R	AIMAG (Z)	Imaginary part of complex number, Z.
R	AINT (X [,K])	Truncate X to a real whole number, of the given kind.
L	ALL (M [,D])	True if all mask, M, elements are true, in dimension D.
L	ALLOCATED (*_ARRAY_P)	True if the array or pointer is allocated.

(continued)

Alphabetic Table of Fortran90 Intrinsic Functions (continued)

Type	Intrinsic	Description
R	ANINT (X [,K])	Real whole number nearest to X, of the given kind.
L	ANY (M [,D])	True if any mask, M, element is true, in dimension D.
R	ASIN (X)	Arcsine (inverse sine) function of real X.
L	ASSOCIATED (P [,T])	True if pointer, P, is associated with any target, or T.
R	ATAN (X)	Arctangent (inverse tangent) function of real X.
R	ATAN2 (Y,X)	Arctangent for argument of complex number (X, Y).
I	BIT_SIZE (I)	Maximum number of bits integer I can hold, e.g. 32.
L	BTEST (I,I_POS)	True if bit location I_POS of integer I has value 1.
I	CEILING (X)	Least integer $\geq$ real X, of the given kind.
C	CHAR (I [,K])	Character in position I of processor collating sequence.
Z	CMPLX (X [,Y][,K])	Convert real(s) to complex type, of given kind.
Z	CONJG (Z)	Conjugate of complex number Z.
R	COS (R_Z)	Cosine function of real or complex argument.
R	COSH (X)	Hyperbolic cosine function of real X.
I	COUNT (M [,D])	Number of true mask, M, elements, in dimension D.
⋆	CSHIFT (⋆_ARAY,I_SHIF [,D])	Circular shift out and in for I_SHIF elements.
call	DATE_AND_TIME ([S_DATE] [,S_TIME] [,S_ZONE] [,I_V_VALUES])	Real-time clock date, time, zone, and vector with year, month, day, UTC, hour, minutes, seconds, and milliseconds.
R	DBLE (A)	Convert A to double precision real.
N	DIGITS (N)	Number of significant digits for N, e.g. 31.
R	DIM (X,Y)	The difference, MAX (X – Y, 0.0).
N,L	DOT_PRODUCT (V,V_2)	Dot product of vectors V and V_2.
R	DPROD (X,Y)	Double precision real product of two real scalars.
⋆	EOSHIFT (⋆_ARRAY, I_SHIFT [,⋆_FILL][,D])	Perform vector end-off shift by ± I_shift terms, and fill, in dimension D.
R	EPSILON (X)	Number $\ll$ 1, for numbers like X, e.g. 2⋆⋆–23.
R,Z	EXP (R_Z)	Exponential function of real or complex argument.
I	EXPONENT (X)	Exponent part of the model for real X.
I	FLOOR (X)	Greatest integer less than or equal to X.
R	FRACTION (X)	Fractional part of the model for real X.
N	HUGE (N)	Largest number for numbers like N, e.g. 2⋆⋆128.
I	IACHAR (C)	Position of character C in ASCII collation.
B	IAND (I,I_2)	Logical AND on the bits of I and I_2.
B	IBCLR (I,I_POS)	Clear bit I_POS to zero in integer I.
B	IBITS (I,I_POS,I_LEN)	Extract an I_LEN sequence of bits at I_POS in I.
B	IBSET (I,I_POS)	Set bit I_POS to one in integer I.
I	ICHAR (C)	Position of character C in processor collation.
B	IEOR (I,I_2)	Exclusive OR on the bits of I and I_2.
I	INDEX (S,S_SUB [,L_BACK])	Left starting position of S_SUB within S (right).
I	INT (A [,K])	Convert A to integer type, of given kind.
B	IOR (I,I_2)	Inclusive OR on the bits of I and I_2.
B	ISHFT (I,I_SHIFT)	Logical shift of bits of I by I_SHIFT, pad with 0.
B	ISHFTC (I,I_SHIFT [,I_SIZE])	Logical circular shift of I_SIZE rightmost bits of I.
I	KIND (ANY)	Kind type integer parameter value for any argument.
I,V	LBOUND (⋆_ARRAY [,D])	ARRAY lower bound(s) vector, along dimension D.
I	LEN (S)	Total character string length.
I	LEN_TRIM (S)	Length of S without trailing blanks.
L	LGE (S,S_2)	True if S > or equal to S_2 in ASCII sequence.
L	LGT (S,S_2)	True if S follows S_2 in ASCII collating sequence.

(continued)

Alphabetic Table of Fortran90 Intrinsic Functions (continued)

Type	Intrinsic	Description
L	LLE (S,S_2)	True if S < or equal to S_2 in ASCII sequence.
L	LLT (S,S_2	True if S precedes S_2 in ASCII collating sequence.
R	LOG (R_Z)	Natural (base e) logarithm of real or complex number.
L	LOGICAL (L [,K])	Convert L to logical of kind K.
R	LOG10 (X)	Common (base 10) logarithm function of real X.
N,L	MATMUL (MATRIX,MATRIX_2)	Conformable matrix multiplication.
N	MAX (N,N_2 [,N_3,...])	Maximum value of two or more numbers same type.
I	MAXEXPONENT (X)	Maximum exponent for real numbers like X, e.g. 128.
I,V	MAXLOC (N_ARRAY [,M])	Location(s) of maximum ARRAY element, passing M.
N	MAXVAL (N_ARRAY [,D] [,M])	Maximum ARRAY term, in dimension D, passing M.
⋆	MERGE (⋆_TRUE,⋆_FALSE,M)	Use ⋆_TRUE when M is true; ⋆_FALSE otherwise.
N	MIN (N,N_2 [,N_3,...])	Minimum value of two or more same type numbers.
I	MINEXPONENT (X)	Minimum exponent for real numbers like X, e.g. –125.
I,V	MINLOC (N_ARRAY [,M])	Location(s) of minimum ARRAY term, passing M.
N	MINVAL (N_ARRAY [,D] [,M])	Minimum ARRAY term, in dimension D, passing M.
N	MOD (N,N_2)	Remainder for N_2. That is, N–INT(N/N_2)⋆N_2.
N	MODULO (N,N_2)	Modulo, that is, N–FLOOR(N/N_2)⋆N_2.
call	MVBITS (I_FROM,I_LOC, I_LEN,I_TO,I_POS)	Copy I_LEN bits at I_LOC in I_FROM to I_TO at I_POS.
R	NEAREST (X,Y)	Nearest number at X in the direction of sign Y.
I	NINT (X [,K])	Integer nearest to real X, of the stated kind.
I	NOT (I)	Logical complement of the bits of integer I.
⋆,V	PACK (⋆_ARRAY,M [,V_PAD])	Pack ARRAY at true M into vector, using V_PAD.
I	PRECISION (R_Z)	Decimal precision for a real or complex R_Z, e.g. 6.
L	PRESENT (OPTIONAL)	True if optional argument is present in call.
A	PRODUCT (A_ARRAY [,D] [,M])	Product of ARRAY elements, along D, for mask M.
I	RADIX (N)	Base of the model for numbers like N, e.g. 2.
call	RANDOM_NUMBER (X)	Pseudo-random numbers in range $0 < X < 1$.
call	RANDOM_SEED ([I_SIZE] [,I_V_PUT][,I_V_GET])	Initialize random number generator, defaults to processor initialization.
I	RANGE (A)	Decimal exponent range in the model for A, e.g. 37.
R	REAL (A [,K])	Convert A to real type, of type K.
S	REPEAT (S,I_COPIES)	Concatenates I_COPIES of string S.
⋆	RESHAPE (⋆_ARAY,I_V_SHAP [,⋆_PAD] [,V_ORDER])	Reshape ARAY, using vector SHAP, pad from an array, and re-order.
R	RRSPACING (X)	Relative spacing reciprocal of numbers near X.
R	SCALE (X,I)	Return X times b⋆⋆I, for base of b = RADIX (X).
I	SCAN (S,S_SET [,L_BACK])	Leftmost character index in S found in S_SET; (rightmost).
I	SELECTED_INT_KIND (I_r)	Integer kind with range, –(10⋆⋆I_r) to (10⋆⋆I_r).
I I	SELECTED_REAL_KIND ([I] [,I_r])	Kind for real of decimal precision, I, and exponent range, I_r.
R	SET_EXPONENT (X,I)	Number with mantissa of X and exponent of I.
I,V	SHAPE (⋆_ARRAY)	ARRAY (or scalar) shape vector.
N	SIGN (N,N_2)	Absolute value of N times sign of same type N_2.
R,Z	SIN (R_Z)	Sine function of real or complex number.
R	SINH (X)	Hyperbolic sine function of real X.
I	SIZE (⋆_ARRAY [,D])	ARRAY size, along dimension D.
R	SPACING (X)	Absolute spacing of numbers near real X, e.g. 2⋆⋆–17.
⋆	SPREAD (⋆_ARAY,D,I_COPIES)	I_COPIES along dimension D of ARAY into an array of rank 1 greater.

(continued)

Alphabetic Table of Fortran90 Intrinsic Functions (continued)		
Type	**Intrinsic**	**Description**
R,Z	SQRT (R_Z)	Square root function, of real or complex number.
A	SUM (A_ARRAY [,D] [,M])	Sum of ARRAY elements, along D, passing mask M.
call	SYSTEM_CLOCK ([I_NOW] [,I_RATE] [,I_MAX])	Integer data from real-time clock. CPU time is (finish_now - start_now) / rate.
R	TAN (X)	Tangent function of real X.
R	TANH (X)	Hyperbolic tangent function of real X.
R	TINY (N)	Smallest positive number, like N, e.g. 2⋆⋆–126.
⋆	TRANSFER (⋆_ARAY, V_MOLD [,I_SIZE])	Same representation as ARAY, but type of MOLD, in vector of length SIZE.
⋆	TRANSPOSE (MATRIX)	Matrix transpose of any type matrix.
S	TRIM (S)	Remove trailing blanks from a single string.
I,V	UBOUND (⋆_ARRAY [,D])	ARRAY upper bound(s) vector, along dimension D.
⋆	UNPACK (V,M,⋆_USE)	Unpack vector V at true elements of M, into USE.
I	VERIFY (S,S_SET [,L_BACK])	First position in S not found in S_SET (or last).

Subject Table of Fortran 90 Intrinsic Routines

The following KEY symbols are utilized to denote the TYPE of the intrinsic function, or subroutine, and its arguments: A-complex, integer, or real; B-integer bit; C-character; D-dimension; I-integer; K-kind; L-logical; M-mask (logical); N-integer, or real; P-pointer; R-real; S-string; T-target; V-vector (rank one array); X-real; Y-real; Z-complex; and *-any type. For more detailed descriptions and example uses of these intrinsic functions see Adams, J.C., et al., *Fortran 90 Handbook*, McGraw-Hill, New York, 1992, ISBN 0–07–000406–4.

Type	**Intrinsic**	**Description**
ALLOCATION		
L	ALLOCATED (⋆_ARRAY)	True if the array is allocated.
ARGUMENT		
L	PRESENT (OPTIONAL)	True if optional argument is present in the call.
ARRAY: CONSTRUCTION		
⋆	MERGE (⋆_TRUE,⋆_FALSE,M)	Use ⋆_TRUE if M is true; ⋆_FALSE otherwise.
⋆,V	PACK (⋆_ARRAY,M [,V_PAD])	Pack ARRAY for true M into vector, pad from V_PAD.
⋆	RESHAPE (⋆_ARRAY,I_V_SHAPE [,⋆_PAD] [,V_ORDER])	Reshape ARRAY using vector SHAPE, pad from an array, and re-order.
⋆	SPREAD (⋆_ARRAY,D,I_COPIES)	I_COPIES along D of ARRAY to rank 1 greater array.
⋆	UNPACK (V,M,⋆_USE)	Unpack V at true elements of M, into USE.
ARRAY: DIMENSIONS		
I,V	LBOUND (⋆_ARRAY [,D])	ARRAY lower bound(s vector), along dimension D.
I,V	SHAPE (⋆_ARRAY)	ARRAY (or scalar) shape vector.
I	SIZE (⋆_ARRAY [,D])	ARRAY size, along dimension D.
I,V	UBOUND (⋆_ARRAY [,D])	ARRAY upper bound(s vector), along dimension D.
ARRAY: INQUIRY		
L	ALL (M [,D])	True if all mask, M, elements are true, along D.
L	ALLOCATED (⋆_ARRAY)	True if the array is allocated.
L	ANY (M [,D])	True if any mask, M, element is true, along D.
I,V	LBOUND (⋆_ARRAY [,D])	ARRAY lower bound(s) vector, along dimension D.
I,V	SHAPE (⋆_ARRAY)	ARRAY (or scalar) shape vector.

(continued)

Subject Table of Fortran 90 Intrinsic Functions (continued)		
Type	**Intrinsic**	**Description**
I,V	UBOUND (⋆_ARRAY [,D])	ARRAY upper bound(s) vector, along dimension D.
ARRAY: LOCATION		
I,V	MAXLOC (N_ARRAY [,M])	Location(s) of maximum ARRAY term, passing M.
I,V	MINLOC (N_ARRAY [,M])	Location(s) of minimum ARRAY term, passing M.
ARRAY: MANIPULATION		
⋆	CSHIFT (⋆_ARRAY,I_SHIFT [,D])	Circular shift out and in for I_SHIFT elements.
⋆	EOSHIFT (⋆_ARRAY,I_SHIFT [,⋆_FIL][,D])	End-off shift ARRAY, and fill, in dimension D.
⋆	TRANSPOSE (MATRIX)	Matrix transpose of any type matrix.
ARRAY: MATHEMATICS		
N,L	DOT_PRODUCT (V,V_2)	Dot product of vectors V and V_2.
N,L	MATMUL (MATRIX,MATRIX_2)	Conformable matrix multiplication.
N	MAXVAL (N_ARRAY [,D] [,M])	Value of max ARRAY term, along D, passing M.
N	MINVAL (N_ARRAY [,D] [,M])	Value of min ARRAY term, along D, passing M.
A	PRODUCT (A_ARRAY [,D] [,M])	Product of ARRAY terms, along D, for mask M.
A	SUM (A_ARRAY [,D] [,M])	Sum of ARRAY terms, along D, passing mask M.
ARRAY: PACKING		
⋆,V	PACK (⋆_ARRAY,M [,V_PAD])	Pack ARRAY for true M into vector, pad from V_PAD.
⋆	UNPACK (V,M,⋆_USE)	Unpack V at true elements of M, into USE.
ARRAY: REDUCTION		
L	ALL (M [,D])	True if all mask, M, terms are true, along D.
L	ANY (M [,D])	True if any mask, M, term is true, along D.
I	COUNT (M [,D])	Number of true mask, M, terms, along dimension D.
N	MAXVAL (N_ARRAY [,D] [,M])	Value of max ARRAY term, along D, passing M.
N	MINVAL (N_ARRAY [,D] [,M])	Value of min ARRAY term, along D, passing M.
A	PRODUCT (A_ARRAY [,D] [,M])	Product of ARRAY terms, along D, for mask M.
A	SUM (A_ARRAY [,D] [,M])	Sum of ARRAY terms, along D, passing mask M.
BACK SCAN		
I	INDEX (S,S_SUB [,L_BACK])	Left starting position of S_SUB within S (or right).
I	SCAN (S,S_SET [,L_BACK])	Left character index in S also in S_SET (or right).
I	VERIFY (S,S_SET [,L_BACK])	First position in S not belonging to S_SET (or last).
BIT: INQUIRY		
I	BIT_SIZE (I)	Max number of bits possible in integer I, e.g. 32.
BIT: MANIPULATION		
L	BTEST (I,I_POS)	True if bit location I_POS of integer I has value one.
B	IAND (I,I_2)	Logical AND on the bits of I and I_2.
B	IBCLR (I,I_POS)	Clear bit I_POS to zero in integer I.
B	IBITS (I,I_POS,I_LEN)	Extract I_LEN bits at I_POS in integer I.
B	IBSET (I,I_POS)	Set bit I_POS to one in integer I.
B	IEOR (I,I_2)	Exclusive OR on the bits of I and I_2.
B	IOR (I,I_2)	Inclusive OR on the bits of I and I_2.
B	ISHFT (I,I_SHIFT)	Logical shift of bits of I by I_SHIFT, pad with 0.
B	ISHFTC (I,I_SHIFT [,I_SIZE])	Logical circular shift of I_SIZE rightmost bits of I.
call	MVBITS (I_GET, I_LOC, I, I_TO,I_POS)	Copy I bits at I_LOC in I_GET to I_TO at I_POS.
I	NOT (I)	Logical complement of the bits of integer I.
⋆	TRANSFER (⋆_ARRAY,	

(continued)

Subject Table of Fortran 90 Intrinsic Functions (continued)

Type	Intrinsic	Description
	V_MOLD [,I_SIZE])	Same representation as ARRAY, but type of MOLD.
BOUNDS		
I	CEILING (X)	Least integer greater than or equal to real X.
I	FLOOR (X)	Greatest integer less than or equal to X.
I,V	LBOUND ($\star$_ARRAY [,D])	ARRAY lower bound(s) vector, along dimension D.
N	MAX (N,N_2 [,N_3,...])	Maximum value of two or more numbers same type.
N	MAXVAL (N_ARRAY [,D] [,M])	Value of max ARRAY term, along D, passing M.
N	MINVAL (N_ARRAY [,D] [,M])	Value of min ARRAY term, along D, passing M.
I,V	UBOUND ($\star$_ARRAY [,D])	ARRAY upper bound(s) vector, along dimension D.
CALLS		
call	MVBITS (I_GET,I_LOC,I, I_TO,I_POS)	Copy I bits at I_LOC in I_GET to I_TO at I_POS.
call	DATE_AND_TIME ([S_DATE] [,S_TIME] [,S_ZONE] [,I_V_VALUES])	Real-time clock data.
call	RANDOM_NUMBER (X)	Pseudo-random numbers in range $0 < X < 1$.
call	RANDOM_SEED ([I_SIZE] [,I_V_P] [,I_V_G])	Initialize random number generator.
call	SYSTEM_CLOCK ([I_NOW] [,I_RAT] [,I_MX])	Integer data from real-time clock.
CHARACTERS		
C	ACHAR (I)	Character in position I of ASCII collating sequence.
C	CHAR (I [,K])	Character in position I of processor collation.
I	IACHAR (C)	Position of character C in ASCII collating sequence.
I	ICHAR (C)	Position of character C in processor collation.
CLOCK		
call	SYSTEM_CLOCK ([I_NOW] [,I_RAT] [,I_MX])	Integer data from real-time clock.
COMBINING		
$\star$	MERGE ($\star$_TRUE,$\star$_FALSE,M)	Use $\star$_TRUE term if M is true or $\star$_FALSE otherwise.
COMPLEX		
R	AIMAG (Z)	Imaginary part of complex number.
Z	CMPLX (X [,Y][,K])	Convert real(s) to complex type, of given kind.
Z	CONJG (Z)	Conjugate of complex number Z.
R	COS (R_Z)	Cosine function of real or complex argument.
R,Z	EXP (R_Z)	Exponential function of real or complex argument.
R	LOG (R_Z)	Natural (base e) logarithm of real or complex number.
I	PRECISION (R_Z)	Decimal precision of real or complex value, e.g. 6.
R,Z	SIN (R_Z)	Sine function of real or complex number.
R,Z	SQRT (R_Z)	Square root function, of real or complex number.
CONVERSIONS		
R	AIMAG (Z)	Imaginary part of complex number.
R	AINT (X [,K])	Truncate X to a real whole number.
Z	CMPLX (X [,Y][,K])	Convert real (s) to complex type, of given kind.
R	DBLE (A)	Convert A to double precision real.
R	DPROD (X,Y)	Double precision product of two default real scalars.

