A FORTRAN PRIMER

David A. Clarke Department of Astronomy and Physics Saint Mary's University Halifax, NS, Canada January, 2002 Revised December, 2005

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A FORTRAN PRIMER

I INTRODUCTION

FORTRAN is a FORmula TRANslator which translates formulæ written in the human language of mathematics to the machine language of binary code. FORTRAN allows the programmer to type in expressions at the keyboard reminiscent to how they appear on paper, and through the steps of pre-compiling, compiling, and linking, a binary code executable by the machine is generated.

FORTRAN was designed for scientific computing. Other languages like C, C⁺⁺, Basic, Cobol, PL1, *etc.* all have their proponents, the most militant of which will waste no time in telling you that as a computer language, FORTRAN is on its way out. Yet, at the time of this writing, 90% of all flops¹ "flopped" by scientific applications worldwide are "flopped" by code generated by a FORTRAN compiler². Evidently, as Mark Twain might have put it: *The report of FORTRAN's demise has been greatly exaggerated*!³.

In all likelihood, FORTRAN is the only scientific computer language you will ever *need* to learn. You may want to pick up C^{++} at some time, but it won't be necessary if you know FORTRAN thoroughly. The biggest complaint about FORTRAN by its detractors is that it leads to unstructured, undecipherable "spaghetti code" (*e.g.*, the all-dreaded and overly maligned GOTO statements). Untrue. FORTRAN allows the programmer to write "spaghetti code", but also allows highly structured coding and whether a program is written as "spaghetti code" or not is a function of the programmer's laziness, not of any inherent shortfalls in the language.

The first release of FORTRAN was FORTRAN66 in, perhaps you can guess, 1966. This language was limited, and was used by a relatively small circle of programmers. But demand for the new language grew, and in 1977, FORTRAN77 was released. This was the first comprehensive version of the language, allowing for virtually all functions a scientific programmer could need.

As "structured programming" became the buzz and demand for more abstract programming grew, FORTRAN90 was released, but not until 1994. This long-awaited version underwent many unexpected revisions as the international committee charged with its content haggled over the details. In the 17 years between FORTRAN77 and FORTRAN90, many "nonstandard" features were built into various versions of the language by various vendors. Thus,

¹Flops is "computerese" for FLoating point OPerationS, one of which is required for each add or subtract, four for each multiply, 10 or so for each divide, *etc.*

²To those C users who may doubt this statistic, look carefully at your C compiler. Many C compilers, especially in supercomputing environments, will actually translate some or all of your C to FORTRAN, then use a FORTRAN compiler which is better suited for optimisation!

³Actually, what Mark Twain wrote was *The report of my death was an exaggeration*, but the words *demise* and *greatly* are commonly added, as though Mark Twain's writings weren't colourful enough!

IBM, DEC, Cray, Sun, *etc.*, all offered F77 compilers that contained standard FORTRAN77 plus their own special features, upon which many programmers came to rely. This made FORTRAN much less portable, and some abandoned the language for this reason.

FORTRAN90 was designed to include most of the specialised features invented by some of the largest vendors of FORTRAN77 as well as all the features of FORTRAN77 itself. Thus, programmers who used an extended version of FORTRAN77 suddenly found that their code was again portable, at least with very minor changes to conform to the new standards, and the use of the language began to grow again.

A year after FORTRAN90 was released, FORTRAN95 came out, in large part to respond to the rapidly rising use of massively parallel architecture. FORTRAN95 was also the first version of the language to drop features of FORTRAN66 (*e.g.*, "hollerith strings"), and so is not completely "downwardly compatible". On the other hand, FORTRAN90 is completely compatible with FORTRAN66 and FORTRAN77.

In this primer, a subset of standard FORTRAN77 is described. Any F90 compiler can compile any program written in standard FORTRAN77 (*e.g.*, without any of the vendor-specific extensions used), and if your code is written with only the statements found in this primer, it can be compiled by an F95 compiler as well. This primer assumes the reader has a rudimentary knowledge of UNIX, and in a UNIX environment knows how to create files, directories, move files around, edit text files, and submit commands. No detailed knowledge of UNIX script language is assumed, though the more the reader is familiar with UNIX, the better.

The next section lists the typical steps required to design, develop, and execute a computer program (written in FORTRAN or otherwise), without reference to details of the computer language. Section III is the most important section in this primer, and should be read and understood thoroughly. It gives a sample FORTRAN program that the reader can use as a template for their first programs, and includes a careful description of the code line by line. Attention is paid to what the FORTRAN statements do, and to programming style. Finally, the last two sections, meant as a reference, give more details on the syntax of the language. Section IV discusses variables, variable types, arrays, *etc.*, while Section V gives descriptions of the most commonly used FORTRAN statements. These discussions are by no means exhaustive, and the more experienced programmer will want to consult one of the many comprehensive FORTRAN texts, vendor manuals, and websites available.

II STEPS TO COMPUTER PROGRAMMING

In order to execute a computer program (code), one must:

- 1. Develop the algorithm (*e.g.*, with pen and paper);
- 2. Write the code (using your favourite text editor in your favourite computer language—FORTRAN!);
- 3. Precompile the code (optional);
- 4. Compile the code (f77 -c myprob.f);
- 5. Link the code (f77 myprob.o mylib.a);
- 6. Execute the code (a.out).

f77 refers to the FORTRAN77 compiler which, with the -c option, generates what is called "object code", unreadable by humans and unexecutable by computers. It is an intermediate stage to which other object files can be linked (*e.g.*, mathematical or graphical libraries). The "link" step also uses f77. If there are no libraries to be linked, steps 4 and 5 can be combined into one step, namely f77 myprob.f, in which case no object code is generated, only the executable.

FORTRAN files should end with the suffix '.f'. The corresponding object code, if any, will have the same name, but with suffix .o. Thus, the object code for myprob.f will be in a file called myprob.o. As given above, the link steps generate an "executable" file called a.out, which is the default name (*i.e.*, that given if none is specified). By typing a.out at your cursor, your program will execute. If you wish to call your executable something other than a.out, you can either rename the file once created (*e.g.*, mv a.out myprob.x), or use the -o option in the f77 command (*e.g.*, f77 -o myfile.x myfile.f). If the compile and link steps are split as in the list above, specify the -o option in the link step.

At each step, minor or extensive debugging may be necessary. There are also issues of optimisation, readability, and generality.

- Debugging: the "art" of eliminating errors in syntax (misuse of the FORTRAN language), logic (unintentional "zero-divides" or square roots of negative numbers), implementation (code does not match algorithm), and design (problems with the algorithm itself);
- Optimisation: The "art" of modifying the code without changing the algorithm to take advantage of compiler and hardware features to make best use of your machine (speed and memory);
- Readability: The "art" of designing your code so that others may read, understand, and use what you have created;
- Generality: The "art" of designing your code to be as flexible and general as possible.

Indeed, developing good software is as much of an art as anything else, and your programming skills will be honed more by doing, rather than by pouring over programming texts. This primer is therefore designed to get you started with the least amount of details possible. As such, debugging and optimisation techniques are left beyond the scope of this primer. Instead, emphasis is placed on developing general-use FORTRAN code, a consistent, readable programming style, and ways of avoiding some of the more common traps often encountered by beginning programmers.

III SAMPLE ALGORITHM AND FORTRAN PROGRAM

The mathematical problem of determining the number of prime numbers less than a given integer was known to the Greeks, and to this day, there is no solution, other than by brute force. This section illustrates a computer "solution" to this problem. It is not general because one cannot ask for an arbitrarily high integer; the machine can only handle integers less than roughly 2 billion; anything bigger requires more than 31 bits (the 32nd bit in a four-byte integer is reserved for the sign).

However, this primer is not here to make history, but to illustrate algorithm design and its FORTRAN implementation for a "simple" (easy to pose, if not solve) problem.

3.1 Designing an Algorithm

Algorithm design can take on many forms. In a Computer Science class, your instructor may take great pains to convey to you what key words you should use, or whether a certain step should be encircled by a diamond, oval, rectangle, rounded rectangle, *etc.* We do none of that here. An algorithm starts off as an idea or a problem you wish to solve, and then consists of various stages in which the method of solution is fleshed out. At some point, there is enough meat on the bones that you can use the algorithm you have developed to generate code.

It is probably a good idea not to write your algorithm in the language of computer code (*e.g.*, FORTRAN), but instead in plain English. Invariably, though, as the algorithm develops, most people will start to pepper the English with FORTRAN- or C-type statements, mostly because the computer language is usually so much briefer than grammatically correct English!

In this section, I show you how I went about designing my algorithm to find out how many prime numbers there are below a certain integer, and after this, I give you two versions of the associated FORTRAN code, both fully debugged (*i.e.*, they execute properly), but only one I would be happy to share with a colleague!

Step 1: Statement of the problem

Find all prime numbers less than a given integer.

Report each prime found.

Report the total number of prime numbers found.

Step 2: First refinement

For a given integer, n, one need only examine divisors greater than 1 and less than the square root of n (think about it!).

Check to see if each divisor divides evenly into n.

As soon as one divisor is found, n is not prime. Continue on to the next candidate.

If no divisors are found, n is prime. Report each prime found to both the screen and

a disc file.

Step 3: Second refinement

Open disc file.

Ask user for maximum integer, n_{max} .

Echo input integer to both screen and discfile.

For each integer n less than n_{max} , do:

Find greatest integer less than $\sqrt{n_{\text{max}}}$; call this i_{max} .

For each i, $2 \leq i \leq i_{\text{max}}$, do:

If i goes evenly into n, n is not a prime. Exit loop, and go onto n + 1.

i goes evenly into n if n/i truncated times i equals n.

If there are no even divisors of n, n is prime. List n as a prime integer, add one to the counter, and go onto n + 1.

Close disc file.

At this point, the algorithm is sufficiently refined to generate code, which starts on the next page.

You might wonder how you would go about solving this problem for numbers of truly arbitrary size; that is, how the algorithm presented above might be modified so that it is not limited by the internal representation of integers. This is not a trivial problem!

3.2 Converting the Algorithm to FORTRAN with good Programming Style

My FORTRAN77 implementation of this algorithm is written in my own personal style that I have developed over the past fifteen years, and is full of comments, headers, vertical alignment, indentation of do-loops and if-then-else-endif structures, sensibly chosen variable names, *etc.*, all to make the code as readable as possible by a human. One of the nice things about FORTRAN is it largely reads like English; no crazy punctuation conventions or made-up words to throw you. After the code, I give some description of what each segment does, and after that I give another version of the code written without any regard to readability so that you can compare two extremes of coding style.

You do not need to adopt my programming style, although you may if you wish. However, for the purposes of assignments, no-style coding (*e.g.*, similar to the second version of the program below) will be given very low grades, regardless of whether it works or not! Note that strict adherence of the rules of FORTRAN requires *none* of these styles to be adopted; style is entirely self-imposed.

So why this emphasis on coding style? Two reasons. First, it makes finding errors (bugs) much easier. Second, the code is much more readable. By whom, you might ask? Primarily by you! Much of the coding I generated as a scientist in the last 15 years, I still use today, or

at least some modified version of it. Try digging up some old coding you generated several years ago without comments, structure, or algorithm description, and see how long it takes you to get it going again! In my case, there are probably about 100,000 lines of my coding that are used by other scientists worldwide. These would have been of very little use to anyone had I not adopted a strict set of programming guidelines for myself when I started out. This is true of anybody who has made any impact on the scientific public domain. In this game, it is not at all a bad thing to be a little anally retentive!

As for the program listing which starts below, the first four columns are not part of the FORTRAN statement. I have added these columns to allow for line numbers so I can refer to various lines in my description following the code. Thus, the first character in each FORTRAN statement below actually starts in column 5, so if you are typing the program in at your terminal (problem 1 at the end of the section), the first column you should type for each line is column 5.

FORTRAN statements are never more than 72 columns wide. Any and all characters beyond the 72nd column are ignored. The first six columns are reserved for special "instruction" characters. For example, if the line is to be a comment, the first character must be a 'c', 'C', or a '*'. If the statement is a continuation of the previous line (because 72 characters wasn't enough), then the sixth character should be a non-zero digit (1-9), or the ampersand (&), or the period (.). Finally, if the statement is referred to by another statement (*e.g.*, by a goto statement), then the reference number (target) for that statement goes in the first five columns. There are numerous examples of this in the code below.