(continued)

Subject Table of Fortran 90 Intrinsic Functions (continued)		
Type	**Intrinsic**	**Description**
I	INT (A [,K])	Convert A to integer type, of given kind.
L	LOGICAL (L [,K])	Convert L to logical of kind K.
I	NINT (X [,K])	Integer nearest to real X, of the stated kind.
R	REAL (A [,K])	Convert A to real type, of type K.
N	SIGN (N,N_2)	Absolute value of N times sign of same type N_2.
⋆	TRANSFER (⋆_ARRAY, V_MOLD [,I_SIZ])	Same representation as ARRAY, but type of MOLD.
COPIES		
⋆	MERGE (⋆_TRUE,⋆_FALSE,M)	Use ⋆_TRUE if M is true or ⋆_FALSE otherwise.
call	MVBITS (I_FROM,I_LOC, I, I_TO,I_POS)	Copy I bits at I_LOC in I_FROM to I_TO at I_POS.
S	REPEAT (S,I_COPIES)	Concatenates I_COPIES of string S.
⋆	SPREAD (⋆_ARRAY,D,I_COPIES)	I_COPIES along D of ARRAY to rank 1 greater array.
COUNTING		
I	COUNT (M [,D])	Number of true mask, M, terms, along dimension D.
DATE		
call	DATE_AND_TIME ([S_DATE] [,S_TIME] [,S_ZONE] [,I_V_VALUES])	Real-time clock data.
DIMENSION OPTIONAL ARGUMENT		
L	ALL (M [,D])	True if all mask, M, terms are true, along D.
L	ANY (M [,D])	True if any mask, M, term is true, along D.
I	COUNT (M [,D])	Number of true mask, M, terms, along dimension D.
⋆	CSHIFT (⋆_ARRAY,I_SHIFT [,D])	Perform circular shift out and in for I_SHIFT terms.
⋆	EOSHIFT (⋆_ARRAY, I_SHIFT [,⋆_FIL][,D])	Perform end-off shift, and fill, in dimension D.
I,V	LBOUND (⋆_ARRAY [,D])	ARRAY lower bound(s) vector, along dimension D.
N	MAXVAL (N_ARRAY [,D] [,M])	Value of max ARRAY term, along D, passing M.
N	MINVAL (N_ARRAY [,D] [,M])	Value of min ARRAY term, along D, passing M.
A	PRODUCT (A_ARRAY [,D] [,M])	Product of ARRAY terms, along D, for mask M.
I	SIZE (⋆_ARRAY [,D])	ARRAY size, along dimension D.
A	SUM (A_ARRAY [,D] [,M])	Sum of ARRAY terms, along D, passing mask M.
I,V	UBOUND (⋆_ARRAY [,D])	ARRAY upper bound(s) vector, along dimension D.
DIMENSIONS		
I,V	LBOUND (⋆_ARRAY [,D])	ARRAY lower bound(s) vector, along dimension D.
I,V	SHAPE (⋆_ARRAY)	ARRAY (or scalar) shape vector.
I	SIZE (⋆_ARRAY [,D])	ARRAY size, along dimension D.
I,V	UBOUND (⋆_ARRAY [,D])	ARRAY upper bound(s) vector, along dimension D.
DOUBLE PRECISION		(see SELECTED_REAL_KIND)
R	DBLE (A)	Convert A to double precision real.
R	DPROD (X,Y)	Double precision product of two default real scalars.
EXISTENCE		
L	ALLOCATED (⋆_ARRAY)	True if the array is allocated.
L	ASSOCIATED (P [,T])	True if pointer, P, is associated with any target, or T.
L	PRESENT (OPTIONAL)	True if optional argument is present in call.
FILE		

(continued)

Type	Intrinsic	Description
Subject Table of Fortran 90 Intrinsic Functions (continued)		
FILL IN		
⋆	EOSHIFT (⋆_ARRAY,I_SHIFT [,⋆_FIL][,D])	End-off shift ARRAY, and fill, in dimension D.
INQUIRY: ARRAY		
L	ALL (M [,D])	True if all mask, M, terms are true, along D.
L	ALLOCATED (⋆_ARRAY)	True if the array is allocated.
L	ANY (M [,D])	True if any mask, M, term is true, along D.
I,V	LBOUND (⋆_ARRAY [,D])	ARRAY lower bound(s) vector, along dimension D.
I,V	SHAPE (⋆_ARRAY)	ARRAY (or scalar) shape vector.
I	SIZE (⋆_ARRAY [,D])	ARRAY size, along dimension D.
I,V	UBOUND (⋆_ARRAY [,D])	ARRAY upper bound(s) vector, along dimension D.
INQUIRY: BIT		
I	BIT_SIZE (I)	Max number of bits possible in integer I, e.g. 32.
INQUIRY: CHARACTER		
I	LEN (S)	Total character string length.
I	LEN_TRIM (S)	Length of S without trailing blanks.
INQUIRY: NUMBER MODEL		
N	DIGITS (N)	Number of significant digits in number N, e.g. 31.
R	EPSILON (X)	Number $\ll$ 1, for numbers like X, e.g. 2⋆⋆–23.
N	HUGE (N)	Largest number for numbers like N, e.g. 2⋆⋆128.
I	MAXEXPONENT (X)	Max exponent for real numbers like X, e.g. 128.
I	MINEXPONENT (X)	Min exponent for real numbers like X, e.g. –125.
I	PRECISION (R_Z)	Decimal precision for real or complex value, e.g. 6.
I	RADIX (N)	Base of the model for numbers like N, e.g. 2.
I	RANGE (A)	Decimal exponent range for A, e.g. 37.
I,V	SHAPE (⋆_ARRAY)	ARRAY (or scalar) shape vector.
I	SIZE (⋆_ARRAY [,D])	ARRAY size, along dimension D.
R	TINY (N)	Smallest positive number, like N, e.g. 2⋆⋆–126.
INQUIRY: MISCELLANEOUS		
I	COUNT (M [,D])	Number of true mask, M, elements, along D.
I	INDEX (S,S_SUB [,L_BACK])	Left starting position of S_SUB within S (or right).
I	SCAN (S,S_SET [,L_BACK])	Left character index in S also in S_SET; (or right).
I	VERIFY (S,S_SET [,L_BACK])	First position in S not belonging to S_SET, (or last).
INTEGERS		
I	CEILING (X)	Least integer greater than or equal to real X.
I	FLOOR (X)	Greatest integer less than or equal to X.
I	MAX1 (X,X2 [,X3])	Maximum integer from list of reals
I	MIN1 (X,X2 [,X3])	Minimum integer from list of reals
N	MODULO (N,N_2)	Modulo, N-FLOOR(N/N_2)⋆N_2.
I	SELECTED_INT_KIND (I_r)	Integer with exponent, –(10⋆⋆I_r) to (10⋆⋆I_r).
KIND: INQUIRY		
I	KIND (ANY)	Kind type integer parameter value for any argument.
KIND: DEFINITION		
I	SELECTED_INT_KIND (I_r)	Integer with exponent, –(10⋆⋆I_r) to (10⋆⋆I_r).
I	SELECTED_REAL_KIND ([I] [,I_r])	Real with precision, I, and exponent range, I_r.
KIND: USE OPTION		

(continued)

Subject Table of Fortran 90 Intrinsic Functions (continued)		
Type	**Intrinsic**	**Description**
R	AINT (X [,K])	Truncate X to a real whole number.
R	ANINT (X [,K])	Real whole number nearest to X.
C	CHAR (I [,K])	Character in position I of processor collation.
Z	CMPLX (X [,Y][,K])	Convert real(s) to complex type, of given kind.
I	INT (A [,K])	Convert A to integer type, of given kind.
L	LOGICAL (L [,K])	Convert L to logical of kind K.
I	NINT (X [,K])	Integer nearest to real X, of the stated kind.
R	REAL (A [,K])	Convert A to real type, of type K.
LOCATION		
I	IACHAR (C)	Position of character C in ASCII collating sequence.
I	ICHAR (C)	Position of character C in processor collation.
I	INDEX (S,S_SUB [,L_BACK])	Left starting position of S_SUB within S (or right).
I,V	MAXLOC (N_ARRAY [,M])	Vector location(s) of ARRAY maximum, passing M.
I,V	MINLOC (N_ARRAY [,M])	Vector location(s) of ARRAY minimum, passing M.
I	SCAN (S,S_SET [,L_BACK])	Left character index in S found in S_SET; (or right).
LOGICAL		
L	ALL (M [,D])	True if all mask, M, terms are true, along D.
L	ALLOCATED (⋆_ARRAY)	True if the array is allocated.
L	ANY (M [,D])	True if any mask, M, term is true, along D.
L	ASSOCIATED (P [,T])	True if pointer, P, is associated with any target, or T.
L	BTEST (I,I_POS)	True if bit location I_POS of integer I has value one.
N,L	DOT_PRODUCT (V,V_2)	Dot product of vectors V and V_2.
B	IAND (I,I_2)	Logical AND on the bits of I and I_2.
B	IEOR (I,I_2)	Exclusive OR on the bits of I and I_2.
B	IOR (I,I_2)	Inclusive OR on the bits of I and I_2.
B	ISHFT (I,I_SHIFT)	Logical shift of bits of I by I_SHIFT, pad with 0.
L	LGE (S,S_2)	True if S is $\geq$ S_2 in ASCII collating sequence.
L	LGT (S,S_2)	True if S follows S_2 in ASCII collating sequence.
L	LLE (S,S_2)	True if S is $\leq$ to S_2 in ASCII collating sequence.
L	LLT (S,S_2)	True if S precedes S_2 in ASCII collating sequence.
N,L	MATMUL (MATRIX,MATRIX_2)	Conformable matrix multiplication.
L	LOGICAL (L [,K])	Convert L to logical of kind K.
I	NOT (I)	Logical complement of the bits of integer I.
L	PRESENT (OPTIONAL)	True if optional argument is present in call.
MASK, or MASK OPTIONAL ARGUMENT		
L	ALL (M [,D])	True if all mask, M, terms are true, along D.
L	ANY (M [,D])	True if any mask, M, term is true, along D.
I	COUNT (M [,D])	Number of true mask, M, terms, along dimension D.
I,V	MAXLOC (N_ARRAY [,M])	Vector of location(s) of ARRAY max's, passing M.
N	MAXVAL (N_ARRAY [,D] [,M])	Value of ARRAY maximum, along D, passing M.
⋆	MERGE (⋆_TRUE,⋆_FALSE,M)	Use ⋆_TRUE if M is true or ⋆_FALSE otherwise.
I,V	MINLOC (N_ARRAY [,M])	Vector location(s) of ARRAY minimum, passing M.
N	MINVAL (N_ARRAY [,D] [,M])	Value of ARRAY minimum, along D, passing M.
⋆,V	PACK (⋆_ARRAY,M [,V_PAD])	Pack ARRAY for true M into vector, pad from V_PAD.
A	PRODUCT (A_ARRAY [,D] [,M])	Product of ARRAY terms, along D, for mask M.
A	SUM (A_ARRAY [,D] [,M])	Sum of ARRAY terms, along D, passing mask M.
MATHEMATICAL FUNCTIONS		
R	ACOS (X)	Arc cosine (inverse cosine) function of real X.

(continued)

Subject Table of Fortran 90 Intrinsic Functions (continued)		
Type	**Intrinsic**	**Description**
R	ASIN (X)	Arcsine (inverse sine) function of real X.
R	ATAN (X)	Arctangent (inverse tangent) function of real X.
R	ATAN2 (Y,X)	Arctangent for argument of complex number (X, Y).
R	COS (R_Z)	Cosine function of real or complex argument.
R	COSH (X)	Hyperbolic cosine function of real X.
R,Z	EXP (R_Z)	Exponential function of real or complex argument.
R	LOG (R_Z)	Natural logarithm of real or complex number.
R	LOG10 (X)	Common (base 10) logarithm function of real X.
R,Z	SIN (R_Z)	Sine function of real or complex number.
R	SINH (X)	Hyperbolic sine function of real X.
R	TAN (X)	Tangent function of real X.
R	TANH (X)	Hyperbolic tangent function of real X.
MATRICES (See ARRAYS)		
N,L	DOT_PRODUCT (V,V_2)	Dot product of vectors V and V_2.
N,L	MATMUL (MATRIX,MATRIX_2)	Conformable matrix multiplication.
⋆	TRANSPOSE (MATRIX)	Matrix transpose of any type matrix.
NUMBER MODEL		
N	DIGITS (N)	Number of significant digits for N, e.g. 31.
R	EPSILON (X)	Number $\ll$ 1, for numbers like X, e.g. 2⋆⋆–23.
I	EXPONENT (X)	Exponent part of the model for real X.
R	FRACTION (X)	Fractional part of the model for real X.
N	HUGE (N)	Largest number for numbers like N, e.g. 2⋆⋆128.
R	NEAREST (X,Y)	Nearest number at X in the direction of sign Y.
I	RADIX (N)	Base of the model for numbers like N, e.g. 2.
I	RANGE (A)	Decimal exponent range for A, e.g. 37.
R	RRSPACING (X)	Reciprocal of relative spacing of numbers near X.
R	SCALE (X,I)	Return X times b⋆⋆I, where base b = RADIX (X).
R	SET_EXPONENT (X,I)	Real with mantissa part of X and exponent part of I.
R	SPACING (X)	Absolute spacing of numbers near X, e.g. 2⋆⋆-17.
R	TINY (N)	Smallest positive number, like N, e.g. 2⋆⋆–126.
NUMERIC FUNCTIONS		
A	ABS (A)	Absolute value of A.
R	AIMAG (Z)	Imaginary part of complex number.
R	ANINT (X [,K])	Real whole number nearest to X.
I	CEILING (X)	Least integer greater than or equal to real X.
Z	CMPLX (X [,Y][,K])	Convert real(s) to complex type, of given kind.
Z	CONJG (Z)	Conjugate of complex number Z.
R	DBLE (A)	Convert A to double precision real.
R	DPROD (X,Y)	Double precision real product of two real scalars.
I	FLOOR (X)	Greatest integer less than or equal to X.
I	INT (A [,K])	Convert A to integer type, of given kind.
N	MAX (N,N_2 [,N_3,...])	Maximum value of two or more numbers same type.
N	MIN (N,N_2 [,N_3,...])	Minimum value of two or more same type numbers.
N	MOD (N,N_2)	Remainder for N_2, *i.e.*, N-INT(N/N_2)⋆N_2.
N	MODULO (N,N_2)	Modulo, N-FLOOR(N/N_2)⋆N_2.
R	REAL (A [,K])	Convert A to real type, of type K.
N	SIGN (N,N_2)	Absolute value of N times sign of same type N_2.
PADDING		
B	ISHFT (I,I_SHIFT)	Logical shift of bits of I by I_SHIFT, pad with 0.

(continued)

Subject Table of Fortran 90 Intrinsic Functions (continued)		
Type	**Intrinsic**	**Description**
⋆,V	PACK (⋆_ARRAY,M [,V_PAD])	Pack ARRAY for true M into vector, pad from V_PAD.
⋆	RESHAPE (⋆_ARRAY,I_V_SHAPE [,⋆_PAD] [,V_ORDER])	Reshape ARRAY to vector SHAPE, pad, re-order.
POINTER		
L	ASSOCIATED (P [,T])	True if pointer, P, is associated with any target, or T.
PRESENCE		
L	PRESENT (OPTIONAL)	True if optional argument is present in call.
RANDOM NUMBER		
call	RANDOM_NUMBER (X)	Pseudo-random numbers in range $0 < X < 1$.
call	RANDOM_SEED ([I_SIZE] [,I_V_P][,I_V_G])	Initialize random number generator.
REALS		
R	AINT (X [,K])	Truncate X to a real whole number.
R	ANINT (X [,K])	Real whole number nearest to X.
R	AMAX0 (I,I2 [,I3])	Maximum real from list of integers.
R	AMIN0 (I,I2 [,I3])	Minimum real from list of integers.
R	REAL (A [,K])	Convert A to real type, of type K.
I	SELECTED_REAL_KIND ([I] [,I_r])	Real with precision, I, and exponent range, I_r.
REDUCTION		
L	ALL (M [,D])	True if all mask, M, terms are true, along D.
L	ANY (M [,D])	True if any mask, M, term is true, along D.
I	COUNT (M [,D])	Number of true mask, M, terms, along dimension D.
N	MAXVAL (N_ARRAY [,D] [,M])	Value of max ARRAY term, along D, passing M.
N	MINVAL (N_ARRAY [,D] [,M])	Value of min ARRAY term, along D, passing M.
A	PRODUCT (A_ARRAY [,D] [,M])	Product of ARRAY terms, along D, for mask M.
A	SUM (A_ARRAY [,D] [,M])	Sum of ARRAY terms, along D, passing mask M.
RESHAPING ARRAYS		
⋆	CSHIFT (⋆_ARRAY,I_SHIFT [,D])	Perform circular shift out and in for I_SHIFT terms.
⋆	EOSHIFT (⋆_ARRAY,I_SHFT [,⋆_FIL] [,D])	End-off shift ARRAY, and fill, in dimension D.
⋆,V	PACK (⋆_ARRAY,M [,V_PAD])	Pack ARRAY for true M into vector, pad from V_PAD.
⋆	RESHAPE (⋆_ARRAY,I_V_SHAPE [,⋆_PAD] [,V_ORDER])	Reshape ARRAY to vector SHAPE, pad, re-order.
⋆	UNPACK (V,M,⋆_USE)	Unpack V for true elements of M, into USE.
REVERSE ORDER		
I	INDEX (S,S_SUB [,L_BACK])	Left starting position of S_SUB within S (rightmost).
I	SCAN (S,S_SET [,L_BACK])	Left character index in S found in S_SET; (rightmost).
I	VERIFY (S,S_SET [,L_BACK])	First position in S not found in S_SET, (or last).
SHIFTS		
⋆	CSHIFT (⋆_ARRAY,I_SHIFT [,D])	Perform circular shift out and in for I_SHIFT terms.
⋆	EOSHIFT (⋆_ARRAY,I_SHIFT [,⋆_FILL][,D])	Perform end-off shift, and fill, in dimension D.
B	ISHFT (I,I_SHIFT)	Logical shift of bits of I by I_SHIFT, pad with 0.
B	ISHFTC (I,I_SHIFT [,I_SIZE])	Logical circular shift of I_SIZE rightmost bits of I.

(continued)

Type	Intrinsic	Description
Subject Table of Fortran 90 Intrinsic Functions (continued)		
STRING		
C	ADJUSTL (S)	Adjust S left, move leading blanks to trailing blanks.
C	ADJUSTR (S)	Adjust S right, move trailing to leading blanks.
I	INDEX (S,S_SUB [,L_BACK])	Left starting position of S_SUB within S (or right).
I	LEN (S)	Total character string length.
I	LEN_TRIM (S)	Length of S without trailing blanks.
L	LGE (S,S_2)	True if S is $\geq$ to S_2 in ASCII collating sequence.
L	LGT (S,S_2)	True if S follows S_2 in ASCII collating sequence.
L	LLE (S,S_2)	True if S is $\leq$ to S_2 in ASCII collating sequence.
L	LLT (S,S_2)	True if S precedes S_2 in ASCII collating sequence.
S	REPEAT (S,I_COPIES)	Concatenates I_COPIES of string S.
I	SCAN (S,S_SET [,L_BACK])	Left character index in S found in S_SET; (or right).
S	TRIM (S)	Remove trailing blanks from a single string.
I	VERIFY (S,S_SET [,L_BACK])	First position in S not found in S_SET, (or last).
TARGET		
L	ASSOCIATED (P [,T])	True if pointer, P, is associated with any target, or T.
TIME		
call	DATE_AND_TIME ([S_DATE] [,S_TIME] [,S_ZONE] [,I_V_VALUES])	Real-time clock data.
call	SYSTEM_CLOCK ([I_NOW] [,I_RAT] [,I_MX])	Integer data from real-time clock.
VECTOR (See ARRAYS)		
N,L	DOT_PRODUCT (V,V_2)	Dot product of vectors V and V_2.
I,V	LBOUND (⋆_ARRAY [,D])	ARRAY lower bound(s) vector, along D.
I,V	MAXLOC (N_ARRAY [,M])	Location(s) of maximum ARRAY term, passing M.
I,V	MINLOC (N_ARRAY [,M])	Location(s) of minimum ARRAY term, passing M.
⋆,V	PACK (⋆_ARRAY,M [,V_PAD])	Pack ARRAY for true M into vector, pad from V_PAD.
⋆	RESHAPE (⋆_ARRAY,I_V_SHAPE [,⋆_PAD] [,V_ORDER])	Reshape ARRAY to vector SHAPE, pad, re-order.
I,V	SHAPE (⋆_ARRAY)	ARRAY (or scalar) shape vector.
⋆	TRANSFER (⋆_ARRAY, V_MOLD [,I_SIZE])	Same representation as ARRAY, but type of MOLD.
I,V	UBOUND (⋆_ARRAY [,D])	ARRAY upper bound(s) vector, along dimension D.

B.3 Syntax of Fortran 90 Statements

The following is a list of the recommended Fortran90 statements. Additional statements are allowed, but have been declared obsolete, and are expected to be deleted in future standards. Thus, they should not be utilized in new programs. They are appended to the end of this list. Below we list the standard syntax for the Fortran90 statements. In some cases the most common simple form of a statement is shown before it's more general options. Such optional features are shown included in brackets, `[ ]`, and a vertical bar | means "or." Note that the new attribute terminator symbol `::` is always optional, but its use is recommended.

The following abbreviations are employed: arg=argument, attr=attribute, exp=expression, i_=integer, r_=real, s_=string, spec=specifier, and here [type] means CHARACTER | COMPLEX | INTEGER | LOGICAL | REAL, or a user defined name given in a TYPE statement. Recall that F90 allows variable names to be 31 characters long and they may include an underscore (but F77 allows only 6 characters and no underscore). F90 lines may contain up to 132 characters (but just 72 in F77). All

	MATLAB	C++	F90
Pre-allocate linear array	A(100)=0	int A[100]; [a]	integer A(100)
Initialize to a constant value of 12	for j=1:100 % slow A(j)=12 end % better way A=12*ones(1,100)	for (j=0; j<100; j++) A[j]=12;	A=12
Pre-allocate two-dimensional array	A=ones(10,10)	int A[10][10];	integer A(10,10)

[a] C++ has a starting subscript of 0, but the argument in the allocation statement is the array's size.

Table B.41: Array initialization constructs.

Action	MATLAB	C++	F90
Define size	A=zeros(2,3) [a]	int A[2][3];	integer,dimension(2,3)::A
Enter rows	A=[1,7,-2; 3, 4, 6];	int A[2][3]={ {1,7,2}, {3,4,6} };	A(1,:)=(/1,7,-2/) A(2,:)=(/3,4,6/)

[a] Optional in MATLAB, but improves efficiency.

Table B.42: Array initialization constructs.

standard F77 statements are a sub-set of F90. Attribute options, and their specifiers, for each statement are given in the companion table "Fortran 90 Attributes and Specifiers". The numerous options for the INQUIRE statement are given in the table entitled "Options for F90 INQUIRE."

In addition to the statements given below F90 offers intrinsic array operations, implied do loops, vector subscripts, and about 160 intrinsic functions. Those functions, with their arguments, are given in tables "Alphabetical Table of Fortran 90 Intrinsic Functions and Subroutines," and "Subject Table of Fortran 90 Intrinsic Functions and Subroutines."

F90 Syntax
! preceeds a comment in F90 in column one denotes a comment line in F77 & continues a line in F90 (must be in column 6 for F77) ; terminates a statement in F90 (allows multiple statements per line) variable = expression_or_statement ! is an assignment (column 7 in F77)
ALLOCATABLE [::] array_name[(extents)] [, array_name[(extents)]] ALLOCATE (array_name) ALLOCATE (array_name [, STAT=status] [,array_name [, STAT=status]]) BACKSPACE i_exp ! file unit number BACKSPACE ([UNIT=]i_value [, IOSTAT=i_variable] [, ERR=i_label]) C in column one denotes a comment line in F77 CALL subroutine_name [([args])] CASE (range_list) [select_name] ! purpose CASE DEFAULT [select_name] ! purpose CHARACTER LEN=i_value [::] s_list CHARACTER [(LEN=i_value | * [, KIND=]i_kind)] [[, attr_list] ::] s_list CHARACTER [(i_value | *, [KIND=]i_kind)] [[, attr_list] ::] s_list

(continued)

F90 *Syntax (continued)*
CHARACTER [([KIND=i_kind] [, LEN=i_value | *])] [[, attr_list] ::] s_list
CLOSE (i_value) ! unit number
CLOSE ([UNIT=]i_value [, ERR=i_label] [, IOSTAT=i_variable] [, STATUS=exp])
COMPLEX [::] variable_list
COMPLEX [([KIND=]i_kind)] [[, attr_list] ::] variable_list
CONTAINS ! internal definitions follow
CYCLE ! current do only for a purpose
CYCLE [nested_do_name] ! and terminate its sub_do's for a purpose
DEALLOCATE (array_name)
DEALLOCATE (array_name [, STAT=status] [, array_name [, STAT=status]])
DIMENSION array_name(extents) [, array_name(extents)]
DO ! forever
DO i_variable = i_start, i_stop ! loop_name_or_purpose
DO [i_variable = i_start, i_stop [, i_inc]] ! loop_name_or_purpose
DO [i_label,] [i_variable = i_start, i_stop [, i_inc]] ! loop_name
[loop_name:] DO [i_variable = i_start, i_stop [, i_inc]] ! purpose
[loop_name:] DO [i_label,] [i_variable = i_start, i_stop [, i_inc]]
DO WHILE (logical_expression) ! obsolete, use DO-EXIT pair
DO [i_label,] WHILE (logical_expression) ! obsolete-obsolete
[name:] DO [i_label,] WHILE (logical_expression) ! obsolete
ELSE [if_name]
ELSE IF (logical_expression) THEN [if_name]
ELSE WHERE (logical_expression)
END [name] ! purpose
END DO [do_name] ! purpose
END FUNCTION [function_name] ! purpose
END IF [if_name] ! purpose
END INTERFACE ! purpose
END MODULE [module_name] ! purpose
END PROGRAM [program_name] ! purpose
END SELECT [select_name] ! purpose
END SUBROUTINE [name] ! purpose
END TYPE [type_name] ! purpose
END WHERE ! purpose
ENDFILE i_exp ! for file unit number
ENDFILE ([UNIT=]i_value [, IOSTAT=i_variable] [, ERR=i_label])
ENTRY entry_name [([args])] [RESULT(variable_name)]
EXIT ! current do only for a purpose
EXIT [nested_do_name] ! and its sub_do's for a purpose
EXTERNAL program_list
i_label FORMAT (specification_and_edit_list)
FUNCTION name ([args]) ! purpose
FUNCTION name ([args]) [RESULT(variable_name)] ! purpose
[type] [RECURSIVE] FUNCTION name ([args]) [RESULT(variable_name)]
[RECURSIVE] [type] FUNCTION name ([args]) [RESULT(variable_name)]
GO TO i_label ! for_a_reason
IF (logical_expression) executable_statement
[name:] IF (logical_expression) THEN ! state_purpose
IMPLICIT type (letter_list) ! F77 (a-h,o-z) real, (i-n) integer
IMPLICIT NONE ! F90 recommended default
INCLUDE source_file_path_name ! purpose
INQUIRE ([FILE=]'name_string' [, see_INQUIRE_table]) ! re file

(continued)

F90 *Syntax (continued)*
INQUIRE ([NAME=]s_variable [, see_INQUIRE_table]) ! re file
INQUIRE (IOLENGTH=i_variable [, see_INQUIRE_table]) ! re output
INQUIRE ([UNIT=]i_value [, see_INQUIRE_table]) ! re unit
INTEGER [::] variable_list
INTEGER [([KIND=]i_kind)] [[, attr_list] ::] variable_list
INTENT ([IN | INOUT | OUT]) argument_list
INTERFACE ASSIGNMENT (+ | - | * | / | = | **) ! user extension
INTERFACE OPERATOR (.operator.) ! user defined
INTERFACE [interface_name]
INTRINSIC function_list
LOGICAL [::] variable_list
LOGICAL [([KIND=]i_kind)] [[, attr_list] ::] variable_list
MODULE PROCEDURE program_list
MODULE module_name ! purpose
NULLIFY (pointer_list)
OPEN (i_value) ! unit number
OPEN ([UNIT=]i_value [, ERR=i_label] [, IOSTAT=i_variable] [, other_spec])
OPTIONAL [::] argument_list
PARAMETER (variable=value [, variable=value])
POINTER [::] name[(extent)] [, name[(extent)]] ! purpose
PRINT * , output_list ! default free format
PRINT * , (io_implied_do) ! default free format
PRINT '(formats)' , output_list ! formatted
PRINT '(formats)' , (io_implied_do) ! formatted
PRIVATE [[::] module_variable_list] ! limit access
PROGRAM [program_name] ! purpose
PUBLIC [[::] module_variable_list] ! default access
READ * , input_list ! default free format
READ * , (io_implied_do) ! default free format
READ '(formats)', input_list ! formatted
READ '(formats)', (io_implied_do) ! formatted
READ ([UNIT=]i_value, [FMT=]i_label [, io_spec_list]), input_list ! formatted
READ ([UNIT=]i_value, s_variable [, io_spec_list]), input_list ! formatted
READ ([UNIT=]i_value, '(formats)' [, io_spec_list]), input_list ! formatted
READ (i_value), input_list ! binary read
READ ([UNIT=]i_value, [, io_spec_list]), input_list ! binary read
READ (s_variable, [FMT=]i_label), input_list ! internal file type change
READ ([UNIT=]s_variable, [FMT=]i_label [, io_spec_list]), input_list ! internal file change
REAL [::] variable_list
REAL [([KIND=]i_kind)] [[, attr_list] ::] variable_list
RECURSIVE FUNCTION name ([args]) [RESULT(variable_name)] ! purpose
[type] RECURSIVE FUNCTION name ([args]) [RESULT(variable_name)] ! purpose
RECURSIVE SUBROUTINE name [([args])] ! purpose
RETURN ! from subroutine_name
REWIND i_exp ! file unit number
REWIND ([UNIT=]i_value [, IOSTAT=i_variable] [, ERR=i_label])
SAVE [[::] variable_list]
[name:] SELECT CASE (value)
SEQUENCE
STOP ['stop_message_string']
SUBROUTINE name [([args])] ! purpose
SUBROUTINE name [([args])] [args, optional_args] ! purpose

(continued)

F90 *Syntax (continued)*
[RECURSIVE] SUBROUTINE name [([args])] ! purpose
TARGET [::] name[(extent)] [, name[(extent)]]
TYPE (type_name) [[, attr_list] ::] variable_list
TYPE [, PRIVATE | PUBLIC] name
USE module_name [, ONLY: list_in_module_name] ! purpose
USE module_name [, new_var_or_sub=>old_name] ! purpose
WHERE (logical_array_expression) ! then
WHERE (logical_array_expression) array_variable = array_expression
WRITE * , output_list ! default free format
WRITE * , (io_implied_do) ! default free format
WRITE '(formats)', output_list ! formatted write
WRITE '(formats)', (io_implied_do) ! formatted write
WRITE ([UNIT=]i_value, [FMT=]i_label [, io_spec_list]), output_list ! formatted write
WRITE ([UNIT=]i_value, s_variable [, io_spec_list]), output_list ! formatted write
WRITE ([UNIT=]i_value, '(formats)' [, io_spec_list]), output_list ! formatted write
WRITE (i_value), output_list ! binary write
WRITE (i_value), (io_implied_do) ! binary write
WRITE ([UNIT=]i_value, [, io_spec_list]), output_list ! binary write
WRITE (s_variable, [FMT=]i_label), output_list ! internal file type change
WRITE ([UNIT=]s_variable, [FMT=]i_label [, io_spec_list]), output_list ! internal file change

Obsolescent statements are those from Fortran77 that are redundant and for which better methods are available in both Fortran77 and Fortran90.

Obsolete Syntax
ASSIGN i_label TO i_variable
BLOCK DATA [block_data_name]
COMMON [/common_block_name/] r_variable_list, i_variable_list
[i_label] CONTINUE ! from do [do_name]
DATA variable_list / value_list /
DATA (array_implied_do) / value_list /
DOUBLE PRECISION [[, attr_list] ::] variable_list
DO [i_label,] [r_variable = r_start, r_stop [, r_inc]] ! real control
DO_CONTINUE_pair
[name:] DO [i_label,] WHILE (logical_expression) ! obsolete
END BLOCK DATA [block_data_name]
EQUIVALENCE (variable_1, variable_2) [, (variable_3, variable_4)]
GO TO (i_label_1,i_label_2,...,i_label_n)[,] i_variable
IF (arithmetic_exp) i_label_neg, i_label_zero, i_label_pos
NAMELIST /group_name/ variable_list
PAUSE ! for human action
RETURN alternates
statement_function (args) = expression

The attributes lists for the type declarations, e.g. `REAL`, are `ALLOCATABLE`, `DIMENSION`, `INTENT`, `OPTIONAL`, `KIND`, `POINTER`, `PARAMETER`, `PRIVATE`, `PUBLIC`, `SAVE`, and `TARGET`; those for `OPEN` and `CLOSE` are `ACCESS`, `ACTION`, `BLANK`, and `DELIM`; while those for `READ` and `WRITE` are `ADVANCE`, `END`, `EOR`, `ERR`, and `FMT`.

	MATLAB	C++	F90
Addition $\mathbf{C} = \mathbf{A} + \mathbf{B}$	`C=A+B`	`for (i=0; i<10; i++){` `  for (j=0; j<10; j++){` `    C[i][j]=A[i][j]+B[i][j];` `    }` `  }`	`C=A+B`
Multiplication $\mathbf{C} = \mathbf{AB}$	`C=A*B`	`for (i=0; i<10; i++){` `  for (j=0; j<10; j++){` `    C[i][j] = 0;` `    for (k=0; k<10; k++){` `      C[i][j] += A[i][k]*B[k][j];` `      }` `    }` `  }`	`C=matmul(A,B)`
Scalar multiplication $\mathbf{C} = a\mathbf{B}$	`C=a*B`	`for (i=0; i<10; i++){` `  for (j=0; j < 10; j++){` `    C[i][j] = a*B[i][j];` `    }` `  }`	`C=a*B`
Matrix inverse $\mathbf{B} = \mathbf{A}^{-1}$	`B=inv(A)`	[a]	`B=inv(A)`[a]

[a]Neither C++ nor F90 have matrix inverse functions as part of their language definitions nor as part of standard collections of mathematical functions (like those listed in Table 4.7). Instead, a special function, usually drawn from a library of numerical functions, or a user defined operation, must be used.

Table B.43: Elementary matrix computational routines.

C++	`int*  point, vector, matrix` `...` `point = new type_tag` `vector = new type_tag [space_1]` `if (vector == 0) {error_process}` `matrix = new type_tag [space_1 * space_2]` `...` `delete matrix` `...` `delete vector` `delete point`
F90	`type_tag, pointer, allocatable :: point` `type_tag, allocatable :: vector (:), matrix (:,:)` `...` `allocate (point)` `allocate (vector (space_1), STAT = my_int)` `if (my_int /= 0) error_process` `allocate (matrix (space_1, space_2))` `...` `deallocate (matrix)` `if (associated (point, target_name)) pointer_action...` `if (allocated (matrix)) matrix_action...` `...` `deallocate (vector)` `deallocate (point)`

Table B.44: Dynamic allocation of arrays and pointers.

```
SUBROUTINE AUTO_ARRAYS (M,N, OTHER)
USE GLOBAL_CONSTANTS ! FOR INTEGER K
   IMPLICIT NONE
   INTEGER, INTENT (IN) :: M,N
   type_tag, INTENT (OUT) :: OTHER (M,N) ! dummy array

!  Automatic array allocations
   type_tag :: FROM_USE (K)
   type_tag :: FROM_ARG (M)
   type_tag :: FROM_MIX (K,N)
   ...
!  Automatic deallocation at end of scope
END SUBROUTINE AUTO_ARRAYS
```

Table B.45: Automatic memory management of local scope arrays.

```
module derived_class_name
     use base_class_name
! new attribute declarations, if any
             ...
contains


   ! new member definitions
             ...
end module derived_class_name
```

Table B.46: F90 Single Inheritance Form.

```
module derived_class_name
     use base_class_name, only: list_of_entities
! new attribute declarations, if any
             ...
contains


   ! new member definitions
             ...
end module derived_class_name
```

Table B.47: F90 Selective Single Inheritance Form.

```
module derived_class_name
     use base_class_name, local_name => base_entity_name
! new attribute declarations, if any
             ...
contains


   ! new member definitions
             ...
end module derived_class_name
```

Table B.48: F90 Single Inheritance Form, with Local Renaming.

```
module derived_class_name
      use  base1_class_name
      use  base2_class_name
      use  base3_class_name, only: list_of_entities
      use  base4_class_name, local_name => base_entity_name
! new attribute declarations, if any
              . . .
contains


      ! new member definitions
              . . .
end module derived_class_name
```

Table B.49: F90 Multiple Selective Inheritance with Renaming.

Examples of F90 Statements

The following is a list of examples of the recommended Fortran90 statements. Some have been declared obsolete, and are expected to be deleted in future standards. Thus, they should not be utilized in new programs. They are noted in the comments. In some cases the most common simple form of a statement is shown along with it's more general options. Note that the new attribute terminator symbol :: is always optional, but its use is recommended. While Fortran is not case-sensitive, this table employs upper case letters to denote standard features, and lower case letters for user supplied information. The following abbreviations are employed: arg=argument, attr=attribute, exp=expression, i_=integer, l_=logical, r_=real, s_=string, spec=specifier, z_=complex.

Recall that F90 allows variable names to be 31 characters long and they may include an underscore (but F77 allows only six characters and no underscore). F90 lines may contain up to 132 characters (but just 72 in F77). All standard F77 statements are a sub-set of F90.

The attributes lists for the type declariations, e.g. `REAL`, are `ALLOCATABLE, DIMENSION, INTENT, OPTIONAL, KIND, POINTER, PARAMETER, PRIVATE, PUBLIC, SAVE`, and `TARGET`. Those optional attributes for `OPEN` are `ACCESS` = [`DIRECT, SEQUENTIAL`], `ACTION` = [`READ, READWRITE, WRITE`], `BLANK` = [`NULL, ZERO`], `DELIM` = [`APOSTROPHE, NONE, QUOTE`], `ERR` = i_label, `FILE` = s_name, `FORM` = [`FORMATTED, UNFORMATTED`], `IOSTAT` = i_var, `PAD` = [`NO, YES`], `POSITION` = [`APPEND, ASIS, REWIND`], `RECL` = i_len, `STATUS` = [`NEW, OLD, REPLACE, SEARCH, UNKNOWN`], and `UNIT` = i_unit; while `CLOSE` utilizes only `ERR, IOSTAT, STATUS`, and `UNIT`.

The io_spec_list options for `READ` and `WRITE` are `ADVANCE` = [`NO, YES`], `END` = i_label, `EOR` = i_label, `ERR` = i_label, `FMT` = [*, i_label, s_var], `IOSTAT` = i_var, `NML` = var_list, `REC` = i_exp, `SIZE` = i_size, and `UNIT` = i_unit.

Fortran Statement Examples

Name	*Examples*	*Comments*
Allocatable	ALLOCATABLE :: force, stiffness	By name
	ALLOCATABLE :: force(:), stiffness(:,:)	Ranks
Allocate	ALLOCATE (hyper_matrix(5, 10, 3))	
	ALLOCATE (force(m))	
	ALLOCATE (array_name(3, 3, 3, 3), STAT=i_err)	Error status
Assign	ASSIGN 9 TO k	Obsolete
Assignment	c = 'b'	Character
	s = "abc"	String
	s = c // 'abc'	Concatenation
	s = string(j:m)	Sub-string
	s_fmt = '(2F5.1)'	Stored format
	l = l_1 .OR. l_2	Logical
	l = m < = 80	
	poor = (final > = 60) .AND. (final < 70)	
	proceed = .TRUE.	
	n = n + 1	Arithmetic
	x = b'1010'	Binary
	z = (0.0, 1.0)	Complex
	r = SQRT (5.)	Function
	converged = (ABS (x0 – x) < 2*SPACING (x))	
	x = z'B'	Hexadecimal
	k = 123	Integer
	x = o'12'	Octal
	r = 321.	Real
	a = 23. ; j = 120 ; ans = .TRUE.;	Semicolon
	k = SELECTED_INTEGER_KIND (20)	Kind
	m = SELECTED_REAL_KIND (16, 30)	

(continued)

Fortran Statement Examples (continued)

Name	*Examples*	*Comments*
	long = SELECTED_REAL_KIND (9, 20)	
	pi = 3.1459265_long	
	a = b + c	Matrix add
	d = MATMUL (a, b)	Matrix multiply
	e = TRANSPOSE (d)	Matrix transpose
	f = 0 ; g = (/ 2. , 4. , 6. /)	Matrix initialize
	B = Al:, n:(:–1)	Matrix flipped
	x = (/ (k, k = 0, n) /) * d	Implied do
	kth_row => a(k,:)	Pointer
	corners => a(1:n:(n-1), 1:m:(m-1))	
	p_2 => r	
	student_record%rank = 51	Defined type
	patient_data%city = 'houston'	
	sqrt(x) = DSQRT(x) ! function statement	Obsolete
Backspace	BACKSPACE i_exp	Compute unit
	BACKSPACE 8	Unit
	BACKSPACE (UNIT=9, IOSTAT=i, ERR=5)	Error go to
	BACKSPACE (9, IOSTAT=io_ok, ERR=99)	
	BACKSPACE (UNIT=9, IOSTAT=io_ok, ERR=99)	
	BACKSPACE (8, IOSTAT=io_ok)	I/O status
Block Data	BLOCK DATA ! Obsolete	
	BLOCK DATA winter ! Obsolete	Named
C	C in column one denotes a comment line in F77	Obsolete
	* in column one denotes a comment line in F77	Obsolete
	! anywhere starts a comment line in F90	
Call	CALL sub1 (a, b)	
	CALL sub2 (a, b, *5) ! Obsolete, use CASE	Alt return to 5
	CALL sub3	No arguments
	CALL subroutine_name (args, optional_args)	Optional arg
Case	CASE (range_list)	See SELECT
	CASE (range_list) select_name	Named
Case Default	CASE DEFAULT	See SELECT
	CASE DEFAULT select_name	Named
Character	CHARACTER (80) s, s_2*3(4)	
	CHARACTER *16 a, b, c	
	CHARACTER * home_team	:: recommended
	CHARACTER (*), INTENT(IN) :: home_team	Intent
	CHARACTER (LEN=3) :: b = 'xyz'	Initialize b
	CHARACTER LEN=40 :: monday, wednesday, friday	
	CHARACTER (LEN=40), attr_list :: last, first, middle	
	CHARACTER (40), attr_list :: name, state	
	CHARACTER (*), PARAMETER :: reply = "Invalid Data"	
	CHARACTER (*, KIND=greek), attr_list :: s1_list	Kind
	CHARACTER (*, KIND=greek), attr_list :: last, first, middle	
	CHARACTER (KIND=cyrillic, LEN=40) :: name, state	
	CHARACTER (KIND=cyrillic, *), attr_list :: s_list	
Close	CLOSE (7)	Unit number
	CLOSE (UNIT=k)	
	CLOSE (UNIT=8, ERR=90, IOSTAT=i)	Error go to
	CLOSE (8, ERR=99, IOSTAT=io_ok, STATUS='KEEP')	I/O status

(continued)

Fortran Statement Examples (continued)		
Name	*Examples*	*Comments*
	CLOSE (9, ERR=99, IOSTAT=io, STATUS='DELETE') CLOSE (UNIT=8, ERR=95, IOSTAT=io_ok)	File status
Common	COMMON / name / h, p, t ! Obsolete COMMON p, d, q(m,n) ! Obsolete	Named common Blank common
Complex	COMPLEX u, v, w(3, 6) COMPLEX :: u = (1.0,1.0), v = (1.0,10.0) COMPLEX :: variable_list COMPLEX attr_list :: variable_list COMPLEX (KIND=i2_kind), attr_list :: variable_list	:: recommended Initialize u and v Kind
Contains	CONTAINS	Internal definitions
	CONTAINS FUNCTION mine (b) . . . END FUNCTION mine	 Or subroutines
Continuation	! any non-block character in column 6 flags continuation & at the end flags continuation to next line & at the beginning flags continuation from above line	F77 obsolete F90 standard
	a_long_name = a_constant_value* & another_value ! on following line	
	a_long_name_here_is_set_to = value & * another_value ! continued from above	
Continue	100 CONTINUE	Obsolete
Cycle	CYCLE CYCLE nested_do_name	Current do only Terminate sub_dos
Data	DATA a, s / 4.01, 'z' / DATA s_fmt / '(2F5.1)' / DATA (r(k), k=1,3) / 0.7, 0.8, 1.9 / DATA array (4,4) / 1.0 / DATA bit_val / b'0011111' /	Obsolete Stored format Implied do Single value Binary
Deallocate	DEALLOCATE (force) DEALLOCATE (force, STAT=i_err)	File name Error status
Dimension	DIMENSION array (4, 4) DIMENSION v(1000), w(3) = (/ 1., 2., 4. /) DIMENSION force(20), stiffness(:,:) DIMENSION (5,10,3) :: triplet	 Initialize w :: recommended
	INTEGER, DIMENSION (:,:) :: material, nodes_list REAL, DIMENSION(m, n) :: a, b REAL, DIMENSION (:,:) :: force, stiffness `REAL, DIMENSION` (5,10,3), `INTENT(IN)` :: triplet	Typed Intent
Do	DO 100 j = init, last, incr ! Obsolete . . . 100 CONTINUE	Labeled do Obsolete
	DO j = init, last . . . END DO	Unlabeled do
	DO ! forever . . . END DO ! forever	Unlabeled do
	DO WHILE (diff <= delta) . . . END DO	Unlabeled while
	DO 100 WHILE (diff < = delta) ! Obsolete	Labeled while

(continued)

Fortran Statement Examples (continued)		
Name	*Examples*	*Comments*
	. . . 100 CONTINUE	 Obsolete
	DO	Forever
	DO k = i_start, i_stop DO k = i_start, i_stop, i_inc DO 10, k = i_start, i_stop	Integer range Increment Obsolete
	do_name: DO k = i_start, i_stop, i_inc do_name: DO 10, k = i_start, i_stop, i_inc	Named Named label
	DO 10, r_variable = r_start, r_stop, r_inc ! Obsolete	Real range
Do While	DO WHILE (.NOT. converged) DO 10, WHILE (.NOT. converged) do_name: DO 10, WHILE (.NOT. converged)	Use DO-EXIT pair Obsolete Obsolete
Double Precision	DOUBLE PRECISION a, d, y(2) DOUBLE PRECISION :: a, d = 1.2D3, y(2) DOUBLE PRECISION, attr_list :: variable_list	Obsolete Initialize D Obsolete
Else	ELSE ELSE leap_year	Then Named
Else If	ELSE IF (k > 50) THEN ELSE IF (days_in_year == 364) THEN ELSE IF (days_in_year == 364) THEN leap_year	 Named
Elsewhere	ELSEWHERE	See WHERE
End	END END name	 Named
End Block Data	END BLOCK DATA END BLOCK DATA block_data_name	Obsolete Obsolete
End Do	END DO END DO do_name	 Named
End Function	END FUNCTION function_name END FUNCTION	
End If	END IF leap_year END IF	Named
End Interface	END INTERFACE	
End Module	END MODULE my_matrix_operators END MODULE	
End Program	END PROGRAM program_name END PROGRAM	
End Select	END SELECT select_name END SELECT	Named
End Subroutine	END SUBROUTINE name END SUBROUTINE	
End Type	END TYPE type_name END TYPE	See TYPE
End Where	END WHERE	See WHERE
Endfile	ENDFILE i_exp ENDFILE (UNIT=k) ENDFILE k ENDFILE (UNIT=8, ERR=95) ENDFILE (7, IOSTAT=io_ok, ERR=99) ENDFILE (UNIT=8, IOSTAT=k, ERR=9) ENDFILE (UNIT=9, IOSTAT=io_ok, ERR=99)	Compute unit Unit number Error go to I/O status

(continued)