The actual FORTRAN statement must start in column 7. However, I always start in column 8, so that any continuation character in column 6 is not butt up against the leading character in my FORTRAN statement. Again, this rule is not *imposed* by FORTRAN, but is *allowed*, and improves readability of the code by human eyes.

1 c =2 c 3 c BEGIN PROGRAM 4 c PRIME \\\\\\\\\\\ 5 c 7 c 8 program prime 9 c ----- lists all prime numbers .le. nmax 10 c abcd:prime <----11 c september, 2001 12 c 13 c written by: A Busy Code Developer 14 c modified 1: by ADCD, October 2001; modularised program by placing the coding that searches for divisors into a separate 15 c 16 c subroutine. 17 c 18 c PURPOSE: This routine generates all prime numbers less than or equal 19 c to the input integer, and reports these in a list printed both to the 20 c screen and a datafile. 21 c 22 c EXTERNALS:

```
23 c
     DIVISOR
24 c
25 c-----
26 c
27
        implicit
                  none
28 c
29
       character*9
                  filename
30
        logical
                   lflag
                  nmax , icount , n
cputot , etime
31
       integer
32
       real
33 c
34
                  tdummy (
       real
                            2)
35 c
                  divisor , etime
36
       external
37 c
38 c-----
39 c
40 c
       Start up CPU time counter.
41 c
42
       cputot = etime ( tdummy )
43 c
44 c
       Open disc file.
45 c
46
        filename = 'prime.txt'
        open (10, file=filename, status='unknown')
47
48 c
49 c
        Input parameter 'nmax', and write opening line to standard output
50 c and 'filename'.
51 c
52
        write( 6,2010)
       read ( 5, *) nmax
write( 6,2011) nmax, filename
53
54
55
        write(10,2020) nmax
56 c
57 c
        Loop over all integers .le. nmax, and report all the prime
58 c numbers.
59 c
        icount = 0
60
        do 10 n=2,nmax
61
62
         call divisor ( n, lflag )
63
         if (lflag .eq. .true.) then
64
           icount = icount + 1
           write(10,2030) n
65
66
         endif
67 10
       continue
68
        write( 6,2040) icount, nmax
69
        write(10,2040) icount, nmax
70 c
        close (10)
71
72 c
73 c
       End CPU time counter, and report time used.
74 c
        cputot = etime ( tdummy ) - cputot
75
        write( 6,2050) cputot
76
77 c
78 c-----
79 c----- Write format statements -----
80 c-----
81 c
```

82 2010 format('PRIME : Enter the maximum integer to be checked for ' 83 1 ,'prime.') 84 2011 format('PRIME : All prime numbers less than or equal to ',i4 85 1 ,' are listed in file ',/ ,'PRIME : ''',a9,'''.') 86 2 87 2020 format('PRIME : The following is a list of all prime numbers ' o/ 2020 format('PRIME : ine following is a list of all prime numbers
88 1 ,'.le. ',i8,'.',/)
89 2030 format('PRIME : ',i9)
90 2040 format('PRIME :',/
91 1 ,'PRIME : There are ',i8,' prime numbers less than or '
92 2 ,'equal to ',i8,'.')
93 2050 format('PRIME :',/
94 1 ,'PRIME : Total cpu usage for this run is ',1pg12.5
95 2 ,' seconds ') ,' seconds.') 95 2 96 c 97 stop 98 end 99 c 101 c 102 c \\\\\\\\\\ END PROGRAM 103 c PRIME \\\\\\\\\\ 104 c 106 c 107 c 109 c 112 c 114 c subroutine divisor (number, lflag) 115 116 c 117 c abcd:prime.divisor <----- determines if input has any divisors 118 c october, 2001 119 c written by: A Busy Code Developer 120 c 121 c modified 1: 122 c 123 c PURPOSE: This routine searches the input number for any divisors 124 c other than 1 and itself. 125 c 126 c INPUT VARIABLES: 127 c number integer for which divisors are sought 128 c 129 c OUTPUT VARIABLES: lflag = .false. if a divisor is found 130 c = .true. if no divisors are found 131 c 132 c 133 c EXTERNALS: [none] 134 c 135 c-----136 c 137 implicit none 138 c logical lflag 139 integer number, imax, i, num 140

```
141
        real
                   \texttt{rnum}
                          , sqrtnum , small
                                         , qty
142 c
                           / 0.0001 /
143
        data
                    small
144 c
145 c-----
146 c
147
        lflag = .true.
148
        if (number .le. 3) return
149 c
150 c
        The maximum divisor that needs to be checked is the greatest
151 c
     integer less than or equal to the square root of the number ('imax').
     The lowest divisor is 2. Thus, check all divisors between 2 and
152 c
     'imax'. As soon as one divisor is found, set 'lflag' to .false.,
153 c
     (i.e., "number" is not prime) and return to the calling program.
154 c
155 c
156
               = real ( number )
        rnum
157
        sqrtnum = sqrt ( rnum )
158
              = int
                    ( sqrtnum + small )
        imax
159
        do 10 i=2,imax
160
          qty = rnum / real ( i )
161
          num = i * int ( qty + small )
162
          if ( num .eq. number ) then
163
            lflag = .false.
164
           return
165
          endif
166 10
        continue
167 c
168
        return
169
        end
170 c
172 c
110 c
       \\\\\\\\\\\
                     ΕND
                          SUBROUTINE
                                                  DIVISOR
174 c
       \\\\\\\\\\\
175 c
```

3.2.1 Delineating Program Modules

Lines 1–7 and 99–105 are how I delineate the beginning and end of the main program, while lines 108–114 and 171–176 delineate the subroutine. These are all "comment" statements, which can be placed anywhere in the code, and must have the character 'c', 'C', or '*' in the first column. There is nothing that makes reading a program more difficult than when you can't tell when you've passed from one module to another.

FORTRAN programs are divided up into the "main" program, and various "subroutines" or "functions" that help modularise the program. Subroutines and functions are useful if a particular programming unit appears more than once in a program, if a program module needs to be used by more than one program, or if you wish to encapsulate logical units in separate modules. The latter use makes a program read more like the algorithm, and thus makes it more readable in general by a human. In this example, I have relegated the search for divisors to a separate subroutine for this very reason.