Fortran Statement Examples (continued)		
Name	*Examples*	*Comments*
Entry	ENTRY sec1 (x, y)	Arguments
	ENTRY sec2 (a1, a2, *4) ! Obsolete, use CASE	Alternate return to 4
	ENTRY section	No arguments
	ENTRY entry_name RESULT(variable_name)	Result
Equivalence	EQUIVALENCE (v (1), a (1,1))	Obsolete
	EQUIVALENCE (v, a)	
	EQUIVALENCE (x, v(10)), (p, q, d)	
Exit	EXIT	Current do only
	EXIT nested_do_name	Current & sub-dos
External	EXTERNAL my_program	
Format	10 FORMAT (2X, 2I3, 3F6.1, 4E12.2, 2A6, 3L2)	X I F E A L
	10 FORMAT (// 2D6.1, 3G12.2)	D, G
	10 FORMAT (2I3.3, 3G6.1E3, 4E12.2E3)	Exponent w
	10 FORMAT ('a quoted string', "another", I2)	Strings
	10 FORMAT (1X, T10, A1, T20, A1)	Tabs
	10 FORMAT (5X, TR10, A1, TR10, A1, TL5, A1)	Tab right, left
	10 FORMAT ("Init=", I2, :, 3X, "Last=", I2)	: stop if empty
	10 FORMAT ('Octal ', o6, ', Hex ' z6)	Octal, hex
	10 FORMAT (specification_and_edit_list)	
Function	FUNCTION z (a, b)	Arguments
	FUNCTION w (e, d) RESULT (a)	Result
	FUNCTION name (args)	
	FUNCTION name	No argument
	FUNCTION name (args) RESULT(variable_name)	
	INTEGER FUNCTION n (j, k)	Type
	INTEGER FUNCTION name (args)	
	COMPLEX RECURSIVE FUNCTION dat (args)	
	RECURSIVE REAL FUNCTION name (args)	
Go To	GO TO 99	Unconditional
	GO TO (10,20,35,95), i_variable ! Obsolete	Computed
If	IF (arithmetic_exp) 95, 10, 20 ! Obsolete	Arithmetic
	IF (logic) RETURN	Logical if
	IF (logic) n = n + 2	
	IF (logic) THEN	if block
	n = n + 1	
	k = k + 1	
	END IF	
	leap_year: IF (logical_expression) THEN	Named
	IF (logic) THEN	if else block
	n = n + 1	
	ELSE	
	k = k + 1	
	END IF	
	IF (c == 'a') THEN	if else-if block
	na = na + 1	
	CALL sub_a	
	ELSE IF (c == 'b') THEN	(Use CASE)
	nb = nb + 1	
	ELSE IF (c == 'c') THEN	
	nc = nc + 1	

(continued)

Fortran Statement Examples (continued)		
Name	*Examples*	*Comments*
	CALL sub_c END IF	
Implicit Type	IMPLICIT INTEGER (i-n) IMPLICIT REAL (a-h,o-z) IMPLICIT NONE IMPLICIT CHARACTER *10 (f,l) IMPLICIT COMPLEX (a-c,z) IMPLICIT TYPE (color) (b,g,r) IMPLICIT LOGICAL (KIND=bit) (m)	F77 default F77 default Recommended F90 Character Complex Derived type Logical
Include	INCLUDE 'path/source.f'	
Inquire	INQUIRE (UNIT=3, OPENED=t_or_f) INQUIRE (FILE='mydata', EXIST=t_or_f) INQUIRE (UNIT=3, OPENED=ok, IOSTAT=k)	Opened Exists I/O status
	INQUIRE (FILE='name_string', see_INQUIRE_table) INQUIRE (NAME=s_variable, see_INQUIRE_table)	Re file Re file
	INQUIRE (IOLENGTH=i_var, see_INQUIRE_table)	Re output
	INQUIRE (7, see_INQUIRE_table) INQUIRE (UNIT=8, see_INQUIRE_table)	Re unit Re unit
Integer	INTEGER c, d(4) INTEGER (long), attr_list :: variable_list INTEGER, DIMENSION (4) :: a, d, e INTEGER, ALLOCATABLE, DIMENSION(:,:) :: a, b INTEGER :: a = 100, b, c = 9 INTEGER :: i, j, k, l, m, n, month, year = 1996 INTEGER, attr_list :: variable_list	:: Recommended Allocatable Initialize a & c
	INTEGER (KIND=i2_kind), attr_list :: variable_list	Kind
Intent	INTENT (IN) :: credit_card_owners INTENT (INOUT) :: amount_due INTENT (OUT) income_rank	
Interface	INTERFACE ASSIGNMENT (=) INTERFACE OPERATOR (+) INTERFACE OPERATOR (–) INTERFACE OPERATOR (/) INTERFACE OPERATOR (*) INTERFACE OPERATOR (**) INTERFACE OPERATOR (.operator.) INTERFACE INTERFACE interface_name	User extension User extension User extension User extension User extension User extension User defined
Intrinsic	INTRINSIC SQRT, EXP	Functions
Logical	LOGICAL c LOGICAL, ALLOCATABLE :: mask(:), mask_2(:,:) LOGICAL (KIND = byte) :: flag, status LOGICAL :: b = .FALSE., c	:: recommended Allocatable Kind Initialize b
Module	MODULE PROCEDURE mat_x_mat, mat_x_vec MODULE my_matrix_operators	Generics
Namelist	NAMELIST /data/ s, n, d	Obsolete
Nullify	NULLIFY (pointer_list)	
Open	OPEN (7) OPEN (UNIT=3, FILE="data.test") OPEN (UNIT=2, FILE="data", STATUS = "old")	Unit number Name File status

(continued)

Fortran Statement Examples (continued)		
Name	*Examples*	*Comments*
	OPEN (UNIT=3, IOSTAT=k)	I/O status
	OPEN (9, ERR = 12, ACCESS ="direct")	Access type
	OPEN (8, ERR=99, IOSTAT=io_ok)	Error go to
	OPEN (UNIT=8, ERR=99, IOSTAT=io_ok)	
Optional	OPTIONAL slow, fast	Argument list
	OPTIONAL :: argument_list	
Parameter	PARAMETER (a="xyz"), (pi=3.14159)	Character
	PARAMETER (a="z", pi=3.14159)	Real
	PARAMETER (x=11, y = x/3)	Computed
	PARAMETER, REAL :: weight = 245.6	Type
Pause	PAUSE ! for human action	Obsolete
Pointer	POINTER current, last	:: recommended
	POINTER :: name(4,5)	Rank
	REAL, POINTER :: y(:), x(:,:,:)	Type
Print	PRINT *, a, j	List-directed
	PRINT *, output_list	Default unformatted
	PRINT *, (io_implied_do)	Implied do
	PRINT *, "The squre root of", n, 'is', SQRT(n)	Function
	PRINT *, (4*k-1, k=1,10,3)	
	PRINT 10, a, j	Formatted
	PRINT 10, m_array	Array
	PRINT 10, (m(i), i = j,k)	Implied do
	PRINT 10, s(j:k)	Substring
	PRINT '(A6, I3)', a, j	Character, integer
	PRINT FMT='(A6, I3)', a, j	Included format
	PRINT data_namelist ! Obsolete	Namelist
	PRINT '(formats)', output_list	Formatted
	PRINT '(formats)', (io_implied_do)	Implied do
	PRINT '(I4)', (2*k, k=1,5)	
Private	PRIVATE	
	PRIVATE :: module_variable_list	Specific items
Program	PROGRAM my_job	
	PROGRAM	
Public	PUBLIC	
	PUBLIC :: module_variable_list	Specific items
Read	READ *, a, j	List-directed
	READ 1, a , j	Formatted
	READ 10, m_array	Formatted array
	READ 10, (m(i), i=j, k)	Implied do
	READ 10, s(i:k)	Substring
	READ '(A6, I3)', a, i	Character, integer
	READ (1, 2) x, y	Formatted file
	READ (UNIT=1, FMT=2) x, y	
	READ (1, 2, ERR=8, END=9) x, y	End of file go to
	READ (UNIT=1, FMT=2, ERR=8, END=9) x, y	Error go to
	READ (*, 2) x, y	Formatted, std out
	READ (*, 10) m_array	Unformatted array
	READ (*, 10) (m(i), i=j, k)	Implied do
	READ (*, 10) s(i:k)	Substring
	READ (1, *) x, y	Unformatted file

(continued)

Fortran Statement Examples (continued)		
Name	*Examples*	*Comments*
	READ (*, *) x, y	Unformatted, std out
	READ (1, '(A6, I3)') x, y READ (1, FMT='(A6, I3)') x, y	Character, integer Included format
	READ (1, s_fmt) x, y READ (1, FMT=s_fmt) x, y	Format in a string
	READ (*, NML=data) ! Obsolete READ (1, NML=data) ! Obsolete	Namelist read Namelist from a file
	READ (1, END=8, ERR=9) x, y	Unformatted
	READ (s2, 1, ERR=9) x	Internal, formatted
	READ (s2, *, ERR=9) x	Unformatted
	READ (s2, REC=4, END=8) x	Internal, direct
	READ (1, REC=3) v	Unformatted direct
	READ (1, 2, REC=3) v	Formatted direct
	READ *, input_list READ *, (io_implied_do) READ *, (a(j,:), j=1, rows)	Default unformatted Implied do
	READ '(formats)', input_list READ '(formats)', (io_implied_do) READ '(5I5, (5I5))', (num(k), k=1, n)	Formatted read Formatted read
	READ (8, FMT=20), input_list READ (8, FMT=20, ADVANCE='NO'), input READ (9, FMT=20, io_spec_list), input_list READ (UNIT=7, 20, io_spec_list), input_list READ (UNIT=8, FMT=10, io_spec_list), input	Formatted Advance I/O Specification
	READ (7, s_fmt, io_spec_list), input_list READ (UNIT=7, s_fmt, io_spec_list), input	Stored format
	READ (9, '(formats)', io_spec_list), input_list READ (UNIT=9, '(formats)', io_spec_list), input	Inline format
	READ (8), input_list READ (UNIT=7), input_list READ (8, io_spec_list), input_list READ (UNIT=9, io_spec_list), input_list	Binary read I/O Specification
	READ (s_variable, FMT=20), input_list READ (UNIT=s_variable, 10, io_spec_list), input	Internal file, type change
Real	REAL*4 REAL :: r, m(9) REAL*16 a, b, c REAL*8, DIMENSION(n) :: a, b, c REAL :: a = 3.14, b, c = 100.0 REAL :: variable_list REAL, attr_list :: variable_list REAL, POINTER :: a(:,:)	:: recommended Quad Precision Double Precision Initialize a & c
	REAL (KIND=i2_kind), attr_list :: variable_list REAL (double), attr_list :: variable_list	Kind
Recursive	RECURSIVE FUNCTION name RECURSIVE FUNCTION a(n) RESULT(fac) INTEGER RECURSIVE FUNCTION name (args)	Function Result
	RECURSIVE SUBROUTINE name (args) RECURSIVE SUBROUTINE name	Subroutine
Return	RETURN	Standard return

(continued)

Fortran Statement Examples (continued)		
Name	*Examples*	*Comments*
Rewind	REWIND i_exp	Compute unit
	REWIND 2	Unit number
	REWIND k	
	REWIND (UNIT=8, IOSTAT=k, ERR=9)	Error go to
	REWIND (UNIT=8, ERR=95)	
	REWIND (8, IOSTAT=io_ok, ERR=99)	I/O status
Save	SAVE a, /name/, c	Scalars, common
	SAVE	Everything
	SAVE :: variable_list	
Select Case	SELECT CASE (value)	
	name: SELECT CASE (value)	Named
	u_or_l SELECT CASE (letter) CASE ("a":"z") ! lower case lower = .TRUE. CASE ("A":"Z") ! upper case lower = .FALSE. CASE DEFAULT ! not a letter PRINT *, "Symbol is not a letter", letter lower = .FALSE. END SELECT u_or_l	Block
Sequence	SEQUENCE	Forced storage
Stop	STOP	
	STOP "invalid data"	With message
Subroutine	SUBROUTINE sub1 (a, b)	
	SUBROUTINE sub1	No arguments
	SUBROUTINE name (args, optional_args)	Optional arguments
	SUBROUTINE sub3 (a, b, *9) ! Obsolete, use CASE	Return to 9
	RECURSIVE SUBROUTINE sub2 (a, b)	Recursive
Target	TARGET :: name, name_2	See Pointer
	TARGET :: name(4,5), name_2(3)	
Type Declaration	TYPE (person) car_pool(5)	User defined type
	TYPE (color), DIMENSION(256) :: hues	
	TYPE (type_name), attr_list :: variable_list	
	TYPE (person), DIMENSION (n) :: address_book	
	TYPE (type_name) :: variable_list	
	TYPE (student_record) CHARACTER (name_len) :: last, first INTEGER :: rank END TYPE student_record	Definition block
Type Statement	TYPE, PRIVATE name	Access
	TYPE, PUBLIC :: name	
Use	USE module_name	
	USE module_name, ONLY: list_in_module_name	Only
	USE module_name, var_subr_fun_name => old_name	Rename
Where	WHERE (logical_array_mask)	Then
	WHERE (a_array > 0.0) sqrt_a = SQRT(a_array) END WHERE	Where block
	WHERE (mask > 0.0) a_array = mask	Elsewhere block

(continued)

Fortran Statement Examples (continued)		
Name	*Examples*	*Comments*
	ELSEWHERE a_array = 0.0 END WHERE	
	WHERE (a_array>0) b_array = SQRT(a_array)	Statement
Write	WRITE (*, 10) s(j:k)	Substring
	WRITE (1, *) x, y WRITE (*, *) x, y	Unformatted file Unformatted
	WRITE (1, ’(A6, I3)’) x, y WRITE (1, FMT=’(A6, I3)’) x, y	Character, integer Included format
	WRITE (1, s_fmt) x, y WRITE (1, FMT=s_fmt) x, y	Stored format string
	WRITE (*, NML=data) ! Obsolete WRITE (1, NML=data) ! Obsolete	Namelist to stdout Namelist to a file
	WRITE (1, END=8, ERR=9) x, y	Unformatted
	WRITE (1, REC=3) v	Unformatted direct
	WRITE (1, 2, REC=3) v	Formatted direct
	WRITE (s2, 1, ERR=9) x	Internal, format
	WRITE (s2, *, ERR=9) x	Unformatted
	WRITE (s2, REC=4, END=8) x	Internal, direct
	WRITE *, output_list WRITE *, (io_implied_do) WRITE *, ((a(i, j), j=1, cols), i=1, rows)	Unformatted Implied do
	WRITE ’(formats)’, output_list WRITE ’(formats)’, (io_implied_do)	Formatted write Implied do
	WRITE (7, 10, ADVANCE=’NO’), output_list WRITE (8, 10, io_spec_list), output_list WRITE (9, FMT=20, io_spec_list), output_list WRITE (UNIT=7, 10, io_spec_list), output_list	Advance I/O specification
	WRITE (9, s_fmt, io_spec_list), output_list WRITE (UNIT=8, s_fmt, io_spec_list), output	Stored format
	WRITE (9, ’(formats)’, io_spec_list), output_list WRITE (UNIT=7, ’(formats)’, io_spec_list), output	Inline format
	WRITE (8), output_list WRITE (7), (io_implied_do) WRITE (8, ADVANCE=’NO’), output_list WRITE (9, io_spec_list), output_list WRITE (UNIT=9, io_spec_list), output_list	Binary write Implied do Advance I/O specification
	WRITE (s_variable, FMT=20), output_list WRITE (UNIT=s_variable, FMT=20), output_list WRITE (s_variable, 20, io_spec_list), output_list WRITE (UNIT=s_var, FMT=20, io_spec), output	Internal file I/O specification

Appendix C

Selected Exercise Solutions

C.1 Problem 1.8.1 : Checking trigonometric identities

The Fortran 90 program and output follow. The error levels are due to the fact that F90 defaults to single precision reals. F90 is easily extended to double precision, and in theory supports any level of user specified precision. For simplicity the F77 default naming convention for integers and reals is used. That is not a good practice since safety dictates declaring the type of each variable at the beginning of each program. (Try changing the reals to double precision to verify that the error is indeed reduced.)

```
implicit none
integer :: k,n = 16
real, parameter :: pi = 3.141592654 ! set constant
 print *,'  Theta        sin^2+cos^2         error'
 do k = 0, n            ! Loop over (n+1) points
   theta = k*pi/n
   sint  = sin( theta )
   cost  = cos( theta )
   test  = sint*sint + cost*cost
   write (*, '( 3(1pe14.5) )') theta, test, 1.-test
 end do ! over k
```

```
Theta          sin^2+cos^2   error
0.00000E+00   1.00000E+00   0.00000E+00
1.96350E-01   1.00000E+00   5.96046E-08
3.92699E-01   1.00000E+00   0.00000E+00
5.89049E-01   1.00000E+00   0.00000E+00
7.85398E-01   1.00000E+00   5.96046E-08
9.81748E-01   1.00000E+00   0.00000E+00
1.17810E+00   1.00000E+00   5.96046E-08
1.37445E+00   1.00000E+00   0.00000E+00
1.57080E+00   1.00000E+00   0.00000E+00
1.76715E+00   1.00000E+00   5.96046E-08
1.96350E+00   1.00000E+00   0.00000E+00
2.15985E+00   1.00000E+00   0.00000E+00
2.35619E+00   1.00000E+00   5.96046E-08
2.55254E+00   1.00000E+00   0.00000E+00
2.74889E+00   1.00000E+00   0.00000E+00
2.94524E+00   1.00000E+00   0.00000E+00
3.14159E+00   1.00000E+00   0.00000E+00
```

C.2 Problem 1.8.2 : Newton-Raphson algorithm

The most convenient form of loop is the post-test loop, which allows each iteration to be calculated and the error checked at the end.

```
xnew = x
do {
    x = xnew
    xnew = x - f(x)/fprime(x)
    }
    while (abs(xnew-x) < tolerance)
```

The alternate logic constructs employ tests at the end of the loop and transfer out the end of the loop when necessary. MATLAB and C++ transfer using the “break” command while F90 uses the “exit” command.

A F90 program with an infinite loop, named `testnewton.f90`, and its result is given below. Be warned that this version uses the IMPLICIT name styles for integers and reals instead of the better strong typing that results from the recommended use of IMPLICIT NONE.

```
function f(x) result(y)
  real, intent (in) :: x
  real              :: y
    y = exp(2*x) - 5*x - 1
end function f
!
function fprime(x) result(y)
  real, intent (in) :: x
  real              :: y
    y = 2*exp(2*x) - 5
end function fprime
!
program main
implicit none
real, parameter :: tolerance = 1.e-6  ! set constant
real :: x, xnew = 3.  ! Initial value
integer :: iteration
  iteration = 0
! Iteration count
  do ! forever until true
    iteration = iteration + 1
    x         = xnew
    xnew      = x - f(x)/fprime(x)
    if ( abs(xnew - x) < tolerance ) exit ! converged is true
  end do ! forever
  print *, 'Solution: ', xnew, ', Iterations:', iteration
end program main
```

```
>>f90 -o newton testnewton.f90
>>newton
 Solution:    0.8093941 , Iterations: 10
```

C.3 Problem 1.8.3 : Game of life

```
program  game_of_life   ! procedural version
implicit none
 integer, parameter :: boardsize = 10
 integer            :: board    (boardsize, boardsize) = 0
 integer            :: newboard (boardsize, boardsize)
 character(len=1)   :: ok         ! page prompt
 integer            :: k, number  ! loops

!           Initial life data, the "Glider"
  board (3, 3) = 1; board (4, 4) = 1; board (5, 4) = 1
  board (5, 3) = 1; board (5, 2) = 1

  print *, "Initial Life Display:"
  call spy (board) ! show initial lifeforms
  print *, "Initially alive = ", sum (board); print *, " "

  print *, "Enter number of generations to display:"
  read  *, number
  do k = 1, number
    newboard = next_generation (board)
    board    = newboard ! save current lifeforms
    call spy (board)    ! show current lifeforms
    print * ; print *, "Generation number = ", k
    print *, "Currently alive = ", sum (newboard)

    print *, 'continue? (y, n)'
    read *, ok ! read any character to continue
    if ( ok == 'n' ) exit ! this do loop only
  end do ! on k for number of generations

contains  ! internal (vs external) subprograms

 function next_generation (board) result (newboard)
!  Compute the next generation of life
 integer, intent(in) :: board    (:, :)
 integer             :: newboard (size(board, 1), size(board, 2))
 integer             :: i, j, neighbors  ! loops

  newboard = 0  ! initialize next generation
  do i = 2, boardsize - 1
    do j = 2, boardsize - 1
      neighbors = sum (board (i - 1:i + 1, j - 1:j + 1))  %
                -  board (i, j)
      if ( board (i, j) == 1 ) then ! life in the cell
```

```
        if ( (neighbors > 3 .or. neighbors < 2) ) then
          newboard (i, j) = 0       ! it died
        else
          newboard (i, j) = 1       ! newborn
        end if ! on number of neighbors
      else ! no life in the cell
        if ( neighbors == 3 ) then
          newboard (i, j) = 1       ! newborn
        else
          newboard (i, j) = 0       ! died
        end if ! on number of neighbors
      end if ! life status
    end do ! on column j
  end do ! on row i
 end function next_generation

 Subroutine spy (board)   ! model matlab spy function
! Show an X at each non-zero entry of board, else show -
 integer, intent(in) :: board (:, :)
 character (len=1)   :: line (size(board, 1))   ! a line on screen
 integer             :: i                       ! loops

  line = ' '                                  ! blank out the line
  do i = 1, size (board, 1 )                  ! loop over each row
    line (1:size (board, 2 )) = '-'          ! current board width
    where ( board (i, :) /= 0 ) line = 'X'   ! mark non-zero columns
    write (*, '(80a1)') line                 ! print current row
  end do ! over all rows
 end subroutine spy
end program  ! game_of_life

! Running gives:
!  Initial Life Display:
! ----------
! ----------
! --X-------
! ---X------
! -XXX------
! ----------
! ----------
! ----------
! ----------
! ----------
!  Initially alive = 5
!
!  Enter number of generations to display: 4
! ----------
! ----------
! ----------
! -X-X------
! --XX------
! --X-------
! ----------
! ----------
! ----------
! ----------
!
!  Generation number = 1
!  Currently alive = 5
!   continue? (y, n) n
```

C.4 Problem 2.5.1 : Conversion factors

This code illustrates the type of global units conversion factors that you can define for your field of study. They can be accessed by any program that includes a `use Conversion_Constants` line and cites a parameter name, as shown on line 16.

```
[ 1]  Module Conversion_Constants     ! DefineUnits Conversion
[ 2]  ! Define selected precision
[ 3]      INTEGER, PARAMETER :: DP = KIND (1.d0) ! Alternate form
[ 4]  ! ========= Metric Conversions =========
[ 5]  real(DP), parameter:: cm_Per_Inch      = 2.54_DP
[ 6]  real(DP), parameter:: kg_Per_Pound     = 0.45359237_DP
[ 7]  real(DP), parameter:: kg_Per_Short_Ton = 907.18474_DP
[ 8]  real(DP), parameter:: kg_Per_Long_Ton  = 1016.0469088_DP
[ 9]  real(DP), parameter:: m_Per_Foot       = 3.048_DP
[10]  real(DP), parameter:: m_Per_Mile       = 1609.344_DP
[11]  real(DP), parameter:: m_Per_Naut_Mile  = 1852.0_DP
[12]  real(DP), parameter:: m_Per_Yard       = 0.9144_DP
[13]  end Module Conversion_Constants
[14]  Program Test
```

```
  use Conversion_Constants
  print *, 'cm_Per_Inch = ', cm_Per_Inch ; End Program Test
! Running gives:  cm_Per_Inch = 2.54000000000000004
```

This code illustrates the type of common physical constants that can be made available as global variables that you can define for your field of study. They can be accessed by any program that includes a `use Physical_Constants` line and cites a parameter name, as shown on line 60 below.

```
[ 1]  Module Physical_Constants     ! Define Physical Constants
[ 2]  ! Define selected precision
[ 3]      INTEGER, PARAMETER :: DP = KIND (1.d0) ! Alternate form
[ 4]
[ 5]  ! ========== Physics Constants and units ==========
[ 6]  real(DP), parameter:: AMU_Value          = 1.6605402E-27_DP   ! kg
[ 7]  real(DP), parameter:: Atmosphere_Pres    = 9.80665E+04_DP     ! Pa
[ 8]  real(DP), parameter:: Avogadro          = 6.0221367E+23_DP   ! 1/mol
[ 9]  real(DP), parameter:: Bohr_Magneton      = 9.2740154E-24_DP   ! J/T
[10]  real(DP), parameter:: Bohr_Radius        = 5.29177249E-11_DP  ! m
[11]  real(DP), parameter:: Boltzmann         = 1.380657E-23_DP    ! J/K
[12]  real(DP), parameter:: c_Light            = 2.997924580E+8_DP  ! m/s
[13]  real(DP), parameter:: Electron_Compton   = 2.42631058E-12_DP  ! m
[14]  real(DP), parameter:: Electron_Angular   = 5.2729E-35_DP      ! J*s
[15]  real(DP), parameter:: Electron_Charge    =-1.60217738E-19_DP  ! coul
[16]  real(DP), parameter:: Electron_Mass_Rest = 9.1093897E-31_DP   ! kg
[17]  real(DP), parameter:: Electron_Moment    = 9.2847700E-24_DP   ! J/T
[18]  real(DP), parameter:: Electron_Radius    = 2.81794092E-15_DP  ! m
[19]  real(DP), parameter:: Faraday           = 9.6485309E+04_DP   ! C/mo
[20]  real(DP), parameter:: G_Universal        = 6.67260E-11_DP     ! m^3/(s^2*kg)
[21]  real(DP), parameter:: Light_Year         = 9.46073E+15_DP     ! m
[22]  real(DP), parameter:: Mech_equiv_Heat    = 4.185E+3_DP        ! J/kcal
[23]  real(DP), parameter:: Molar_Volume       = 0.02241410_DP      ! m^3/mol
[24]  real(DP), parameter:: Neutron_Mass       = 1.6749286E-27_DP   ! kg
[25]  real(DP), parameter:: Permeability      = 1.25663706143E-06_DP ! H/m
[26]  real(DP), parameter:: Permittivity      = 8.85418781762E-12_DP ! F/m
[27]  real(DP), parameter:: Planck_Const       = 6.6260754E-34_DP   ! J*s
[28]  real(DP), parameter:: Proton_Mass        = 1.6726230E-27_DP   ! kg
[29]  real(DP), parameter:: Proton_Moment      = 1.41060761E-26_DP  ! J/T
[30]  real(DP), parameter:: Quantum_charge_r   = 4.13556E+12_DP     ! J*s/C
[31]  real(DP), parameter:: Rydberg_inf        = 1.0973731534E+07_DP! 1/m
[32]  real(DP), parameter:: Rydberg_Hydrogen   = 1.09678E+07_DP     ! 1/m
[33]  real(DP), parameter:: Std_Atmosphere     = 1.01325E+05_DP     ! Pa
[34]  real(DP), parameter:: Stefan_Boltzmann   = 5.67050E-08_DP     ! W/(m^2*K^4)
[35]  real(DP), parameter:: Thomson_cross_sect = 6.6516E-29_DP      ! m^2
[36]  real(DP), parameter:: Universal_Gas_C    = 8.314510_DP        ! J/mol*K
[37]
[38]  ! ========== Astronomy Constants and units ==========
[39]  real(DP), parameter:: AU_Earth_Sun       = 1.4959787E+11_DP ! m
[40]  real(DP), parameter:: Anomal_Month       = 27.5546_DP       ! days
[41]  real(DP), parameter:: Anomal_Year        = 365.2596_DP      ! days
[42]  real(DP), parameter:: Dracon_Month       = 27.2122_DP       ! days
[43]  real(DP), parameter:: Earth_G            = 9.80665_DP       ! m/s^2
[44]  real(DP), parameter:: Earth_Mass         = 5.974E+24_DP     ! kg
[45]  real(DP), parameter:: Earth_Radius_Eq    = 6.37814E+6_DP    ! m
[46]  real(DP), parameter:: Earth_Radius_Mean  = 6.371E+6_DP      ! m
[47]  real(DP), parameter:: Earth_Radius_Polar = 6.356755E+6_DP   ! m
[48]  real(DP), parameter:: Julian_Year        = 365.25_DP        ! days
[49]  real(DP), parameter:: Rotation_Day       = 23.93447222_DP   ! hours
[50]  real(DP), parameter:: Sidereal_Day       = 23.93446944_DP   ! hours
[51]  real(DP), parameter:: Sidereal_Month     = 27.3217_DP       ! days
[52]  real(DP), parameter:: Sidereal_Ratio     = 1.0027379092558_DP
[53]  real(DP), parameter:: Sidereal_Year      = 365.2564_DP      ! days
[54]  real(DP), parameter:: Solar_Day          = 24.06571111_DP   ! hours
[55]  real(DP), parameter:: Synodic_Month      = 29.5306_DP       ! days
[56]  real(DP), parameter:: Tropical_Year      = 365.2422_DP      ! days
[57]  end Module Physical_Constants     ! Define Physical Constants
[58]  Program Test
[59]    use Physical_Constants
[60]    print *, 'Avogadro = ', Avogadro ; End Program Test
[61]  ! Running gives: Avogadro =  0.602213669999999967E+24
```

C.5 Problem 3.5.3 : Creating a vector class

We begin by defining the components to be included in our vector object. They include the length of each vector and a corresponding real array of pointers to the vector components:

```
 module class_Vector    ! filename: class_Vector.f90
 ! public, everything by default, but can specify any
  implicit none
   type Vector
      private
```

```
[  6]      integer                     :: size   ! vector length
[  7]      real, pointer, dimension(:) :: data   ! component values
[  8]   end type Vector
```

For persons familiar with vectors the use of overloaded operators makes sense (but it often does not make sense). Thus we overload the addition, subtraction, multiplication, assignment, and logical equal to operators by defining the correct class members to be used for different argument types:

```
[  9]  !              Overload common operators
[ 10]  interface operator (+)                   ! add others later
[ 11]   module procedure add_Vector, add_Real_to_Vector; end interface
[ 12]  interface operator (-)                   ! add unary versions later
[ 13]   module procedure subtract_Vector, subtract_Real; end interface
[ 14]  interface operator (*)                   ! overload *
[ 15]   module procedure dot_Vector, real_mult_Vector, Vector_mult_real
[ 16]  end interface
[ 17]  interface assignment (=)                 ! overload =
[ 18]   module procedure equal_Real; end interface
[ 19]  interface operator (==)                  ! overload ==
[ 20]   module procedure is_equal_to; end interface
[ 21]
```

Then we encapsulate the supporting member functions, beginning with two constructors, assign and make_Vector:

```
[ 22]  contains  ! functions & operators
[ 23]
[ 24]  function assign (values) result (name) ! array to vector constructor
[ 25]    real, intent(in) :: values(:)        ! given rank 1 array
[ 26]    integer          :: length           ! array size
[ 27]    type (Vector)    :: name             ! Vector to create
[ 28]     length = size(values); allocate ( name%data(length) )
[ 29]     name % size = length; name % data = values; end function assign
[ 30]
[ 31]  function make_Vector (len, values) result(v) ! Optional Constructor
[ 32]    integer, optional, intent(in) :: len       ! number of values
[ 33]    real,    optional, intent(in) :: values(:) ! given values
[ 34]    type (Vector)                 :: v
[ 35]     if ( present (len) ) then                ! create vector data
[ 36]       v%size = len ; allocate ( v%data(len) )
[ 37]       if ( present (values)) then ; v%data = values    ! vector
[ 38]         else                      ; v%data = 0.d0      ! null vector
[ 39]       end if ! values present
[ 40]     else                                     ! scalar constant
[ 41]       v%size = 1                  ; allocate ( v%data(1) ) ! default
[ 42]       if ( present (values)) then ; v%data(1) = values(1)  ! scalar
[ 43]         else                      ; v%data(1) = 0.d0       ! null
[ 44]       end if ! value present
[ 45]     end if ! len present
[ 46]  end function make_Vector
[ 47]
```

The remainder of the members are given in alphabetical order:

```
[ 48]   function add_Real_to_Vector (v, r) result (new) ! overload +
[ 49]    type (Vector), intent(in) :: v
[ 50]    real,          intent(in) :: r
[ 51]    type (Vector)             :: new          ! new = v + r
[ 52]     if ( v%size < 1 ) stop "No sizes in add_Real_to_Vector"
[ 53]     allocate ( new%data(v%size) ) ; new%size = v%size
[ 54]   ! new%data = v%data + r       ! as array operation
[ 55]     new%data(1:v%size) = v%data(1:v%size) + r ; end function
[ 56]
[ 57]  function add_Vector (a, b) result (new)    ! vector + vector
[ 58]    type (Vector), intent(in) :: a, b
[ 59]    type (Vector)             :: new          ! new = a + b
[ 60]     if ( a%size /= b%size ) stop "Sizes differ in add_Vector"
[ 61]     allocate ( new%data(a%size) ) ; new%size = a%size
[ 62]     new%data = a%data + b%data    ; end function add_Vector
```

Note that lines 55 and 62 above are similar ways to avoid writing serial loops that would have to be used in most languages. This keeps the code cleaner and shorter, and more importantly it lets the compiler carry out those operations in parallel on some machines.

While copy members are very important to C++ programmers the following `copy_Vector` should probably be omitted since you would not usually pass big arrays as copies and F90 defaults to passing by reference unless forced to pass by value.

```
[ 63]
[ 64]  function copy_Vector (name) result (new)
[ 65]    type (Vector), intent(in) :: name
```

```
   type (Vector)             :: new
    allocate ( new%data(name%size) ) ; new%size = name%size
    new%data = name%data             ; end function copy_Vector
```

The routine `delete_Vector` is the destructor for this class. In some sense it is incomplete because it does not delete the `size` attribute. It was decided that while the actual array of data may take a huge amount of storage, the single integer was not important. To be more complete one would have to have to make `size` an integer pointer and allocate and deallocate it at numerous locations within this module.

```

 subroutine  delete_Vector (name) ! deallocate allocated items
   type (Vector), intent(inout) :: name
   integer                      :: ok ! check deallocate status
    deallocate (name%data, stat = ok )
    if ( ok /= 0 ) stop "Vector not allocated in delete_Vector"
      name%size = 0 ; end subroutine delete_Vector

 function dot_Vector (a, b) result (c)      ! overload *
   type (Vector), intent(in) :: a, b
   real                      :: c
    if ( a%size /= b%size ) stop "Sizes differ in dot_Vector"
      c = dot_product(a%data, b%data); end function dot_Vector

 subroutine equal_Real (new, R)   ! overload =, real to vector
   type (Vector), intent(inout) :: new
   real,          intent(in)    :: R
    if ( associated (new%data) ) deallocate (new%data)
    allocate ( new%data(1) ); new%size = 1
     new%data = R            ; end subroutine equal_Real

 logical function is_equal_to (a, b) result (t_f) ! overload ==
   type (Vector), intent(in) :: a, b        ! left & right of ==
    t_f = .false.                          ! initialize
    if ( a%size /= b%size ) return          ! same size ?
      t_f = all ( a%data == b%data )       ! and all values match
 end function is_equal_to

 function length (name) result (n)          ! accessor member
   type (Vector), intent(in) :: name
   integer                   :: n
    n = name % size ; end function length

 subroutine list (name)  ! accessor member, for prettier printing
   type (Vector), intent(in) :: name
    print *,"[", name % data(1:name%size), "]"; end subroutine list

 function normalize_Vector (name)  result (new)
   type (Vector), intent(in) :: name
   type (Vector)             :: new
   real                      :: total, nil = epsilon(1.0) ! tolerance
    allocate ( new%data(name%size) ) ; new%size = name%size
    total = sqrt ( sum ( name%data**2 ) )     ! intrinsic functions
    if ( total < nil ) then ; new%data = 0.d0 ! avoid division by 0
      else                  ; new%data = name%data/total
    end if                  ; end function normalize_Vector

 subroutine read_Vector (name)              ! read array, assign
   type (Vector), intent(inout) :: name
   integer, parameter           :: max = 999
   integer                      :: length
    read (*,'(i1)', advance = 'no') length
    if ( length <= 0 )   stop "Invalid length in read_Vector"
    if ( length >= max ) stop "Maximum length in read_Vector"
     allocate ( name % data(length) ) ; name % size = length
     read *, name % data(1:length)    ; end subroutine read_Vector

 function real_mult_Vector (r, v) result (new) ! overload *
   real,          intent(in) :: r
   type (Vector), intent(in) :: v
   type (Vector)             :: new         ! new = r * v
    if ( v%size < 1 ) stop "Zero size in real_mult_Vector"
     allocate ( new%data(v%size) ) ; new%size = v%size
     new%data = r * v%data         ; end function real_mult_Vector

 function size_Vector (name) result (n)     ! accessor member
   type (Vector), intent(in) :: name
   integer                   :: n
    n = name % size ; end function size_Vector

 function subtract_Real(v, r) result(new) ! vector-real, overload -
   type (Vector), intent(in) :: v
   real,          intent(in) :: r
   type (Vector)             :: new         ! new = v + r
```

```
[143]     if ( v%size < 1 ) stop "Zero length in subtract_Real"
[144]      allocate ( new%data(v%size) ) ; new%size = v%size
[145]      new%data = v%data - r         ; end function subtract_Real
[146]
[147]  function subtract_Vector (a, b) result (new) ! overload -
[148]    type (Vector), intent(in) :: a, b
[149]    type (Vector)             :: new
[150]     if ( a%size /= b%size ) stop "Sizes differ in subtract_Vector"
[151]      allocate ( new%data(a%size) ) ; new%size = a%size
[152]      new%data = a%data - b%data    ; end function subtract_Vector
[153]
[154]  function values (name) result (array)        ! accessor member
[155]    type (Vector), intent(in) :: name
[156]    real                      :: array(name%size)
[157]     array = name % data ; end function values
```

The routine delete_Vector is the manual constructor for this class. It has no optional arguments so both arguments must be supplied, and it duplicates the constructor on line 31, but it uses the naming convention preferred by the author.

```
[158]
[159]  function Vector_ (length, values) result(name) ! constructor
[160]    integer,      intent(in) :: length           ! array size
[161]    real, target, intent(in) :: values(length)   ! given array
[162]    real, pointer            :: pt_to_val(:)    ! pointer to array
[163]    type (Vector)            :: name           ! Vector to create
[164]    integer                  :: get_m           ! allocate flag
[165]      allocate ( pt_to_val (length), stat = get_m )  ! allocate
[166]      if ( get_m /= 0 ) stop 'allocate error'        ! check
[167]      pt_to_val = values                    ! dereference values
[168]      name      = Vector(length, pt_to_val) ! intrinsic constructor
[169]  end function Vector_
[170]
[171]  function Vector_max_value (a) result (v)       ! accessor member
[172]    type (Vector), intent(in) :: a
[173]    real                      :: v
[174]     v = maxval ( a%data(1:a%size) ) ; end function Vector_max_value
[175]
[176]  function Vector_min_value (a) result (v)       ! accessor member
[177]    type (Vector), intent(in) :: a
[178]    real                      :: v
[179]     v = minval ( a%data(1:a%size) ) ; end function Vector_min_value
[180]
[181]  function Vector_mult_real(v, r) result(new) ! vec*real, overload *
[182]    type (Vector), intent(in) :: v
[183]    real,          intent(in) :: r
[184]    type (Vector)             :: new             ! new = v * r
[185]     if ( v%size < 1 ) stop "Zero size in Vector_mult_real"
[186]       new = Real_mult_Vector(r, v); end function Vector_mult_real
[187]
[188]  end module class_Vector
```

A first test of this class is given below along with comments that give the verifications of the members.

```
!        Testing Vector Class Constructors & Operators
include 'class_Vector.f90'        ! see previous figure
program check_vector_class
 use class_Vector
 implicit none

 type (Vector) :: x, y, z

!        test optional constructors: assign, and copy
 x = make_Vector ()                ! single scalar zero
 write (*,'("made scalar x = ")',advance='no'); call list(x)

 call delete_Vector (x) ; y = make_Vector (4)  ! 4 zeros
 write (*,'("made null y = ")',advance='no'); call list(y)

 z = make_Vector (4, (/11., 12., 13., 14./) )  ! 4 non-zeros
 write (*,'("made full z = ")',advance='no'); call list(z)
 write (*,'("assign [ 31., 32., 33., 34. ] to x")')

 x = assign( (/31., 32., 33., 34./) )         ! (4) non-zeros
 write (*,'("assigned  x = ")',advance='no'); call list(x)

 x = Vector_(4, (/31., 32., 33., 34./) )       ! 4 non-zeros
 write (*,'("public    x = ")',advance='no'); call list(x)
 write (*,'("copy x to y =")',advance='no')
 y = copy_Vector (x) ; call list(y)                     ! copy

!               test overloaded operators
 write (*,'("z * x gives ")',advance='no'); print *, z*x  ! dot
 write (*,'("z + x gives ")',advance='no'); call list(z+x) ! add
```

```
  y = 25.6                              ! real to vector
  write (*,'("y = 25.6 gives ")',advance='no'); call list(y)
  y = z                                 ! equality
  write (*,'("y = z gives y as ")',  advance='no'); call list(y)
  write (*,'("logic y == x gives ")',advance='no'); print *, y==x
  write (*,'("logic y == z gives ")',advance='no'); print *, y==z

!                 test destructor, accessors
  call delete_Vector (y)                            ! destructor
  write (*,'("deleting y gives y = ")',advance='no'); call list(y)
  print *, "size of x is ", length (x)            ! accessor
  print *, "data in x are [", values (x), "]"     ! accessor
  write (*,'("2. times x is ")',advance='no'); call list(2.0*x)
  write (*,'("x times 2. is ")',advance='no'); call list(x*2.0)
  call delete_Vector (x); call delete_Vector (z)  ! clean up
end program check_vector_class
!  Running gives the output:   ! made scalar x = [0]
! made null y = [0, 0, 0, 0]   ! made full z = [11, 12, 13, 14]
! assign [31, 32, 33, 34] to x ! assigned x  = [31, 32, 33, 34]
! public  x = [31, 32, 33, 34] ! copy x to y = [31, 32, 33, 34]
! z * x gives 1630             ! z + x gives   [42, 44, 46, 48]
! y = 256 gives [256000004]    ! y = z,   y =  [11, 12, 13, 14]
! logic y == x gives F         ! logic y == z gives T
! deleting y gives y = []      ! size of x is 4
! data in x : [31, 32, 33, 34] ! 2 times x is [62, 64, 66, 68]
! x times 2 is [62, 64, 66, 68]
```

Having tested the vector class we will now use it in some typical vector operations. We want a program that will work with arrays of vectors to read in the number of vectors. The array of vectors will use an automatic storage mode. That could be risky because if the system runs out of memory we get a fatal error message and the run aborts. If we made the alternate choice of allocatable arrays then we could check the allocation status and have a chance (but not a good chance) of closing down the code is some ”friendly” manner. Once the code reads the number of vectors then for each one it reads the number of components and the the component values. After testing some simple vector math we compute a more complicated result know as the orthonormal basis for the given set of vectors:

```
!     Test Vector Class Constructors, Operators and Basis
include 'class_Vector.f'

program check_basis ! demonstrate a typical Vector class
  use class_Vector
  implicit none

  interface
     subroutine testing_basis (N_V)
       integer, intent(in) :: N_V
     end subroutine testing_basis
  end interface

  print *, "Test automatic allocate, deallocate"
  print *, " " ; read  *, N_V
  print *, "The number of vectors to be read is: ", N_V
  call  testing_basis ( N_V) ! to use automatic arrays
end program check_basis

subroutine testing_basis (N_V)
! test vectors AND demo automatic allocation/deallocation
  use class_Vector

  integer, intent(in) :: N_V
  type (Vector)       :: Input(N_V) ! automatic array
  type (Vector)       :: Ortho(N_V) ! automatic array
  integer             :: j
  real                :: norm

interface
  subroutine  orthonormal_basis (Input, Ortho, N_given)
    use class_Vector
    type (Vector), intent(in)  :: Input(N_given)
    type (Vector), intent(out) :: Ortho(N_given)
    integer, intent(in)        :: N_given
  end subroutine  orthonormal_basis
end interface

  print *, " " ; print *, "The given ", N_V, " vectors:"
  do j = 1, N_V
     call read_Vector ( Input(j) )
     call list        ( Input(j) )
  end do ! for j

  print *, " "
```

```
  print *, "The Orthogonal Basis of the original set is:"

  call orthonormal_basis (Input, Ortho, N_V)
  do j = 1, N_V              ! list new orthogonal basis
     call list ( Ortho(j) )
  end do ! for j

       ! use vector class features & operators
  print *, ' ' ; print *,"vector 1 + vector 2 = "
  call list (Input(1)+Input(2))
  print *,"vector 1 - vector 2 = "
  call list (Input(1)-Input(2))
  print *,"vector 1 dot vector 2 = ", Input(1)*Input(2)
  print *,"vector 1 * 3.5 = "
  call list (3.5*Input(1))
  norm = sqrt ( dot_Vector( Input(1), Input(1) ))
  print *,"norm(vector 1) = ", norm
  print *,"normalized vector 1 = "
  call list (normalize_Vector(Input(1)))
  print *,"max(vector 1) = ", vector_max_value (Input(1))
  print *,"min(vector 1) = ", vector_min_value (Input(1))
  print *,"length of vector 1 = ", length ( Input(1) )
end subroutine testing_basis

subroutine  orthonormal_basis (Input, Ortho, N_given)
!     Find Orthonormal Basis of a Set of Vector Classes
  use class_Vector
!*******************************************************
! =, -, +, * are overloaded operators from class_Vector
!*******************************************************

  type (Vector), intent(in)  :: Input(N_given)
  type (Vector), intent(out) :: Ortho(N_given)
  integer, intent(in)        :: N_given
  integer                    :: i, j  ! loops
  real                       :: dot
  do i = 1, N_given         ! original set of vectors
    Ortho(i) = Input(i)      ! copy input vector class
    do j = 1, i              ! for previous copies
      dot      = dot_Vector(Ortho(i), Ortho(j))
      Ortho(i) = Ortho(i) - (dot*Ortho(j))
    end do ! for j
    Ortho(i) = normalize_Vector ( Ortho(i) )
  end do ! over i
end subroutine  orthonormal_basis

! Compiling and inputting :
! 4
! 3 0.625 0 0
! 3 7.5 3.125 0
! 3 13.25 -7.8125 6.5
! 3 14.0 3.5 -7.5
!            Gives:
! Test automatic allocate, deallocate
!
! The number of vectors to be read is:  4
! The given  4  vectors:
! [  0.6250   0.0000   0.0000 ]
! [  7.5000   3.1250   0.0000 ]
! [ 13.2500  -7.8125   6.5000 ]
! [ 14.0000   3.5000  -7.5000 ]
!
! The Orthogonal Basis of the original set is:
! [  1.0000   0.0000   0.0000 ]
! [  0.0000  -1.0000   0.0000 ]
! [  0.0000   0.0000  -1.0000 ]
! [  0.0000   0.0000   0.0000 ]
!
! vector 1 + vector 2    = [ 8.1250   3.1250   0.0000 ]
! vector 1 - vector 2    = [-6.8750  -3.1250   0.0000 ]
! vector 1 dot vector 2  =   4.6875
! vector 1 * 3.5         = [ 2.1875   0.0000   0.0000 ]
! norm(vector 1)         =   0.6250
! normalized vector 1    = [ 1.0000   0.0000   0.0000 ]
! max(vector 1)          =   0.6250
! min(vector 1)          =   0.0000
! length of vector 1     =  3
```