3.2.2 The Program Statement and Selecting a Name for your Program

The program statement (line 8) is always the first non-comment statement in a program. The name of the program is entirely up to you, but keep it, and names of all subroutines and functions, to eight characters or less. FORTRAN is case insensitive, and I tend to use lower case for everything. You can mix lower and upper case as you like, the FORTRAN compiler makes no distinction. Thus, program modules PRIME and prime are the same, variables NMAX and nmax are the same.

Usually, I name the file containing the program (main routine plus its subroutines and functions) the same as the main routine with a .f appended to it, though this is not necessary. Thus, the above program exists on my disc as a file named prime.f. If the compiler should find syntax errors (illegal FORTRAN usage) anywhere in your program, it will refer to the name of the program module (*e.g.*, prime or divisor), not the name of the file (*e.g.*, prime.f), when it tells you where the syntax errors are.

3.2.3 Program History

The comments in lines 9-24 provide a history of the module **prime**. This is not 'fluff'. If you ever use any of your software again after several months of non-usage, you will breathe a sigh of relief when you find some history information in the header. This will reassure you that you have found the right version of the code, that the module does what you think it does, *etc.*

3.2.4 Declaration Statements

I start and end my declaration sections (lines 25–38 and 135–145) with a single line clearly demarcating it from the header above and the body of the FORTRAN code below. The declarations are a critical part of the code, and must be easy to spot. There are several items of note here, all in the realm of coding style.

1. The implicit none statement (lines 27 and 137) forces you to declare all your variables as type character, integer, real, or logical. FORTRAN treats variables of these types differently, and so you cannot mix these types in the same statement without due care. Thus, if the variable filename is to contain the name of the file, it is a character string, and cannot be set, for example, to an arithmetical expression involving numbers. While this may seem obvious, what may not be so obvious is that integers and real numbers are treated differently too, and cannot be mixed either. Thus, if nmax is an integer, and sqrtnmax is real, you cannot set

sqrtnmax = sqrt(nmax)

because the intrinsic function⁴ sqrt is expecting a real number, not an integer. Fortunately, there are intrinsic functions that will allow conversions between reals and

⁴Intrinsic functions are operations that come with the compiler; that is you can use these without having to write a separate function or subroutine to do the operation. The most frequently-used intrinsic functions (such as square roots, trig functions, type conversion, *etc.*) are described in \S V.

integers, and so their arithmetic can be mixed when needed. There are examples of this in this program.

Without implicit none, all variables beginning with the letter 'i', 'j', 'k', 'l', 'm', and 'n' are assumed to be integers, and all the rest are assumed to be real. Or, for example, you can use the implicit feature to tell the compiler that all variables starting with the letter 'c' are character*8, and all variables starting with the letter 'l' are logical. While this may be convenient, it is widely recognised as sloppy coding. Declaring implicit none forces you to declare each variable deliberately in the declarations list, and any variable found in the program not declared in the declaration list will generate a compiler error. Thus, you are safeguarded from misspelling a variable somewhere in your program which, had you used implicit declarations, would have been assumed to be a brand new variable, initialised accordingly (usually to zero or the null string), and computation would resume, usually incorrectly and without warning.

- 2. Enforcing vertical alignment means that I allow eight spaces for each variable name in the declaration lists, regardless of whether the variable has eight characters or not (hence the four spaces between **nmax** and the following comma in line 31). Frequently, you will have a program in which there are many similarly named variables, and having them all vertically aligned means that a quick scan can tell whether or not a variable has been forgotten, misspelled, *etc.*
- 3. Line 34 shows how an array (albeit a very small one) is declared.
- 4. External statements (line 36) list all subroutines and functions called by the module, and is used in the spirit that all variables be declared; it is simply good programming practise.
- 5. There is some restriction to the order in which statements must occur. The program statement is always first. Next, is the implicit statement, followed by the declarations of variables and parameters in any order (character, integer, logical, real, real*8, parameter). Next, equivalence, common, data, and external statements, in any order, are given, followed finally by the text of the program.

3.2.5 The Body of the Main Program

Lines 39–98 comprise the "body" of the "main" program. There are a number of things of note here as well:

1. Line 42 initialises the cpu⁵ time counter so that lines 75 and 76 can report the cpu required to execute the program. Note that the function invoked to "glance at the cpu clock" (etime) is *not* an intrinsic function to FORTRAN, but a special extension of the SOLARIS FORTRAN compiler. Each operating system will have their own such extensions, and you will need to consult the relevant manuals to determine what these are.

⁵Computer Processing Unit; the "smarts" of the computer.

2. Line 46 shows how a character variable is set. It is also possible to set a specific portion of the variable, leaving the rest as is. Thus, if later on I wished to change filename to 'prime.num', I could either set:

filename = 'prime.num'

which overwrites the entire value of the variable, including that portion which did not change, or I could reset only that portion I wish to change:

filename(7:9) = 'num'

leaving the first 6 characters (prime.) as they were. Note that the variable filename was declared as a character*9 variable (line 29), and thus filename can contain no more than nine characters.

- 3. Again in line 46, note the single space on each side of the equals sign. This is not required in FORTRAN, but adds enormously to the readability of the program, particularly when there are a lot of equations. In addition, I typically surround + * / operators (plus, minus, multiply, divide) with single spaces to improve readability.
- 4. Line 47 shows how to open a file on disc. It makes a specific link between a disc file filename (set to 'prime.txt' on line 46) and unit 10, which is how the FORTRAN program will refer to this file until it is "closed" in line 71. So later, when I want to write something to the file prime.txt, the write statements in lines 55, 65, and 69 refer to the unit number rather than the file name. The status variable in the open statement indicates whether the file is new, (thus, a new file named prime.txt is created unless such a file already exists, in which case an error message is generated and execution aborted to protect you from unwittingly overwriting a file you may wish to keep), old, (thus an existing file named prime.txt is opened so the file may be modified, unless the file doesn't already exist, in which case an error message is generated and execution aborted), or unknown (in which case a file is created if none exists, or opened if one already exists, as in this example).
- 5. Lines 52-55 are read/write statements. For both, the first argument in parentheses refers to the unit. Since unit 10 is attached to the disc file prime.txt, the write statement to unit 10 (line 55) adds data to this file. For the write statement, unit 6 refers to "standard output" by default (normally the computer screen in front of you), and for the read statement in line 53, unit 5 refers to "standard input" by default (again, the computer screen in front of you, and in particular, the data you type at the cursor).