C.6 Problem 3.5.4 : Creating a sparse vector class

This class begins like the previous Vector class except that we must add a row entry (line 4) for each data value entry (line 5). This is done for efficiency since we expect most values in sparse vectors to be zero (and hence their name). The attribute `non_zero` is the size of both `rows` and `values`.

```
[  1]  module class_sparse_Vector
[  2]   implicit none
[  3]    type sv           ! a sparse vector
[  4]     integer          :: non_zeros
[  5]     integer, pointer :: rows(:)
[  6]     real,    pointer :: values(:)
[  7]    end type
[  8]
```

The overloading process is similar, but now we will see that much more logic is required to deal with the zero entries and new zeros created by addition or multiplication.

```
[  8]    interface assignment (=)
[  9]      module procedure equal_Vector ; end interface
[ 10]    interface operator (.dot.) ! define dot product operator
[ 11]      module procedure dot_Vector ; end interface
[ 12]    interface operator (==) ! Boolean equal to
[ 13]      module procedure is_equal_to ; end interface
[ 14]    interface operator (*) ! term by term product
[ 15]      module procedure el_by_el_Mult, real_mult_Sparse
[ 16]      module procedure Sparse_mult_real
[ 17]    end interface
[ 18]    interface operator (-)   ! for sparse vectors
[ 19]       module procedure Sub_Sparse_Vectors ; end interface
[ 20]    interface operator (+)   ! for sparse vectors
[ 21]       module procedure Sum_Sparse_Vectors ; end interface
[ 22]
[ 23]  contains  ! operators and functionality
```

In the following constructor for the class note that both the pointer array attributes are allocated (line 32) the same amount of storage in memory. One should also include the allocation status flag here and checks its value to raise a possible exception (as seen in lines 41-46).

```
[ 24]    subroutine make_Sparse_Vector (s,n,r,v)
[ 25]    !      allows zero length vectors
[ 26]      type (sv)          :: s     ! name
[ 27]      integer, intent(in) :: n     ! size
[ 28]      integer, intent(in) :: r(n)  ! rows
[ 29]      real,    intent(in) :: v(n)  ! values
[ 30]        if ( n < 0 ) stop &
[ 31]          "Error, negative rows in make_Sparse_Vector"
[ 32]          allocate (s%rows(n), s%values(n))
[ 33]          s%non_zeros = n      ! copy size
[ 34]          s%rows      = r      ! row   array assignment
[ 35]          s%values    = v      ! value array assignment
[ 36]    end subroutine make_Sparse_Vector
[ 37]
```

This is really a destructor. Again, it is incomplete because the integer array size was not made allocatable for simplicity.

```
[ 38]    subroutine delete_Sparse_Vector (s)
[ 39]      type (sv) :: s       ! name of sparse vector
[ 40]      integer   :: error   ! deallocate status flag, 0 no error
[ 41]        deallocate (s%rows, s%values, stat = error) ! memory released
[ 42]        if ( error == 0 ) then
[ 43]          s%non_zeros = 0                           ! reset size
[ 44]        else ! never created
[ 45]          stop "Sparse vector to delete does not exist"
[ 46]        end if ; end subroutine delete_Sparse_Vector
[ 47]
```

This creates a user defined operator call `.dot.` to be applied to sparse vectors.

```
[ 48]    function dot_Vector (u, v) result (d) ! defines .dot.
[ 49]    ! dot product of sparse vectors
[ 50]      type (sv), intent(in) :: u, v ! sparse vectors
[ 51]      type (sv)             :: w    ! sparse vector, temporary
[ 52]      real                  :: d    ! dot product value
[ 53]        d = 0.0                                        ! default
[ 54]        if ( u%non_zeros < 1 .or. v%non_zeros < 1 ) return  ! null
[ 55]          w = el_by_el_Mult (u, v) ! element by element sparse product
[ 56]          if ( w%non_zeros > 0 ) &
[ 57]          d = sum( w%values(1:w%non_zeros) ) ! summed
[ 58]          call delete_Sparse_Vector (w)              ! delete temp
```

```
[ 59]    end function dot_Vector
[ 60]
```

The above `dot_Vector` is more complicated in this format because it is likely that stored non-zero values will be multiplied by (unstored) zeros. Thus, the real work is done in the following member function that employs Boolean logic. The terms for the summation that creates the scalar dot product are first computed in a full vector equal in length to the minimum row number given. Observe that its size is established through the use of the `min` intrinsic, acting on the two given sizes, within the `dimension` attribute for the full array (lines 67,68). Three logical arrays (line 68) are used as "masks" which are `true` when a non-zero exists in the corresponding row of their associated sparse vector (down to the minimum row cited above). The three logical vectors are initialized in lines 77 to 92. That process ends with the third vector being created as a Boolean product (line 91) and the maximum possible number of non-zero products is found from the `count` intrinsic (line 92).

It is also important to note that the working space vector `full` is an `automatic array` and memory for it is automatically allocated for it each time the function is called. It could be an extremely long vector and thus it is possible (but not likely) that there would not be enough memory available. Then the system would abort with an error message. To avoid that possibility one could have declared `full` to be an `allocatable` vector and then allocate its memory by using a similar `min` construct. That allocation request should (always) include the STAT flag so that if the memory allocation fails it would be possible to issue an exception to try to avoid a fatal crash of the system (not likely).

```
[ 61]    function el_by_el_Mult (u, v) result (w) ! defines * operator
[ 62]    ! element by element product of sparse vectors: 0 * real ?
[ 63]      type (sv), intent(in) :: u, v              ! given vectors
[ 64]      type (sv)             :: w                 ! new vector
[ 65]      real :: full( min( u%rows(u%non_zeros),   & ! automatic
[ 66]            &          v%rows(v%non_zeros) ) )  ! workspace
[ 67]      logical, dimension( min( u%rows(u%non_zeros), &
[ 68]        v%rows(v%non_zeros))) :: u_m, v_m, w_m ! logical product masks
[ 69]      integer :: j, k, last, n, row
[ 70]        !  is either u or v null ?
[ 71]        if ( u%non_zeros < 1 .or. v%non_zeros < 1 ) then ! w is null
[ 72]          allocate ( w%rows(0), w%values(0) )
[ 73]          w%non_zeros = 0
[ 74]          return  ! a null sparse vector
[ 75]        end if ! no calculation necessary
[ 76]
[ 77]        !              Initialize logic masks
[ 78]        last = min( u%rows(u%non_zeros), v%rows(v%non_zeros) ) ! max size
[ 79]        u_m = .false.                          ! assume no contributions
[ 80]        do j = 1, size(u%rows)
[ 81]          row = u%rows(j)                      ! get row number to flag
[ 82]          if ( row > last ) exit ! j loop
[ 83]            u_m(row) = .true.                  ! possible contribution
[ 84]        end do  ! to initalize u mask
[ 85]        v_m = .false.                          ! assume no contributions
[ 86]        do j = 1, size(v%rows)
[ 87]          row = v%rows(j)                      ! get row number to flag
[ 88]          if ( row > last ) exit ! j loop
[ 89]            v_m(row) = .true.                  ! possible contribution
[ 90]        end do  ! to initalize v mask
[ 91]        w_m = (u_m .and. v_m )                  ! Boolean product logic
[ 92]        n   = count ( w_m )                    ! count possible products
[ 93]        ! if ( n == 0 ) print *,"Warning: zero length sparse" ! debug
[ 94]
```

The vector `full` is set to zero (line 96) and comparison DO loops (lines 97,101) over the two given vectors are minimized (lines 100,103) by testing where the mask vector `w_m` is `true` (thereby indicating a non-zero product). When all the products are stored in the `full` vector it is converted to the sparse vector storage mode (line 109) for release as the return result. Because `full` is an `automatic array` its memory is automatically released when the function is exited.

```
[ 95]        !             Fill the product workspace, full
[ 96]        full = 0.0                                    ! initialize
[ 97]        do j = 1, size(u%rows)                        ! loop over u
[ 98]          row = u%rows(j)                             ! row in u
[ 99]          if ( row > last ) exit ! this loop in u     ! past end of w
[100]          if ( .not. w_m(row) ) cycle ! to next j      ! not in product
[101]          do k = 1, size(v%rows)                        ! loop over v
[102]            if ( v%rows(k) > last ) exit ! this loop    ! past end of w
[103]            if ( .not. w_m(v%rows(k)) ) cycle ! to k+1  ! not in product
[104]              if ( row == v%rows(k) ) then              ! same row, u & v
[105]                full(row) = u%values(j)*v%values(k)     ! get product
```

```
[106]             end if
[107]           end do ! on k in v
[108]         end do ! on j in u
[109]         w = Vector_To_Sparse (full)                     !delete any zeros
[110]     end function el_by_el_Mult ! deletes full & 3 masks
[111]
```

The operator overloading members are given with the next function (line 112) as well as in lines 140, 231, and 320.

```
[112]     subroutine equal_Vector (new, s) ! overload =
[113]       type (sv), intent(inout) :: new
[114]       type (sv), intent(in)    :: s
[115]         allocate ( new%rows(s%non_zeros) )
[116]         allocate ( new%values(s%non_zeros) )
[117]         new%non_zeros = s%non_zeros
[118]         if ( s%non_zeros > 0 ) then
[119]           new%rows (1:s%non_zeros) = s%rows (1:s%non_zeros) ! array copy
[120]           new%values(1:s%non_zeros) = s%values(1:s%non_zeros) ! copy
[121]         end if ; end subroutine equal_Vector
[122]
[123]     function get_element (name, row) result (v)
[124]       type (sv), intent(in) :: name    ! sparse vector
[125]       integer,   intent(in) :: row     ! row in sparse vector
[126]       integer               :: j       ! loops
[127]       real                  :: v       ! value at row
[128]         v = 0.0                                         ! default
[129]         if ( row < 1 ) stop "Invalid row number, get_element"
[130]         if ( name%non_zeros < 1 ) return               ! not here
[131]         if ( row > name%rows(name%non_zeros) ) return  ! not here
[132]           do j = 1, name%non_zeros
[133]             if ( row == name%rows(j) ) then
[134]               v = name%values(j)                  ! found the value
[135]               return                              ! search done
[136]             end if ! in the vector
[137]           end do ! over possible values
[138]     end function get_element
[139]
[140]     function is_equal_to (a, b) result (t_or_f)  ! define ==
[141]      type (sv), intent(in) :: a, b    ! two sparse vectors
[142]      logical               :: t_or_f
[143]      integer               :: i       ! loops
[144]        t_or_f = .true.                         ! default
[145]      if ( a%non_zeros == b%non_zeros ) then ! also check values
[146]       do i = 1, a%non_zeros  ! or use count function for simplicity
[147]        if (a%rows(i) /= b%rows(i) .or. &
[148]            a%values(i) /= b%values(i)) then
[149]            t_or_f = .false.   ! because rows and/or values differ
[150]            return            ! no additional checks needed
[151]        end if ! same values
[152]       end do ! over sparse rows
[153]      else              ! sizes differ so vectors must be different
[154]        t_or_f = .false.
[155]      end if ! sizes match
[156]     end function is_equal_to
[157]
[158]     function  largest_index (s) result(row)
[159]       type (sv), intent(in) :: s    ! sparse vector
[160]       integer               :: row  ! last non-zero in full vector
[161]       integer               :: j    ! loops
[162]         row = 0                            ! initalize
[163]         if ( s%non_zeros < 1 ) return     ! null vector
[164]         do j = s%non_zeros, 1, -1         ! loop backward
[165]           if ( s%values(j) /= 0.0 ) then  ! last non-zero term
[166]             row = s%rows(j)               ! actual row number
[167]             return                        ! search done
[168]           end if
[169]         end do
[170]     end function  largest_index
[171]
[172]     function  length (name) result (n)
[173]       type (sv), intent(in) :: name
[174]       integer               :: n
[175]         n = name % non_zeros  ! read access to size, if private
[176]     end function  length
[177]
```

Once again we observe that the next two functions employ the colon operator (lines 185,196,199,201) to avoid explicit serial loops which would make them faster on certain vector and parallel computers.

```
[178]   function  norm (name)  result (total)
[179]     type (sv), intent(in) :: name
[180]     real                  :: total
[181]       if ( name%non_zeros < 1 ) then
```

```
      ! print *, "Warning: empty vector in norm"
      total = 0.0
    else
      total = sqrt( sum( name%values(1:name%non_zeros)**2 ))
    end if ! a null vector
end function  norm

function  normalize_Vector (s)  result (new)
  type (sv), intent(in) :: s
  type (sv)             :: new
  real                  :: total, epsilon = 1.e-6
    allocate ( new%rows  (s%non_zeros) )
    allocate ( new%values(s%non_zeros) )
    new%non_zeros          = s%non_zeros           ! copy size
    new%rows(1:s%non_zeros) = s%rows(1:s%non_zeros)  ! copy rows
    total = sqrt( sum( s%values(1:s%non_zeros)**2 )) ! norm
    if ( total <= epsilon ) then               ! divide by 0 ?
      new%values(1:s%non_zeros) = 0.d0         ! set to zero
    else                                       ! or real values
      new%values(1:s%non_zeros) = s%values(1:s%non_zeros)/total
    end if ! division by zero
end function  normalize_Vector

subroutine pretty (s)   ! print all values if space allows
  type (sv), intent(in) :: s          ! sparse vector
  integer, parameter    :: limit = 20 ! for print size
  integer               :: n
  real                  :: full( s%rows(s%non_zeros) ) ! temp
    n = s%non_zeros
    if ( s%non_zeros < 1 .or. s%rows(s%non_zeros) > limit ) then
      print *, "Wrong size to pretty print"
    else
      full = 0.                            ! initialize to zero
      if ( n > 0 ) full(s%rows) = s%values ! array copy non zeros
      print *,"[", full,"]"                ! pretty print
    end if ; end subroutine pretty ! automatic deallocate of full

subroutine read_Vector (name)     ! sparse vector data on unit 1
  type (sv), intent(inout) :: name
  integer                  :: length, j
    read (1,'(i1)', advance = 'no') length
    if ( length <= 0 )   stop "Invalid length in read_Vector"
    name % non_zeros = length
    allocate ( name % rows   (length) )
    allocate ( name % values (length) )
    read (1,*) ( name%rows(j), name%values(j), j = 1, length)
    name%rows = name%rows + 1 ! default to 1 not 0 in F90
end subroutine read_Vector

  function  real_mult_Sparse (a, b) result (new)
  !  scalar * vector
    real,      intent(in) :: a
    type (sv), intent(in) :: b
    type (sv)             :: new
      allocate ( new%rows  (b%non_zeros) )
      allocate ( new%values(b%non_zeros) )
      new%non_zeros = b%non_zeros
      if ( b%non_zeros < 1 ) then
        print *, "Warning: zero size in real_mult_Sparse "
      else  ! copy array components
        new%rows  (1:b%non_zeros) =     b%rows  (1:b%non_zeros)
        new%values(1:b%non_zeros) = a * b%values(1:b%non_zeros)
      end if ! null vector
  end function  real_mult_Sparse

  function rows_of (s)  result(n)  ! copy rows array of s
    type (sv) :: s                 ! sparse vector
    integer   :: n(s%non_zeros)    ! standard array
      if ( s%non_zeros < 1 ) stop "No rows to extract, rows_of"
      n = s%rows                     ! array copy
    end function rows_of

 subroutine set_element  (s, row, value)
  ! Set, or insert, value into row of a sparse vector, s
    type (sv), intent(inout) :: s       ! sparse vector
    integer,   intent(in)    :: row     ! full vector row
    real,      intent(in)    :: value   ! full vector value
    type (sv)                :: new     ! workspace
    logical                  :: found   ! true if row exists
    integer                  :: j, where ! loops, locator
      found = .false.                    ! initialize
      where = 0                          ! initialize
      do  j = 1, s%non_zeros
        if ( s%rows(j) == row ) then     ! found it
          s%values(j) = value            ! value changed
```

```
[267]            return                             ! no insert needed
[268]          end if
[269]          if ( s%rows(j) > row ) then
[270]            where = j                          ! insert before j
[271]            exit ! the loop search
[272]          else ! s%rows(j) < row,               may be next or last
[273]            where = j + 1
[274]          end if
[275]        end do ! over current rows in s
[276]        if ( .not. found ) then ! expand and insert at where
[277]          if ( where == 0 ) stop "Logic error, set_element"
[278]          new%non_zeros = s%non_zeros + 1
[279]          allocate ( new%rows  (new%non_zeros) )
[280]          allocate ( new%values(new%non_zeros) )
[281]          !   copy preceeding rows
[282]          if ( where > 1 ) then  ! copy to front of new
[283]            new%rows  (1:where-1) = s%rows  (1:where-1) ! array copy
[284]            new%values(1:where-1) = s%values(1:where-1) ! array copy
[285]          end if ! copy to front of new
[286]          !   insert, copy following rows of s
[287]          new%rows  (where   ) = row                    ! insert
[288]          new%values(where   ) = value                  ! insert
[289]          new%rows  (where+1:) = s%rows  (where:)       ! array copy
[290]          new%values(where+1:) = s%values(where:)       ! array copy
[291]          !   deallocate s, move new to s, deallocate new
[292]          call delete_Sparse_Vector (s)                  ! delete s
[293]          call equal_Vector         (s, new)            ! s <- new
[294]          call delete_Sparse_Vector (new)                ! delete new
[295]        end if ! an insert is required
[296]    end subroutine set_element
[297]
[298]    subroutine show (s) ! alternating row number and value
[299]      type (sv) :: s    ! sparse vector
[300]      integer   :: j, k ! implied loops
[301]        k = length (s)
[302]        if ( k == 0 ) then
[303]          print *, k ; else ;          ! print in C++ style rows
[304]          print *, k, ( (s%rows(j)-1), s%values(j), j = 1, k )
[305]        end if ; end subroutine show
[306]
[307]    subroutine show_r_v (s) ! all rows then all values
[308]      type (sv) :: s        ! sparse vector
[309]        print *, "Vector has ", s%non_zeros, " non_zero terms."
[310]        if ( s%non_zeros > 0 ) then
[311]          print *, "Rows:   ", s%rows - 1     ! to look like C++
[312]          print *, "Values: ", s%values
[313]        end if ; end subroutine show_r_v
[314]
[315]    function size_of (s)  result(n)
[316]      type (sv) :: s
[317]      integer   :: n
[318]        n = s%non_zeros ; end function size_of
[319]
[320]    function  Sparse_mult_real (a, b) result (new)
[321]    !  vector * scalar
[322]      real,       intent(in) :: b
[323]      type (sv), intent(in) :: a
[324]      type (sv)             :: new
[325]        new = real_mult_Sparse ( b, a)  ! reverse the order
[326]    end function  Sparse_mult_real
[327]
```

In the following subtraction and addition functions we again note that sparse terms with the same values but opposite signs can result in new zero terms in the resulting vector. A temporary automatic workspace vector, `full`, is used to hold the preliminary results. In this case it must have a size that is the maximum of the two given vectors. Thus, the `max` intrinsic is employed in its `dimension` attribute (lines 331,344) which is opposite the earlier multiplication example (line 65).

```
[328]    function Sub_Sparse_Vectors (u, v) result (w) ! defines -
[329]      type (sv), intent(in) :: u, v
[330]      type (sv)             :: w
[331]      real :: full( max( u%rows(u%non_zeros),   & ! automatic
[332]            &            v%rows(v%non_zeros) ) )  ! workspace
[333]        if ( u%non_zeros <= 0 ) stop "First vector doesn't exist"
[334]        if ( v%non_zeros <= 0 ) stop "Second vector doesn't exist"
[335]        full         = 0.0                     ! set to zero
[336]        full(u%rows) = u%values                ! copy first values
[337]        full(v%rows) = full(v%rows) - v%values ! less second values
[338]        w = Vector_To_Sparse (full)             ! delete any zeros
[339]    end function Sub_Sparse_Vectors ! automatically deletes full
[340]
[341]    function Sum_Sparse_Vectors (u, v) result (w) ! defines +
[342]      type (sv), intent(in) :: u, v
```

```
    type (sv)             :: w
      real :: full( max( u%rows(u%non_zeros),   & ! automatic
            &            v%rows(v%non_zeros) ) )  ! workspace
      if ( u%non_zeros <= 0 ) stop "First vector doesn't exist"
      if ( v%non_zeros <= 0 ) stop "Second vector doesn't exist"
      full         = 0.                        ! set to zero
      full(u%rows) = u%values                  ! copy first values
      full(v%rows) = full(v%rows) + v%values  ! add second values
      w = Vector_To_Sparse (full)              ! delete any zeros
  end function Sum_Sparse_Vectors ! automatically deletes full

  function values_of (s)  result(v)  ! copy values of s
    type (sv) :: s                   ! sparse vector
    real      :: v(s%non_zeros)      ! standard array
      if ( s%non_zeros < 1 ) &
         stop "No values to extract, in values_of"
      v = s%values                     ! array copy
  end function values_of

  function Vector_max_value (a) result (v)
    type (sv), intent(in) :: a
    real                  :: v
      v = maxval (a%values(1:a%non_zeros)) ! intrinsic function
      !  is it a sparse vector with a false negative maximum ?
      if ( a%non_zeros < a%rows(a%non_zeros) .and. v < 0. ) v = 0.0
  end function Vector_max_value

  function Vector_min_value (a) result (v)
    type (sv), intent(in) :: a
    real                  :: v
      v = minval ( a%values(1:a%non_zeros) ) ! intrinsic function
      !  is it a sparse vector with a false positive minimum ?
      if ( a%non_zeros < a%rows(a%non_zeros) &
           .and. v > 0. ) v = 0.0
  end function Vector_min_value

```

This function is invoked several times in other member functions. It simply accepts a standard (dense) vector and converts it to the sparse storage mode in the return result.

```
  function Vector_To_Sparse (full) result (sparse)
    real, intent(in) :: full(:)       ! standard array
    type (sv)        :: sparse        ! sparse vector copy
    integer          :: j, n, number  ! loops and counters
      n = count ( full /= 0.0 )       ! count non_zeros
      ! if ( n == 0 ) print *, "Warning: null full vector "
      allocate ( sparse%rows(n), sparse%values(n) )
      sparse%non_zeros = n            ! sparse size
      number           = 0            ! non zeros inserted
      do j = 1, size(full)
        if ( full(j) == 0.0 ) cycle          ! to next j value
          number                 = number + 1 ! non zeros inserted
          sparse%rows(number)   = j          ! row number in full
          sparse%values(number) = full(j)    ! value
          if ( number == n ) exit            ! all non_zeros found
      end do ; end function Vector_To_Sparse

  function zero_sparse ()  result (s)
    type (sv) :: s  ! create sparse null vector
      s%non_zeros = 0
      allocate (s%rows(0), s%values(0)); end function zero_sparse
end module class_sparse_Vector
```