What is read/written by a read/write statement are the values of the variables, if any, following the parentheses (e.g., nmax in lines 53-55). How these data are written is determined by the "format statement" referenced by the second argument in the parentheses. In line 52, the second argument, 2010, refers to line 82 in which the first four columns contain the target number 2010. Since no variables are listed after the parentheses in line 52, format statement 2010 just provides the text (contained in single quotes) to be written to the specified unit, which in this case is 6, your computer screen. This particular write statement prompts you to enter the datum required by the program to do what it is designed to do, namely list off all the primes less than this input value.

Line 53 is the read statement, and execution is paused until you enter the data required (*i.e.*, enough numbers of the right type to assign values to all variables listed after the parentheses, which in this case, is just nmax). With unit 5 (terminal screen) specified, you enter data right at the cursor, and hit return or enter when you are done. If the read statement refers to a unit number attached to a disc file, that disc file would have had to be opened by a previous open statement, and would have to exist on disc with the data in the expected format.

When entering the value for nmax at the screen (unit 5), take care to enter an integer, since nmax is declared as an integer by line 31. Thus, if you want to enter one thousand, enter 1000, not 1000.0 which by virtue of the '.0' is real. Commas are also not allowed. Don't enter 1,000 for example.

The second argument in the parentheses of the **read** statement on line 53 is an asterisk (*), which means you are using an "unformatted **read** statement". This instructs the computer to read in whatever you enter and deal with it in a "sensible" way. This means, of course, that the person who designed this portion of the compiler had to do a lot of programming (the compiler is a computer program too!) to allow for whatever you or I might have had a whim to do, and to generate sensible error messages if we make one of the many possible errors, each of which have to be specifically anticipated. So, for example, the compiler needs to be able to detect if you've entered in a character string when what is required is a real number, and it then has to generate an error message to tell you what you did wrong. What if you use a comma instead of a period for the decimal point? What if you enter too much data, or not enough? And so it goes.

Instead of the asterisk, you may specify the target for a format statement as you did for the write statement. However, if you do use what is called a "formatted read statement", the data you enter must appear *exactly* as specified by the format statement (see §5.8 for details).

Lines 54 and 55 are formatted write statements that write the contents of nmax according to the rules of format statements 2011 and 2020 (discussed below in point 6, and further in §5.7). The first writes to your screen (unit 6) and the second to the file prime.txt (unit 10). The latter will remain as the permanent copy of the results of executing the program long after the results flashed to your screen have scrolled out of sight.

Note the use of vertical alignment; extra spaces are inserted before the * in the read statement so that the close-parentheses will all align in the read and write statements. Obviously, this is hardly needed here. I do it as a matter of habit, without thinking

so that when vertical alignment is needed (to make reading many lines of complicated formulæ a lot easier), it is always there.

6. Lines 60-67 comprise the main loop of the program. The variable icount will be the total number of prime numbers found. Line 60 initialises this counter to zero, then line 64 adds one to icount whenever another prime number is found. Note that line 64 makes no sense algebraically, if one thinks of = as a true 'equals sign'. If 63 were a true algebraic statement, one could then subtract icount from each side, and arrive at the astounding result that 0 = 1! Rather, in FORTRAN, = is an *assignment* symbol, and in a statement such as icount = icount + 1, we read "Replace the contents of the variable icount with icount + 1".

The do-loop structure is one of the most commonly used and powerful structures in FORTRAN (§5.1). Statement 60 states, in English, "Repeat all instructions from here to target 10 (line 67) as many times as required for the counter n to go from 2 to nmax when n is incremented by 1. If n is to be incremented by a number other than 1, the increment must be specified after nmax. Thus, do 10 n=3,nmax,2 would mean "do for every n between 3 and nmax counting by twos". Thus, n=3,5,7,...,nmax or nmax-1, whichever is odd.

While it is not necessary to indent do-loops and if-then-else-endif structures, it vastly improves readability, so we do it. Again, I indent by habit. That way, all my software has the same readability. You may argue, "Well, for this one eensy-weensy program, I don't need to bother with indenting." But what if this program then makes the core of a larger one, that is then expanded again to make a still-larger one? When *do* you start to indent? And then do you have to go back to all the old coding, and retro-indent all that once you have decided the code has grown long enough? What a pain! Like most things in life, it usually takes no more time to do a job well than to do it poorly, so you may as well get into the "indenting, vertical alignment, extra spaces around arithmetical operators habit" right away!

Line 62 is a call to the subroutine divisor which appears after the main program (lines 108–176). Logically, you can think of line 62 as being replaced by the "guts" of the subroutine divisor. The use of subroutines (and functions) is strictly for making your program more useful and readable to the human, not for the computer. We use a subroutine (or a function) for the following reasons:

- If a module appears more than once in a program, the subroutine allows you to write the logic out only once and then call it as often as needed.
- If the module is used by several programs, it makes sense to put it into a separate subroutine in a separate file (library) so that you don't have to have several copies of the same module. This is particularly critical if you ever have to update the algorithm in the affected subroutine. Wouldn't it be a pain if you had to update the same subroutine in twelve different programs, then check and debug each to make sure you updated each right, only to realise months later that there were

four more copies of the same subroutine in four other programs that you don't use very often and forgot about?

• To segregate logically separate modules or ideas of the program from each other. Often, a subroutine call represents a single statement or paragraph of a welldesigned algorithm, and thus relegating each logical unit to a subroutine makes the main program read like the algorithm itself; a laudable goal for any good programmer.

Line 62 is typical of a call to a subroutine. The arguments listed parenthetically beside the subroutine name are variables passed between the calling routine (prime) and the subroutine (divisor). These variables could be data needed by the subroutine to do its task or data generated by the subroutine needed by the calling routine to continue its task. In this case, the variable n is passed to divisor (the quantity to be checked for divisors), and the logical variable lflag is returned to the calling routine to indicate whether n has a divisor nor not.

There must be a one-to-one correspondence between the variable types (integer, real, *etc.*) in the calling statement (line 62) and the subroutine declaration statement (line 115). However, the actual variable names need not be the same. In this case, I have elected to call the input integer number in the subroutine divisor but n in the calling routine prime. Conversely, the logical variable lflag has the same name in both prime and divisor.

A logical variable (*e.g.*, lflag) is different from a real or integer variable. It occupies much less memory (usually only one byte rather than four or eight bytes for a real or integer) and can take on only one of two values, either .true. or .false. (*e.g.*, as set in line 147). Note the periods before and after the variable value; these are as much a part of the value as the digit 1 is part of the real value 1.25. Line 63 then tests the value of lflag as set by the subroutine divisor. In English, we would read "If lflag is true, then perform the statements up to and including the next endif statement. Otherwise, skip on past the next endif statement, and carry on from there." Note the use of .eq. instead of =, again with the periods. This is interpreted by the compiler as a "logical equal" rather than an "assignment" as specified by '='. Other logical comparisons are possible, including .ne., .gt., .lt., .ge., and .le.. For "if-tests" (*i.e.*, the phrases enclosed by parentheses after the word if in the if-statement; see §5.2 and §5.3) involving logical variables, inequalities (.gt., *etc.*) make no sense, and only .eq. and .ne. are legal. Thus, the following three statements are synonymous:

if (lflag .eq. .true.) then
if (lflag .ne. .false.) then
if (lflag) then

While the following three equivalent statements are opposite to those above:

if (lflag .eq. .false.) then
if (lflag .ne. .true.) then
if (.not. lflag) then

In each set of three statements above, the last statement [if (lflag) then and if (.not. lflag) then] are carry-overs from FORTRAN66. In general, it is better practise to avoid these.

7. Lines 82–95 are the format statements. These may be placed *anywhere* in the program, including before the write statement that calls them. I prefer to place them all at the end of the program module rather than cluttering up the program logic by placing them directly after the write or read statement that first references them.

Format statements contain explicit instructions on how the output is to be written, or how the input is to be read. The few statements here provide some examples. Each instruction, or "format code" within a format statement is separated by commas. For example, lines 87–88 comprise one statement that is too long for one line. Thus, column 6 in line 88 contains the digit 1, indicating this is a continuation from line 87. In this format statement, there are five separate format instructions. The first instruction, which fills most of line 87, is to write the text "PRIME : The following is a list of all prime numbers". The second instruction, which starts off continuation line 88, is to write the text ".le. " immediately following the text written by the instruction on line 87. The third instruction is to write the integer variable nmax (line 55), as an eight-digit integer (i8). The fourth instruction is to write a period, and finally the fifth instruction is to add a blank line afterwards (/). The first four instructions together form a complete sentence, while the last instruction is effectively a "carriage return", generating an extra blank line to make the output more readable.

More complete syntax rules for format statements are given in §5.7 and §5.8.

8. Line 97 is the stop statement, which flushes the program out of computer memory and releases the computer chip for the next task. Generally, if there is no stop statement in the program (in either the main routine or any of the subroutines), the compiler will issue an error message. However, it is possible to outsmart the compiler by making it impossible logically for execution to reach a stop statement. In this case, the computer will be left hanging after execution is complete, until some abort signal is sent to the cpu (*e.g.*, control-c).

While the **stop** statement need not be the second last line of the main routine, it often is. The last line of a module, lines 98 and 169, is always an **end** statement which tells the compiler to cease reading statements as part of the current module.

3.2.6 The Subroutine

Line 108–176 comprise the subroutine divisor. Many of these statements have been described or addressed already, but a few additional points of interest remain:

1. The data statement (line 143) is a useful way to set constants that are to remain the same throughout execution (though they could be changed by subsequent assignment statements if desired). In this case, the value for small is set to 0.0001. If there were

other variables to set by the same data statement, one would add them after small separated by commas, and their corresponding values would be listed between the slashes, also separated by commas. For more than one value in the data statement, I often list them "stacked" (with the variable name appearing directly above its value), and/or leave enough blanks between each variable name so that each variable name takes up eight characters. Again, this is strictly for ease of reading by a human. Thus, suppose there were four variables instead of one, namely tiny, small, big, and huge. My data statement would then look like this:

real tiny , small , big , huge data tiny , small , big , huge 1 / 1.0e-32 , 0.0001 , 1000.0 , 1.0e32 /

The vertical alignment allows for no mistaking what value is assigned to each variable. Note also how scientific notation is expressed for single-precision real variables $(1.0e-32 = 1.0 \times 10^{-32})$. For double-precision (real*8) variables, one uses a d instead of the e. Thus, $1.0 \times 10^{99} = 1.0d99$.

- 2. Line 148 acknowledges the fact that 2 and 3 are already prime, and so there is no need to go through the motions to see if these have any divisors. Thus, execution is returned straight away with the logical variable lflag set to .true. (*i.e.*, number is prime).
- 3. Note the vertical alignment in lines 156–158. I want the square root of number, but number is an integer, and I cannot take the square root of an integer because the square root intrinsic function sqrt expects a real number (single or double precision) as an argument (§5.9.2). Thus, by using the intrinsic function real (§5.9.13), line 156 converts the value of the integer number to real, and assigns the real variable rnum that value. Thus, if number=1000, line 156 would assign rnum=1000.000, seven digits of accuracy for a four byte ("single precision") real number.

Now, one thing one has to realise about a computer is it is not always as accurate as you might expect. On some compilers, 1000 might get converted to 999.9999 or 1000.001, rather than 1000.000. These inaccuracies are usually infrequent and innocuous, though on some rare occasions, they can lead to very wrong answers. If high accuracy is required, one can use so-called "double-precision" real numbers (declared as real*8 instead of real), or one can make some minor alterations to the algorithm to account for such potential problems, as done in line 158.

Line 158 converts the square root of **rnum** back to an integer, using the intrinsic function **int** (opposite operation of **real**). This conversion is done by truncation, not by rounding. Thus, **6.928** (the square root of **48**) gets truncated back to **6** when converted to an integer, not rounded up to **7**.

Here is where the addition of small comes in in line 158. Because integer-real (in computerese, "fixed-float") conversions are not 100% accurate, it is quite possible that number=100 gets converted to rnum=100.0000, and then sqrtnum=9.999999 because of floating truncation errors peculiar to the compiler. Thus, because int truncates

always, int(sqrtnum)=9, and not 10 as it should be. Since these truncation errors are always small (1 in the last digit of accuracy at the very most), adding just a very small number (*e.g.*, small=0.0001) to sqrtnum before converting it back to an integer means that the number 10.000099 gets truncated by int to 10 rather than 9.999999 getting truncated to 9. Note that in all other situations, adding small to sqrtnum would not be enough to change the value of imax.