C.7 Problem 4.11.1 : Count the lines in an external file

```
function inputCount(unit) result(linesOfInput)
!-------------------------------------------------------------
! takes a file number, counts the number of lines in that
! file, and returns the number of lines.
!-------------------------------------------------------------
implicit none
integer, intent(in) :: unit         ! file unit number
integer             :: linesOfInput ! result
integer ioResult    ! system I/O action error code
character temp      ! place to hold the character read

  rewind (unit)             ! go to the front of the file
  linesOfInput = 0          ! initially, there are 0 lines

  do  ! Until iostat says we've hit the end_of_file
    read (unit,'(A)', iostat = ioResult) temp    ! one char
```

```

      if ( ioResult == 0 ) then          ! there were no errors
        linesOfInput = linesOfInput + 1  ! increment lines
      else if ( ioResult < 0 ) then      ! we've hit end-of-file
        exit                             ! so exit this loop.
      else   ! ioResult is positive, which is a user error
        write (*,*) 'inputCount: no data at unit =', unit
        stop 'user read error'
      end if
    end do
    rewind(unit)               ! go to the front of the file
  end Function inputCount
```

C.8 Problem 4.11.3 : Computing CPU time useage

While this is mainly designed to show the use of the module `tic_toc` you should note that the intrinsic way of printing a date or time is not "pretty" and could be easily improved.

```
program watch
! -----------------------------------------------
! Exercise DATE_AND_TIME and SYSTEM_CLOCK functions.
! -----------------------------------------------
  use tic_toc
  implicit none
  character* 8  :: the_date
  character*10  :: the_time
  integer       :: j, k
!
   call date_and_time ( DATE = the_date )
   call date_and_time ( TIME = the_time )
   print *, 'The date is ', the_date, &
  &         ' and the time is now ', the_time
!   Display facts about the system clock.
   print *, ' '
   call system_clock ( COUNT_RATE  =  rate )
   print *, 'System clock runs at ', rate,&
  &         ' ticks per second'
!
!   Call the system clock to start an execution timer.
   call  tic
!
!  call run_the_job, or test with next 3 lines
    do k = 1, 9999
       j = sqrt ( real(k*k) )
    end do
!   Stop the execution timer and report execution time.
   print *, ' '
   print *, 'Job took ', toc (), ' seconds to execute.'
 end program watch                  ! Running gives
! The date is 19980313 and the time is now 171837.792
! System clock runs at  100  ticks per second
! Job took  0.9999999776E-02  seconds to execute.
```

C.9 Problem 4.11.4 : Converting a string to upper case

The change from the `to_lower` should be obvious here. It seems desirable to place these two routines, and others that deal with strings into a single strings utility module.

```
function  to_upper (string)  result (new_string) ! like C
! -------------------------------------------------------------
!        Convert a string or character to upper case
!         (valid for ASCII or EBCDIC processors)
! -------------------------------------------------------------
implicit none
character (len = *), intent(in) :: string     ! unknown length
character (len = len(string))   :: new_string ! same length
character (len = 26), parameter ::                 &
          UPPER = 'ABCDEFGHIJKLMNOPQRSTUVWXYZ',  &
          lower = 'abcdefghijklmnopqrstuvwxyz'
integer :: k    ! loop counter
integer :: loc  ! position in alphabet
  new_string = string       ! copy everything
  do k = 1, len(string)     ! to change letters
    loc = index ( lower, string(k:k))               ! locate
    if (loc /= 0 ) new_string(k:k) = UPPER(loc:loc) ! convert
  end do ! over string characters
end function to_upper
```

C.10 Problem 4.11.8 : Read two values from each line of an external file

```
subroutine readData (inFile, lines, x, y)
! ----------------------------------------------------
!   Take a file number, the number of lines to be read,
!      and put the data into the arrays x and y
! ----------------------------------------------------
! inFile     is unit number to be read
! lines      is number of lines in the file
! x          is independent data
! y          is dependent data
  implicit none
  integer, intent(in)  :: inFile,   lines
  real,    intent(out) :: x(lines), y(lines)
  integer              :: j

  rewind (inFile)               ! go to front of the file
  do j = 1, lines               ! for the entire file
    read (inFile, *) x(j), y(j) ! get the x and y values
  end do ! over all lines
end subroutine readData
```

C.11 Problem 4.11.14 : Two line least square fits

The extension of the single-line least squares fit shown in Fig. 4.21 is rather straightforward in that we will call subroutine lsq_fit multiple times. In line 37 we first call it in case a single-line fit may be more accurate than the expected two-line fit.

```
[  1]  program two_line_lsq_fit
[  2]  !-----------------------------------------------------
[  3]  ! Best two-line linear least-squares fit of data in
[  4]  ! file specified by the user, and split in two sets
[  5]  !-----------------------------------------------------
[  6]    implicit none
[  7]    real, allocatable :: x (:)  ! independent data
[  8]    real, allocatable :: y (:)  ! dependent data
[  9]
[ 10]    real    :: fit(3),  fit1(3), fit2(3) ! error results
[ 11]    real    :: left(3), right(3)         ! best results
[ 12]    real    :: error                     ! current error
[ 13]    real    :: error_min                  ! best error
[ 14]    integer :: split                     ! best division
[ 15]
[ 16]    integer, parameter   :: filenumber = 1 ! input unit
[ 17]    character (len = 64) :: filename       ! input file
[ 18]    integer              :: lines          ! of input
[ 19]    integer              :: inputCount, j  ! loops
[ 20]
[ 21]  !   Get the name of the file containing the data.
[ 22]     write (*, *) 'Enter the data input filename:'
[ 23]     read  (*, *) filename
[ 24]
[ 25]  !       Open that file for reading.
[ 26]     open (unit = filenumber, file = filename)
[ 27]
[ 28]  !       Find the number of lines in the file
[ 29]     lines = inputCount (filenumber)
[ 30]     write (*, *) 'There were ',lines,' records read.'
[ 31]
[ 32]  !   Allocate that many entries in the x and y array
[ 33]     allocate (x(lines), y(lines))
[ 34]     call read_xy_file (filenumber, lines, x, y) ! Read data
[ 35]     close (filenumber)
[ 36]
[ 37]     call lsq_fit (lines, x, y, fit)   ! single line fit
[ 38]     print *, "Single line fit"
[ 39]     print *, "the slope is     ", fit(1)
[ 40]     print *, "the intercept is ", fit(2)
[ 41]     print *, "the error is     ", fit(3)
[ 42]
```

After that we want to try all the reasonable choices for breading the data set into two adjacent regions that are each to be fit with a different straight line. Trial variables were defined in lines 10 and 12, while the best results found are in variables declared in lines 11, 13, and 14. Note that on line 48 we have required that at least three points be used to define an approximate straight line. If we allowed two points to be employed we would get a false (or misleading) indication of zero error for such a choice. Thus, in line 48 we begin a loop over all possible sets of three or more data points and call lsq_fit for each of the two segments, as seen in lines 50 and 51.

```
[ 43]  ! Loop to determine the mean squared error for each
[ 44]  ! of the possible two divisions of the data
[ 45]  !
[ 46]     error_min = HUGE(error_min)   ! initialize the error_min
[ 47]     split = 3                    ! initialize split point
[ 48]     do j = 3, lines-3            ! 3 pts to approximate a line
[ 49]  !        least-squares fit of two data subsets
[ 50]        call lsq_fit (j,       x(1:j),       y(1:j),       fit1)
[ 51]        call lsq_fit (lines-j, x(j+1:lines), y(j+1:lines), fit2)
[ 52]        error = fit1(3) + fit2(3)
[ 53]
```

In splitting up the two data regions not that it was not necessary to copy segments of the independent and dependent data. Instead the colon operator, or implied do loops, were used in lines 50 and 51 to pass vectors with *j* and *(lines – j)* entries, respectively to the two calls to lsq_fit. After combining the two errors, in line 52, we update the current best choice for the data set division point in lines 55 through 58.

```
[ 54]  !       does this division gives you a smaller error ?
[ 55]        if ( error < error_min ) then
[ 56]          error_min = error ; split = j
[ 57]          left      = fit1  ; right = fit2
[ 58]        end if ! current best choice
[ 59]      end do ! of split choices
```

After we exit the loop, at line 59, we simply list the best results obtained. In line 73 we have also deallocated the data arrays even though it is just a formality at this point since all memory is released at the program terminates immediately afterwards. Had this been a subroutine or function then we would need to be sure that allocated variables are released when their access scope has terminated. Later versions of Fortran will do that for you, but good programmers should keep up with memory allocations.

```
[ 60]  !       Display the results
[ 61]      print *, "Two line best fit; combined error is ", error_min
[ 62]      print *, "Best division of the data is:"
[ 63]      print *, "data(:j), data(j+1:), where j = ", split
[ 64]      print *, "Left line fit:"
[ 65]      print *, "the slope is     ", left(1)
[ 66]      print *, "the intercept is ", left(2)
[ 67]      print *, "the error is     ", left(3)
[ 68]      print *, "Right line fit:"
[ 69]      print *, "the slope is     ", right(1)
[ 70]      print *, "the intercept is ", right(2)
[ 71]      print *, "the error is     ", right(3)
[ 72]
[ 73]      deallocate (y, x)
[ 74]  end program two_line_lsq_fit
[ 75]
```

For completeness an input routine, read_xy_file, is illustrated. It is elementary since it does not check for any read errors, and thus does not allow for any exception control if the read somehow fails.

```
[ 76]  subroutine read_xy_file (infile, lines, x, y)
[ 77]  !----------------------------------------------------
[ 78]  ! Take a file number, the number of lines to be read,
[ 79]  !   and put the data into the arrays x and y
[ 80]  !----------------------------------------------------
[ 81]    implicit none
[ 82]    integer, intent(in)  :: inFile     ! unit to read
[ 83]    integer, intent(in)  :: lines      ! length of the file
[ 84]    real,    intent(out) :: x(lines)   ! independent data
[ 85]    real,    intent(out) :: y(lines)   ! dependent data
[ 86]    integer j
[ 87]      rewind (inFile)  ! go to front of the file
[ 88]      do j = 1, lines               ! for the entire file
[ 89]        read (infile, *) x(j), y(j) ! get the x and y values
[ 90]      end do ! over all lines
[ 91]  end subroutine read_xy_file
[ 92]
```

If the supplied data file was huge, say argument lines has a value of ten million, the such data would probably have been stored in a binary rather that a formatted file. In that case we would simply invoke a binary read by re-writing line 89 as

```
[ 89]        read (infile) x(j), y(j) ! binary read of x and y
```

Such a change would yield a much faster input, but would still be relatively slow due to being in the loop starting at line 88. To get the fastest posible input we would have had to have saved the binary data on the file such that all the x values were stored first, followed by all the corresponding y values. In that case, we avoid the loop and get the fastest possible input by replacing lines 88–90 with:

```
[ 88]     ! sequential binary read of x and y values
[ 89]        read (infile) x, y
[ 90]     ! input complete, add iostat for exceptions
```

Here we will not go into the details about how we would have to replace subroutine inputCount an equivalent one for binary files. To do that you will have to study the Fortran INQUIRE statement for files, and its IOLENGTH option to get a hardware independent record lenght of a real variable.

```
[ 93]  !  Given test data in file two_line.dat:
[ 94]  !  0.0000000e+00   1.7348276e+01
[ 95]  !  1.0000000e+00   6.5017349e+01
[ 96]  !  2.0000000e+00   8.7237749e+01
[ 97]  !  3.0000000e+00   1.2433478e+02
[ 98]  !  4.0000000e+00   1.5456681e+02
[ 99]  !  5.0000000e+00   1.8956219e+02
[100]  !  6.0000000e+00   2.1740486e+02
[101]  !  7.0000000e+00   2.3138619e+02
[102]  !  8.0000000e+00   2.7995041e+02
[103]  !  9.0000000e+00   3.1885162e+02
[104]  !  1.0000000e+01   3.4628642e+02
[105]  !  1.1000000e+01   3.3522546e+02
[106]  !  1.2000000e+01   3.7626218e+02
[107]  !  1.3000000e+01   3.9577060e+02
[108]  !  1.4000000e+01   4.2217988e+02
[109]  !  1.5000000e+01   4.3388828e+02
[110]  !  1.6000000e+01   4.5897959e+02
[111]  !  1.7000000e+01   4.9506511e+02
[112]  !  1.8000000e+01   5.0747649e+02
[113]  !  1.9000000e+01   5.2168101e+02
[114]  !  2.0000000e+01   5.2976511e+02
```

Assuming the formatted data are stored in file two_line.dat, as shown above we obtain the best two straight ine fit.

```
[115]  ! Running the program gives:
[116]  !
[117]  ! Enter the data input filename: two_line.dat
[118]  ! There were 21 records read.
[119]  ! Single line fit
[120]  ! the slope is     25.6630135
[121]  ! the intercept is 53.2859993
[122]  ! the error is     343.854675
[123]  ! Two line best fit; combined error is 126.096634
[124]  ! Best division of the data is:
[125]  ! data(:j), data(j+1:), where j = 11
[126]  ! Left line fit:
[127]  ! the slope is     31.9555302
[128]  ! the intercept is 24.9447269
[129]  ! the error is     46.060421
[130]  ! Right line fit:
[131]  ! the slope is     21.6427555
[132]  ! the intercept is 112.166664
[133]  ! the error is     80.0362091
[134]
```

Check this out by plotting the data points and the three straight line segments. Just remember that the first line covers the whole domain, while the second goes only up to halfway between points 11 and 12 while the third line runs from there to the end of the independent data.

C.12 Problem 4.11.15 : Find the next available file unit

The INQUIRE statement has a lot of very useful features that return information based on the unit number, or the file name. It can also tell you how much storage a particular type of record requires (like the sizeof function in C and C++). Here we use only the ability to determine if a unit number is currently open. To do that we begin by checking the unit number that follows the last one we utilized. Line 9 declares that variable, last_unit and initializes it to 0. The save attribute in that line assures that the latest value of last_unit will always be saved and available on each subsequent use of the function. Since the standard input/output units have numbers less that ten we allow the unit numbers to be used to range from 10 to 999, as seen in line 8. However, the upper limit could be changed.

Lines 14–18 determine if the unit after last_unit is closed. If so that unit will be used and we are basically finished. We set the return value, next, update last_unit, and return.

```
[ 1]  function get_next_io_unit () result (next)
[ 2]  ! * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
[ 3]  !      find a unit number available for i/o action
[ 4]  ! * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
[ 5]    implicit none
[ 6]    integer :: next   ! the next available unit number
[ 7]
[ 8]    integer, parameter :: min_unit = 10, max_unit = 999
[ 9]    integer, save      :: last_unit = 0   ! initialize
[10]    integer            :: count           ! number of failures
[11]    logical            :: open            ! file status
[12]
[13]    count = 0 ; next = min_unit - 1
[14]    if ( last_unit > 0 ) then ! check next in line
[15]      next = last_unit + 1
[16]      inquire (unit=next, opened=open)
[17]      if ( .not. open ) last_unit = next ! found it
[18]      return
```

Otherwise, if the unit after last_unit is open we must loop over all the higher unit numbers in search of one that is closed. If we succeed then we update last_unit and return by exiting the forever loop, as seen in lines 24 and 25.

```
[19]    else ! loop through allowed units
[20]      do ! forever
[21]        next = next + 1
[22]        inquire (unit=next, opened=open)
[23]        if ( .not. open ) then
[24]          last_unit = next     ! found it
[25]          exit ! the unit loop
[26]        end if
```

At this point it may be impossible to find a unit. However, with 999 units available it is likely that one that was previously in use has now been closed and is available again. Before aborting we reset the search and allow three cycles to find a unit that is now free. That is done in lines 27–31.

```
[27]        if ( next == max_unit ) then ! attempt reset 3 times
[28]          last_unit = 0
[29]          count     = count + 1
[30]          if ( count <= 3 ) next = min_unit - 1
[31]        end if ! reset try
```

In the unlikely event that all allowed units are still in use we abort the function after giving some insight to why.

```
[32]        if ( next > max_unit ) then ! abort
[33]          print *,'ERROR: max unit exceeded in get_next_io_unit'
[34]          stop    'ERROR: max unit exceeded in get_next_io_unit'
[35]        end if ! abort
[36]      end do ! over unit numbers
[37]    end if ! last_unit
[38]  end function get_next_io_unit
```

C.13 Problem 5.4.4 : Polymorphic interface for the class 'Position_Angle'

```
module class_Position_Angle  ! file: class_Position_Angle.f90
  use class_Angle
  implicit none
  type Position_Angle        ! angle in deg, min, sec
    private
    integer   :: deg, min    ! degrees, minutes
    real      :: sec         ! seconds
    character :: dir         ! N | S, E | W
  end type
```

The above type definitions are unchanged. The only new part of the module for this class is the INTERFACE given in the following four lines.

```
  interface Position_Angle_    ! generic constructor
    module procedure Decimal_sec, Decimal_min
    module procedure Int_deg, Int_deg_min, Int_deg_min_sec
  end interface
contains   . . .
```

Returning to the original `main` program:

```
[ 1]  program main
[ 2]   use class_Great_Arc
[ 3]   implicit none
[ 4]    type (Great_Arc)       :: arc
[ 5]    type (Global_Position) :: g1, g2
[ 6]    type (Position_Angle)  :: a1, a2
[ 7]    type (Angle)          :: ang
[ 8]    real                  :: deg, rad
```

We simply replace all the previous constructor calls with the generic function `Position_Angle_` as shown on lines 8 through 17 below.

```
[ 9]      a1 = Position_Angle_ (10, 30, 0., "N")  ! note decimal point
[10]      call List_Position_Angle (a1)
[11]      a1 = Position_Angle_ (10, 30, 0,  "N")
[12]      call List_Position_Angle (a1)
[13]      a1 = Position_Angle_ (10, 30,     "N")
[14]      call List_Position_Angle (a1)
[15]      a1 = Position_Angle_ (20,         "N")
[16]      call List_Position_Angle (a1)
[17]      a2 = Position_Angle_ (30, 48, 0., "N")
[18]      call List_Position_Angle (a2)
```

C.14 Problem 6.4.1 : Using a function with the same name in two classes

```
include 'class_X.f90'
include 'class_Y.f90'
program main  ! modified from Fig. 4.6.2-3F
  use class_Y, Y_f => f ! renamed in main
  implicit none
  type (X_) :: x, z ; type (Y_) :: y
    x%a = 22              ! assigns 22 to the a defined in X
    call X_f(x)          ! invokes the f() defined in X
    print *,"x%a = ", x%a ! lists the a defined in X
    y%a = 44              ! assigns 44 to the a defined in Y
    x%a = 66              ! assigns 66 to the a defined in X
    call Y_f(y)          ! invokes the f() defined in Y
    call X_f(x)          ! invokes the f() defined in X
    print *,"y%a = ", y%a ! lists the a defined in X
    print *,"x%a = ", x%a ! lists the a defined in X
    z%a = y%a             ! assign Y a to z in X
    print *,"z%a = ", z%a ! lists the a defined in X
end program main                    ! Running gives:
! X_ f() executing            ! x%a = 22
! Y_ f() executing            ! X_ f() executing
! y%a = 44                    ! x%a = 66
! z%a = 44
```

C.15 Problem 6.4.3 : Revising the employee-manager classes

.

The changes are relatively simple. First we add two lines in the `Employee` class:

```
interface setData                ! a polymorphic member
  module procedure setDataE      ; end interface
```

Then we change two other lines:

```
[ 8]    empl = setData ( "Burke", "John", 25.0 )
. . .
[14]    mgr = Manager_ ( "Kovacs", "Jan", 1200.0 ) ! constructor
```

The generic `setData` could not also contain `setDataM` because it has the same argument signature as `setDataE` and the compiler would not be able to tell which dynamic binding to select.