4. In lines 159–166, the main loop of the subroutine checks the input integer number for all possible divisors, with the counter of the do-loop being used as the candidate divisor. Lines 160 and 161 are the guts of the algorithm, which use the real and int intrinsic functions to determine if i divides evenly into number. Note the use of small again to avoid unfortunate truncation errors in the conversions.

Line 162 performs the salient test. Should the test be true, then an exact divisor of number has been found, the logical variable lflag is set to .false. (*i.e.*, number is not a prime), and execution is returned to the main program even before do-loop 10 is finished, since there is no need to look further for divisors.

On the other hand, should execution get to line 168, then number was found to have no divisors. Execution is returned to the calling routine with lflag left as .true. (yes, number is a prime) by virtue of line 147 and because line 163 was never reached to reset it to .false..

3.3 Poor Programming Style

I will now give you the same program but without any indentation, comments, *etc.* It is logically identical to the program given at the top of this section, and almost a factor of five shorter! But which would you rather have to face for the first time, and be asked to tell your boss what it does in ten minutes?

1		program main
2		<pre>open(10,file='main.txt',status='unknown')</pre>
3		write(6,8)
4	8	<pre>format('Enter nmax')</pre>
5		read(5,*)nmax
6		m=0
7		do 9 n=1,nmax
8		ii=1
9		if(n.le.3)goto 9
10		r=real(n)
11		s=sqrt(r)
12		<pre>imax=int(s+.0001)</pre>
13		do 1 i=2,imax
14		q=r/real(i)
15		num=i*int(q+.0001)
16		if(num.eq.n)then
17		ii=0
18		goto 1
19		endif

20	1	continue
21		if(ii.eq.1)then
22		m=m+1
23		write(6,17)n
24		write(10,17)n
25	17	format(i9)
26		endif
27	9	continue
28		write(6,3)m
29		write(10,3)m
30	3	<pre>format(/,'m=',i4)</pre>
31		close(10)
32		stop
33		end

IV DATA TYPES AND STRUCTURES

4.1 Variables

Variables play the same role in FORTRAN as they do in algebraic equations; they represent quantities whose values are to be determined by the calculation. In general, most variables you use will be temporary, and represent intermediate steps in what may be a rather complex calculation. A few of the variables will contain the actual data needed, and you as the programmer will have to arrange to have them printed to the screen, disc, or presented in a graphical format.

Unlike variables in algebraic equations, the computer does not actually manipulate the symbols themselves⁶, but instead stores their numerical values. The name of the variable you assign is actually mapped by the compiler to a specific area of memory which will be used to contain the current value of that variable as the calculation proceeds.

Also, unlike algebraic equations, variable names are restricted to letters (a-z, A-Z), digits (0-9), and the underscore $(_)$, with the proviso that all variables shall start with a letter. No other punctuation (!, @, #, etc.) may be used. Thus, variable names can contain no Greek letters, no subscripts, no parentheses, etc. You may use up to eight characters for each variable name. You may use UPPER CASE or lower case or both, knowing that FORTRAN compilers make no distinction; they are case-insensitive. Thus NMAX, Nmax, and nmax would all be treated as the same variable.

When selecting names for your variables, make sure each name describes what the variable is. Thus, if you have a program which deals with the ideal equation of state;

$$PV = NRT; \quad T = \frac{P}{R}\frac{V}{N} = \frac{P}{R\rho_m}$$
 (1)

where $\rho_m = N/V$ is the molar density (moles per unit volume), you might represent this in a FORTRAN code as:

```
temp = pressure / ( gasconst * mol_den )
```

which is preferable to:

$$T = p / (R * rho)$$

since it is considered better programming style to avoid single-character variable names. Ideally, you would like your variable name to be a (nearly) unique combination of characters so that an electronic search in your program file for a particular variable picks up only the variable you are looking for, and not all occurrences of the letter **p**, for example, for which there may be hundreds of occurrences in a long, well-commented program. Still, this is much better than:

a=b/c/d

 $^{^{6}}$ There are so-called *symbolic manipulating* programs, such as *Mathematica* and *Maple*, but we're not talking about these here.

which is perfectly legal in FORTRAN and would still give you the right answer so long as **a** were temperature, **b** were pressure, **c** were the gas constant, and **d** were the molar density, but where nothing about the variable name is a mnemonic for what the variable is.

4.2 Variable types

Variables come in many types, the most common of which are integer, character, logical, real, and real*8. Other types include complex, real*16, integer*2, *etc.*

Variable type is declared using declaration type statements:

ivar
cvar
lvar
rvar
dvar

where *ivar* are the integer variables (separated by commas), *cvar* are the character variables, n is an integer greater than zero to indicate the number of characters in each of the variables listed in the character declaration statement, *lvar* are the logical variables, *rvar* are the real variables, and *dvar* are the double-precision real variables. Double precision variables may also be declared as:

double precision dvar

but I shall stick with the real*8 syntax in this primer.

4.2.1 Integer Type

Integer variables consist of a sign (+ or -) and digits, nothing else. -245 and 4609 are valid integers, -245.0 and 4,609 are not (no decimal points and no commas allowed). Computer manuals refer to integers as *fixed* values, and integer arithmetic as *fixed* arithmetic. Fixed arithmetic is exact; no truncation errors are committed during fixed operations, which include addition, subtraction and multiplication. Division is, strictly speaking, *real* arithmetic, as there is the potential for the result not to be an integer. However, one can still divide integers, with the result being truncated to the largest integer less than or equal to the actual ratio. Thus, 3/2 = 1 in fixed arithmetic.

An integer is stored with four bytes, or 32 bits. The bit is the fundamental unit of computer memory, and is how all computers store data. A bit is either "on" (1) or "off" (0). The first bit of an integer stores the sign of the number (+ or -), leaving 31 bits for the number itself. Since a bit can only have one of two values, the computer stores numbers in "binary code", and with 31 bits, the highest number the computer can store is $2^{31} = 2,147,483,648$.

Finally on integers, if you really had to store an integer much bigger than two billion, you could declare a variable to be integer*8, reserving eight bytes for that integer, thus allowing you to access integers to almost *ten pentillion* (10^{19}) , but even this is finite! Note that integer*8 and integer*4 variables are different types, as different as character and logical.

4.2.2 Character Type

Character variables contain characters only, no numerical values. They may contain the text of the title you wish to put on a plot, or text to be printed to the computer screen or a line from a text file.