Appendix D

Companion C++ Examples

D.1 Introduction

It is necessary to be multilingual in computer languages today. Since C++ is often used in the OOP literature it should be useful to have C++ versions of the same code given earlier in F90. In most cases these examples have the same variable names and the line numbers are usually very close to each other. This appendix will allow you to flip from F90 examples in Chapter 4 of the main body of the text to see similar operations in C++.

```
#include <iostream.h> // system i/o files
#include <math.h>     // system math files
main ()
// Examples of simple arithmetic in C++
{
 int    Integer_Var_1, Integer_Var_2;  // user inputs
 int    Mult_Result, Div_Result, Add_Result
 int    Sub_Result, Mod_Result;
 double Pow_Result, Sqrt_Result;
 cout << "Enter two integers: ";
 cin >>  Integer_Var_1, Integer_Var_2;

 Add_Result = Integer_Var_1 + Integer_Var_2;
 cout << Integer_Var_1 << " + " << Integer_Var_2 << " = "
      << Add_Result << endl;
 Sub_Result = Integer_Var_1 - Integer_Var_2 ;
 cout << Integer_Var_1 << " - " << Integer_Var_2 << " = "
      << Sub_Result << endl;
 Mult_Result = Integer_Var_1 * Integer_Var_2 ;
 cout << Integer_Var_1 << " * " << Integer_Var_2 << " = "
      << Mult_Result << endl;
 Div_Result = Integer_Var_1 / Integer_Var_2 ;
 cout << Integer_Var_1 << " / " << Integer_Var_2 << " = "
      << Div_Result << endl;
 Mod_Result = Integer_Var_1 % Integer_Var_2; // remainder
 cout << Integer_Var_1 << " % " << Integer_Var_2 << " = "
      << Mod_Result << endl;
 Pow_Result = pow ((double)Integer_Var_1, (double)Integer_Var_2);
 cout << Integer_Var_1 << " ^ " << Integer_Var_2 << " = "
      << Pow_Result << endl;
 Sqrt_Result = sqrt( (double)Integer_Var_1 );
 cout << "Square root of " << Integer_Var_1 << " is "
      << Sqrt_Result << endl;
} // end main, Running produces:
// Enter two integers: 25 4
// 25  +  4  =  29
// 25  -  4  =  21
// 25  *  4  =  100
// 25  /  4  =  6, note integer
// 25  %  4  =  1
// 25  ^  4  =  390625
// Square root of  25  =  5
```

Figure D.1: Typical Math and Functions in C++

```
#include <iostream.h> // system i/o files
main ()
// Examples of a simple loop in C++
{
  int  Integer_Var;

  for (Integer_Var = 0; Integer_Var < 5; Integer_Var ++)
  {
    cout << "The loop variable is: " << Integer_Var << endl;
  } // end for

  cout << "The final loop variable is: " << Integer_Var << endl;

} // end main                               // Running produces:
// The loop variable is: 0
// The loop variable is: 1
// The loop variable is: 2
// The loop variable is: 3
// The loop variable is: 4
// The final loop variable is: 5 <- NOTE
```

Figure D.2: Typical Looping Concepts in C++

```
#include <iostream.h> // system i/o files
main ()
//  Examples of simple array indexing in C++
{
  int MAX = 5, loopcount;
  int  Integer_Array[5] ;
  // or, int  Integer_Array[5] = {10, 20, 30, 40, 50 };

  Integer_Array[0] = 10 ;  // C arrays start at zero
  Integer_Array[1] = 20 ; Integer_Array[2] = 30 ;
  Integer_Array[3] = 40 ; Integer_Array[4] = 50 ;

  for ( loopcount = 0; loopcount < MAX; loopcount ++)
    cout << "The loop counter is: " << loopcount
         << " with an array value of: " << Integer
  // end for loop
  cout << "The final loop counter is: " << loopcount << endl ;

} // end main

//  Running produces:
// The loop counter is: 0 with an array value of: 10
// The loop counter is: 1 with an array value of: 20
// The loop counter is: 2 with an array value of: 30
// The loop counter is: 3 with an array value of: 40
// The loop counter is: 4 with an array value of: 50
// The final loop counter is: 5
```

Figure D.3: Simple Array Indexing in C++

```
#include <iostream.h> // system i/o files
main ()
// Examples of relational "if" operator, via C++
{
  int    Integer_Var_1, Integer_Var_2; // user inputs

  cout << "\nEnter two integers: ";
  cin >> Integer_Var_1, Integer_Var_2;

  if ( Integer_Var_1 > Integer_Var_2 )
    cout << Integer_Var_1 << " is greater than " << Integer_Var_2;

  if ( Integer_Var_1 < Integer_Var_2 )
    cout << Integer_Var_1 << " is less than " << Integer_Var_2;

  if ( Integer_Var_1 == Integer_Var_2 )
    cout << Integer_Var_1 << " is equal to " << Integer_Var_2;

} // end main

// Running with 25 and 4 produces: 25 4
// Enter two integers:
// 25 is greater than  4
```

Figure D.4: Typical Relational Operators in C++

```
#include <iostream.h>
main ()
// Illustrate a simple if-else logic in C++
{
  int Integer_Var;

  cout << "Enter an integer: ";
  cin  >>  Integer_Var;

  if ( Integer_Var > 5 && Integer_Var < 10 )
   {
     cout << Integer_Var << " is greater than 5 and less than 10"
    << endl;  }
   else
   {
     cout << Integer_Var << " is not greater than 5 and less than 10"
    << endl;  } // end of range of input

} // end program main

// Running with 3 gives: 3 is not greater than 5 and less than 10
// Running with 8 gives: 8 is greater than 5 and less than 10
```

Figure D.5: Typical If-Else Uses in C++

```
#include <iostream.h>
main ()
// Examples of Logical operators in C++
{
  int Logic_Var_1, Logic_Var_2;

  cout << "Enter logical value of A (1 or 0): ";
  cin >> Logic_Var_1;

  cout << "Enter logical value of B (1 or 0): ";
  cin >> Logic_Var_2;

  cout << "NOT A is " << !Logic_Var_1 << endl;

  if ( Logic_Var_1  && Logic_Var_2 )
   {
    cout << "A ANDed with B is true " << endl;
   }
  else
   {
    cout << "A ANDed with B is false " << endl;
   } // end if for AND

  if ( Logic_Var_1 || Logic_Var_2 )
   {
    cout << "A ORed with B is true " << endl;
   }
  else
   {
    cout << "A ORed with B is false " << endl;
   } // end if for OR

  if ( Logic_Var_1 == Logic_Var_2 )
   {
    cout << "A EQiValent with B is true " << endl;
   }
  else
   {
    cout << "A EQiValent with B is false " << endl;
   } // end if for EQV

  if ( Logic_Var_1 != Logic_Var_2 )
   {
    cout << "A Not EQiValent with B is true " << endl;
   }
  else
   {
    cout << "A Not EQiValent with B is false " << endl;
   } // end if for NEQV

} // end main
// Running with 1 and 0 produces:
// Enter logical value of A (1 or 0): 1
// Enter logical value of B (1 or 0): 0
// NOT A is 0
// A ANDed with B is false
// A ORed with B is true
// A EQiValent with B is false
// A Not EQiValent with B is true
```

Figure D.6: Typical Logical Operators in C++

```
// Program to find the maximum of a set of integers
#include <iostream.h>
#include <stdlib.h> // for exit
#define ARRAYLENGTH 100
long integers[ARRAYLENGTH];

// Function interface prototype
long maxint(long [], long);

// Main routine

main() { // Read in the number of integers
long i, n;

 cout << "Find maximum; type n: "; cin >> n;
 if ( n > ARRAYLENGTH || n < 0 ) {
   cout << "Value you typed is too large or negative." << endl;
   exit(1);
   } // end if

 for (i = 0; i < n; i++) { // Read in the user's integers
    cout << "Integer " << (i+1) << ": "; cin >> integers[i]; cout
    << endl;  } // end for
 cout << "Maximum: ",  cout << maxint(integers, n); cout << endl;
} // end main

// Find the maximum of an array of integers
long maxint(long input[], long input_length) {
long i, max;

 for (max = input[0], i = 1; i < input_length; i++) {
   if ( input[i] > max ) {
     max = input[i]; } // end if
  } // end for
 return(max);
} // end maxint                   // produces this result
// Find maximum; type n: 4
// Integer 1: 9
// Integer 2: 6
// Integer 3: 4
// Integer 4: -99
// Maximum: 9
```

Figure D.7: Search for Largest Value in C++

```
#include <iostream.h>

// declare the interface prototypes
void  Change    ( int& Input_Val);
void  No_Change ( int  Input_Val);

main ()
//  illustrate passing by reference and by value in C++
{
  int Input_Val;

  cout << "Enter an integer: ";
  cin >> Input_Val;
  cout << "Input value was " <<  Input_Val << endl;

  //  pass by value
  No_Change ( Input_Val );  // Use but do not change
  cout << "After No_Change it is " <<  Input_Val << endl;

  //  pass by reference
  Change ( Input_Val );  // Use and change
  cout << "After Change it is " <<  Input_Val << endl;
}

void  Change (int& Value)
{
//  changes Value in calling code IF passed by reference
  Value = 100;
  cout << "Inside Change it is set to " << Value << endl;
}

void  No_Change (int Value)
{
//  does not change Value in calling code IF passed by value
  Value  = 100;
  cout << "Inside No_Change it is set to " << Value << endl;
}
//   Running gives:
// Enter an integer: 12
// Input value was 12
// Inside No_Change it is set to 100
// After No_Change it is 12
// Inside Change it is set to 100
// After Change it is 100
```

Figure D.8: Passing Arguments by Reference and by Value in C++

```
#include <iostream.h>
main ()
// Compare two character strings in C++
// Concatenate two character strings together
{
  char String1[40];
  char String2[20];
  int  length;

  cout << "Enter first string (20 char max):";
  cin >> String1;

  cout << "Enter second string (20 char max):";
  cin >> String2;

  // Compare
  if ( !strcmp(String1, String2) ) {
    cout << "They are the same." << endl;
    }
    else {
    cout << "They are different." << endl;
    } // end if the same

  // Concatenate
  strcat(String1, String2) ; // add onto String1

  cout << "The combined string is: " << String1 << endl;
  length = strlen( String1 );
  cout << "The combined length is: " << length << endl;
  length = strlen( String1 );

} // end main
// Running with "red" and "bird" produces:
// Enter first string (20 char max): red
// Enter second string (20 char max): bird
// They are different.
// The combined string is: redbird
// The combined length is: 7
// But, "the red" and "bird" gives unexpected results
```

Figure D.9: Using Two Strings in C++

```
#include <iostream.h>
#include <stdlib.h>
#include <math.h>  // system math files

main()
// Convert a character string to an integer in C++
{
  char Age_Char[5];
  int  age;

  cout << "Enter your age: ";
  cin >> Age_Char;

  // convert with intrinsic function
  age = atoi(Age_Char);

  cout << "Your integer age is "            << age << endl;
  cout << "Your hexadecimal age is " << hex << age << endl;
  cout << "Your octal age is "       << oct << age << endl;

} // end of main

// Running gives:
// Enter your age: 45
// Your integer age is 45.
// Your hexadecimal age is 2d.
// Your octal age is 55.
```

Figure D.10: Converting a String to an Integer with C++

```
#include <iostream.h>

// Define structures and components in C++

struct Person     // define a person structure type
 {
  char   Name[20];
  int    Age;
 };

struct Who_Where  // use person type in a new structure
 {
  struct Person Guest;
  char   Address[40];
 };

// Fill a record of the Who_Where type components
main ()
{
   struct Who_Where  Record;

   cout << "Enter your name: ";
   cin  >>  Record.Guest.Name;

   cout << "Enter your city: ";
   cin  >>  Record.Address;

   cout << "Enter your age: ";
   cin  >>  Record.Guest.Age;

   cout << "Hello " << Record.Guest.Age << " year old "
        << Record.Guest.Name << " in " << Record.Address << endl;
}
// Running with input: Sammy, Houston, 104 gives
// Hello 104 year old Sammy in Houston
//
// But try: Sammy Owl, Houston, 104 for a bug
```

Figure D.11: Using Multiple Structures in C++

Appendix E

Glossary of Object Oriented Terms

abstract class: A class primarily intended to define an instance, but can not be instantiated without additional methods.

abstract data type: An abstraction that describes a set of items in terms of a hidden data structure and operations on that structure.

abstraction: A mental facility that permits one to view problems with varying degrees of detail depending on the current context of the problem.

accessor: A public member subprogram that provides query access to a private data member.

actor: An object that initiates behavior in other objects, but cannot be acted upon itself.

agent: An object that can both initiate behavior in other objects, as well as be operated upon by other objects.

ADT: Abstract data type.

AKO: A Kind Of. The inheritance relationship between classes and their superclasses.

allocatable array: A named array having the ability to dynamically obtain memory. Only when space has been allocated for it does it have a shape and may it be referenced or defined.

argument: A value, variable, or expression that provides input to a subprogram.

array: An ordered collection that is indexed.

array constructor: A means of creating a part of an array by a single statement.

array overflow: An attempt to access an array element with a subscript outside the array size bounds.

array pointer: A pointer whose target is an array, or an array section.

array section: A subobject that is an array and is not a defined type component.

assertion: A programming means to cope with errors and exceptions.

assignment operator: The equal symbol, “=”, which may be overloaded by a user.

assignment statement: A statement of the form “variable = expression”.

association: Host association, name association, pointer association, or storage association.

attribute: A property of a variable that may be specified in a type declaration statement.

automatic array: An explicit-shape array in a procedure, which is not a dummy argument, some or all of whose bounds are provided when the procedure is invoked.

base class: A previously defined class whose public members can be inherited by another class. (Also called a super class.)

behavior sharing: A form of polymorphism, when multiple entities have the same generic interface. This is achieved by inheritance or operator overloading.

binary operator: An operator that takes two operands.

bintree: A tree structure where each node has two child nodes.

browser: A tool to find all occurrences of a variable, object, or component in a source code.

call-by-reference: A language mechanism that supplies an argument to a procedure by passing the address of the argument rather than its value. If it is modified, the new value will also take effect outside of the procedure.

call-by-value: A language mechanism that supplies an argument to a procedure by passing a copy of its data value. If it is modified, the new value will not take effect outside of the procedure that modifies it.

class: An abstraction of an object that specifies the static and behavioral characteristics of it, including their public and private nature. A class is an ADT with a constructor template from which object instances are created.

class attribute: An attribute whose value is common to a class of objects rather than a value peculiar to each instance of the class.

class descriptor: An object representing a class, containing a list of its attributes and methods as well as the values of any class attributes.

class diagram: A diagram depicting classes, their internal structure and operations, and the fixed relationships between them.

class inheritance: Defining a new derived class in terms of one or more base classes.

client: A software component that users services from another supplier class.

concrete class: A class having no abstract operations and can be instantiated.

compiler: Software that translates a high-level language into machine language.

component: A data member of a defined type within a class declaration

constructor: An operation, by a class member function, that initializes a newly created instance of a class. (See default and intrinsic constructor.)

constructor operations: Methods which create and initialize the state of an object.

container class: A class whose instances are container objects. Examples include sets, arrays, and stacks.

container object: An object that stores a collection of other objects and provides operations to access or iterate over them.

control variable: The variable which controls the number of loop executions.

data abstraction: The ability to create new data types, together with associated operators, and to hide the internal structure and operations from the user, thus allowing the new data type to be used in a fashion analogous to intrinsic data types.

data hiding: The concept that some variables and/or operations in a module may not be accessible to a user of that module; a key element of data abstraction.

data member: A public data attribute, or instance variable, in a class declaration.

data type: A named category of data that is characterized by a set of values. together with a way to denote these values and a collection of operations that interpret and manipulate the values. For an intrinsic type, the set of data values depends on the values of the type parameters.

deallocation statement: A statement which releases dynamic memory that has been previously allocated to an allocatable array or a pointer.

debugger software: A program that allows one to execute a program in segments up to selected breakpoints, and to observe the program variables.

debugging: The process of detecting, locating, and correcting errors in software.

declaration statement: A statement which specifies the type and, optionally, attributes of one or more variables or constants.

default constructor: A class member function with no arguments that assigns default initial values to all data members in a newly created instance of a class.

defined operator: An operator that is not an intrinsic operator and is defined by a subprogram that is associated with a generic identifier.

deque: A container that supports inserts or removals from either end of a queue.

dereferencing: The interpretation of a pointer as the target to which it is pointing.

derived attribute: An attribute that is determined from other attributes.

derived class: A class whose declaration indicates that it is to inherit the public members of a previously defined base class.

derived type: A user defined data type with components, each of which is either of intrinsic type or of another derived type.

destructor: An operation that cleans up an existing instance of a class that is no longer needed.

destructor operations: Methods which destroy objects and reclaim their dynamic memory.

domain: The set over which a function or relation is defined.

dummy argument: An argument in a procedure definition which will be associated with the actual (reference or value) argument when the procedure is invoked.

dummy array: A dummy argument that is an array.

dummy pointer: A dummy argument that is a pointer.

dummy procedure: A dummy argument that is specified or referenced as a procedure.

dynamic binding: The allocation of storage at run time rather than compile time, or the run time association of an object and one of its generic operations..

edit descriptor: An item in an input/output format which specifies the conversion between internal and external forms.

encapsulation: A modeling and implementation technique (information hiding) that separates the external aspects of an object from the internal, implementation details of the object.

exception: An unexpected error condition causing an interruption to the normal flow of program control.

explicit interface: For a procedure referenced in a scoping unit, the property of being an internal procedure, a module procedure, an external procedure that has an interface (prototype) block, a recursive procedure reference in its own scoping unit, or a dummy procedure that has an interface block.

explicit shape array: A named array that is declared with explicit bounds.

external file: A sequence of records that exists in a medium external to the program.

external procedure: A procedure that is defined by an external subprogram.

FIFO: First in, first out storage; a queue.

friend: A method, in C++, which is allowed privileged access to the private implementation of another object.

function body: A block of statements that manipulate parameters to accomplish the subprogram's purpose.

function definition: Program unit that associates with a subprogram name a return type, a list of arguments, and a sequence of statements that manipulate the arguments to accomplish the subprogram's purpose

function header: A line of code at the beginning of a function definition; includes the argument list, and the function return variable name.

generic function: A function which can be called with different types of arguments.

generic identifier: A lexical token that appears in an INTERFACE statement and is associated with all the procedures in the interface block.

generic interface block: A form of interface block which is used to define a generic name for a set of procedures.

generic name: A name used to identify two or more procedures, the required one being determined by the types of the non-optional arguments in the procedure invocation.

generic operator: An operator which can be invoked with different types of operands.

Has-A: A relationship in which the derived class has a property of the base class.

hashing technique: A technique used to create a hash table, in which the array element where an item is to be stored is determined by converting some item feature into an integer in the range of the size of the table.

heap: A region of memory used for data structures dynamically allocated and deallocated by a program.

host: The program unit containing a lower (hosted) internal procedure.

host association: Data, and variables automatically available to an internal procedure from its host.

information hiding: The principle that the state and implementation of an object should be private to that object and only accessible via its public interface.

inheritance: The relationship between classes whereby one class inherits part or all of the public description of another base class, and instances inherit all the properties and methods of the classes which they contain.

instance: A individual example of a class invoked via a class constructor.

instance diagram: A drawing showing the instance connection between two objects along with the number or range of mapping that may occur.

instantiation: The process of creating (giving a value to) instances from classes.

intent: An attribute of a dummy argument that which indicates whether it may be used to transfer data into the procedure, out of the procedure, or both.

interaction diagram: A diagram that shows the flow of requests, or messages between objects.

interface: The set of all signatures (public methods) defined for an object.

internal file: A character string that is used to transfer and/or convert data from one internal storage mode to a different internal storage mode.

internal procedure: A procedure contained within another program unit, or class, and which can only be invoked from within that program unit, or class.

internal subprogram: A subprogram contained in a main program or another subprogram.

intrinsic constructor: A class member function with the same name as the class which receives initial values of all the data members as arguments.

Is-A: A relationship in which the derived class is a variation of the base class.

iterator: A method that permits all parts of a data structure to be visited.

keyword: A programming language word already defined and reserved for a single special purpose.

LIFO: Last in, first out storage; a stack.

link: The process of combining compiled program units to form an executable program.

linked list: A data structure in which each element identifies its predecessor and/or successor by some form of pointer.

linker: Software that combines object files to create an executable machine language program.

list: An ordered collection that is not indexed.

map: An indexed collection that may be ordered.

matrix: A rank-two array.

member data: Variables declared as components of a defined type and encapsulated in a class.

member function: Subprograms encapsulated as members of a class.

method: A class member function encapsulated with its class data members.

method resolution: The process of matching a generic operation on an object to the unique method appropriate to the object's class.

message: A request, from another object, for an object to carry out one of its operations.

message passing: The philosophy that objects only interact by sending messages to each other that request some operations to be performed.

module: A program unit which allows other program units to access variables, derived type definitions, classes and procedures declared within it by USE association.

module procedure: A procedure which is contained within a module, and usually used to define generic interfaces, and/or to overload or define operators.

nested: Placement of a control structure inside another control structure.

object: A concept, or thing with crisp boundaries and meanings for the problem at hand; an instance of a class.

object diagram: A graphical representation of an object model showing relationships, attributes, and operations.

object-oriented (OO): A software development strategy that organizes software as a collection of objects that contain both data structure and behavior. (Abbreviated OO.)

object-oriented programming (OOP): Object-oriented programs are object-based, class-based, support inheritance between classes and base classes and allow objects to send and receive messages.

object-oriented programming language: A language that supports objects (encapsulating identity, data, and operations), method resolution, and inheritance.

octree: A tree structure where each node has eight child nodes.

OO (acronym): Object-oriented.

operand: An expression or variable that precedes or succeeds an operator.

operation: Manipulation of an object's data by its member function when it receives a request.

operator overloading: A special case of polymorphism; attaching more than one meaning to the same operator symbol. 'Overloading' is also sometimes used to indicate using the same name for different objects.

overflow: An error condition arising from an attempt to store a number which is too large for the storage location specified; typically caused by an attempt to divide by zero.

overloading: Using the same name for multiple functions or operators in a single scope.

overriding: The ability to change the definition of an inherited method or attribute in a subclass.

parameterized classes: A template for creating real classes that may differ in well-defined ways as specified by parameters at the time of creation. The parameters are often data types or classes, but may include other attributes, such as the size of a collection. (Also called generic classes.)

pass-by-reference: Method of passing an argument that permits the function to refer to the memory holding the original copy of the argument

pass-by-value: Method of passing an argument that evaluates the argument and stores this value in the corresponding formal argument, so the function has its own copy of the argument value

pointer: A single data object which stands for another (a "target"), which may be a compound object such as an array, or defined type.

pointer array: An array which is declared with the pointer attribute. Its shape and size may not be determined until they are created for the array by means of a memory allocation statement.

pointer assignment statement: A statement of the form "pointer-name $\Rightarrow$ target".

polymorphism: The ability of an function/operator, with one name, to refer to arguments, or return types, of different classes at run time.

post-condition: Specifies what must be true after the execution of an operation.

pre-condition: Specifies the condition(s) that must be true before an operation can be executed.

private: That part of an class, methods or attributes, which may not be accessed by other classes, only by instances of that class.

protected: (Referring to an attribute or operation of a class in C++) accessible by methods of any descendent of the current class.

prototype: A statement declaring a function's return type, name, and list of argument types.

pseudocode: A language of structured English statements used in designing a step-by-step approach to solving a problem.

public: That part of an object, methods or attributes, which may be accessed by other objects, and thus constitutes its interface.

quadtree: A tree structure where each tree node has four child nodes.

query operation: An operation that returns a value without modifying any objects.

rank: Number of subscripted variables an array has. A scalar has rank zero, a vector has rank one, a matrix has rank two.

scope: That part of an executable program within which a lexical token (name) has a single interpretation.

section: Part of an array.

sequential: A kind of file in which each record is written (read) after the previously written (read) record.

server: An object that can only be operated upon by other objects.

service: A class member function encapsulated with its class data members.

shape: The rank of an array and the extent of each of its subscripts. Often stored in a rank-one array.

side effect: A change in a variable's value as a result of using it as an operand, or argument.

signature: The combination of a subprogram's (operator's) name and its argument (operand) types. Does not include function result types.

size: The total number of elements in an array.

stack: Region of memory used for allocation of function data areas; allocation of variables on the stack occurs automatically when a block is entered, and deallocation occurs when the block is exited

stride: The increment used in a subscript triplet.

strong typing: The property of a programming language such that the type of each variable must be declared.

structure component: The part of a data object of derived type corresponding to a component of its type.

sub-object: A portion of a data object that may be referenced or defined independently of other portions. It may be an array element, an array section, a structure component, or a substring.

subprogram: A function or subroutine subprogram.

subprogram header: A block of code at the beginning of a subprogram definition; includes the name, and the argument list, if any.

subscript triplet: A method of specifying an array section by means of the initial and final subscript integer values and an optional stride (or increment).

super class: A class from which another class inherits. (See base class.)

supplier: Software component that implements a new class with services to be used by a client software component.

target: The data object pointed to by a pointer, or reference variable.

template: An abstract recipe with parameters for producing concrete code for class definitions or subprogram definitions.

thread: The basic entity to which the operating system allocates CPU time.

tree: A form of linked list in which each node points to at least two other nodes, thus defining a dynamic data structure.

unary operator: An operator which has only one operand.

undefined: A data object which does not have a defined value.

underflow: An error condition where a number is too close to zero to be distinguished from zero in the floating-point representation being used.

utility function: A private subprogram that can only be used within its defining class.

vector: A rank-one array. An array with one subscript.

vector subscript: A method of specifying an array section by means of a vector containing the subscripts of the elements of the parent array that are to constitute the array section.

virtual function: A genetic function, with a specific return type, extended later for each new argument type.

void subprogram: A C++ subprogram with an empty argument list and/or a subroutine with no returned argument.

work array: A temporary array used for the storage of intermediate results during processing.

Appendix F

Subject Index

In the index the F90/95 intrinsic attributes, functions, subroutines, statements, etc. are shown in upper-case letters even though Fortran is not case sensitive. The page numbers are cited with the chapter (or appendix) number followed by a period, followed by the pages in that chapter separated by commas. Topics that occur frequently are only cited at their first few uses.

Appendix G

Program Index