Each character in a character variable takes one byte, or eight bits thus allowing for as many as $2^8 = 256$ characters. Indeed, the standard "ASCII character set" contains 256 characters, including all lower and upper case Roman letters (52), all digits (10), all punctuation on your keyboard (32), and the blank (1). The remaining 161 characters consist of characters that are not on the standard QWERTY keyboard, including many accented characters used world-wide, other characters used in other alphabets, as well as some characters not found in any alphabet. Consult any comprehensive FORTRAN manual if you need to access the full ASCII set of characters.

Because each character takes one byte of storage, storing the number 2000000000 (two billion) as a character variable would require ten bytes (one for each character). Clearly, the integer type, requiring just four bytes, is a more efficient way of storing numbers than character type.

4.2.3 Logical Type

Logical variables are one byte long, and can have only one of two values: .true. and .false.. Note that the periods are a necessary part of the value, as necessary as the 1 is in the real value 1.25. These values are equivalent to "on" (1) and "off" (0), and in principle should only need one bit, not one byte. However, most computer architecture is such that memory access has one byte resolution, and some hardwares such as some Cray supercomputers can only access its memory with eight-byte resolution. Thus, logical variables consist largely of "unused memory". Still, if the sole purpose of a variable is to act as a toggle, logical type is the most efficient way to go.

4.2.4 Real Type (Single and Double Precision)

Real variables are also referred to as *floating* variables, and real arithmetic as *floating* arithmetic. Like an integer, a real variable uses four bytes of memory, but unlike an integer, a real number is not exact. 1.000000 is the value of one to seven significant digits. What the eighth digit is completely unknown (there is only a one in ten chance of it being a zero), and thus, the real value 1.000000 is not *exactly* one, while the integer 1 is.

The proper syntax of the real number 1.538702×10^{-17} is 1.538702e-17, where the exponent portion may be omitted if it is zero. In general, the first bit of a 32-bit real number is reserved for the sign, the next 25 bits for the mantissa (allowing for seven or eight significant figures), the next bit for the sign of the exponent, and the last 5 bits for the exponent itself⁷ (giving a maximum exponent of $2^5 = 32$). Thus, the greatest number that can be stored as a real number is 3.3554432×10^{32} , or 3.3554432e32 ($2^{25} = 33554432$). Anything larger may generate "overflow" error messages and cause the program to stop, or even worse, generate

 $^{^{7}}$ Some compilers reserve 6 and even 7 bits for the exponent at the expense of the mantissa

no messages and continue erroneously!

So, if 3.3554432×10^{32} is not big enough for your application (the mass of the sun in grams is already too large!), you will have to declare "double precision" (real*8) variables which use eight bytes, or 64 bits per number. In a double precision real value, the first bit is reserved for the sign, the next 52 bits for the mantissa (giving 15 digits of accuracy), the next bit for the exponent sign, and the last 10 bits for the exponent. The largest double precision number you can assign is $4.503599627370496 \times 10^{1024}$ before overflow problems start. If this is still not large enough, redesign your computer program!

These days, most processors use 64-bit technology, making it easier for these machines to process 64-bit numbers than 32-bit numbers. Thus, you may find that double-precision calculations actually run *faster* on 64-bit machines than single-precision calculations. There will come a time when 64-bit numbers are considered "single precision"⁸, and 32-bit numbers "half-precision", just as once upon a time, 2-byte integers were considered "full integers" instead of "half-integers" as they are today. But for now, 32-bit real numbers are still considered single-precision (and therefore the default) and 64-bit real numbers as "double-precision".

When truly accurate (32 digits of accuracy) or truly colossal (up to 10^{10^6}) numbers are required, there is "quad-precision" (real*16). However, I have never come across anyone who has had a legitimate need for these in practise.

Floating arithmetic includes all operations such as square roots (sqrt), trigonometry functions (sin and cos), exponentiation (exp), logarithms (log), *etc.* (§5.9). Floating point arithmetic is approximate, and round-off errors will frequently occur in the last significant digit. This can have annoying consequences when doing logical comparisons. For example, in the following snippet of coding:

```
1 x = 1.0

2 xby4 = x / 4.0

3 if (xby4 .eq. 0.25) then

4 instruction set 1

5 else

6 instruction set 2

7 endif
```

It is quite possible that on some compilers, xby4 might actually be stored as 0.2499999, and the logical test of line 3 would test negative, invoking the second set of instructions (line 6) rather than the intended first (line 4). As it turns out, it is unusual for an algorithm to rely on the exact equality of a real expression; normally one uses inequalities (.lt., *etc.*). However, should an equality such as this be needed, the only fool-proof way of doing it would be to replace line 3 with something like:

3 if ((xby4.lt. 0.2500003).and. (xby4.gt. 0.2499997)) then

where ± 3 in the seventh digit is just from my own personal experience. ± 2 is probably

 $^{^{8}}$ Cray has treated 64-bit (8-byte) numbers as single precision since the 1980s, but at the time of this writing, they remain the only vendor to do so.

fine, while ± 1 may be pushing your luck. Note the introduction of the logical connector .and.. As you might expect, .or. is also available to create more complex logical tests.

4.3 Arrays and Parameters

It is often useful to declare variables analogous to vectors (1-D arrays), matrices (2-D arrays), and beyond (3-D, 4-D, *etc.*)

For example, suppose in a computer program that predicts the weather, you wished to store the temperature at many uniformly spaced points over the surface of the Earth. If your resolution was to be 1 (angular) degree of latitude by 1 degree of longitude, then there would be 180 different latitudes and 360 different longitudes. You could declare $180 \times 360 = 64,800$ different temperature variables, one for each point on the Earth (but don't!), or you could declare a single 2-D temperature array:

real temp (180, 360)

This tells the compiler to reserve enough memory to store 64,800 different real numbers, and that in the program, the variable temp will be treated as an array of 180 columns by 360 rows. Each element of the array, corresponding to a temperature at some point on the Earth, can be addressed individually by specifying temp(i,j), where i is an integer between 1 and 180, and j is an integer between 1 and 360.

Any variable type (integer, logical, *etc.*) can be declared as an array. Arrays are particularly useful when used inside a do-loop ($\S5.1$). Thus, in programming equation (1), you might have:

1	с		implicit	none
3 4	с			idim , jdim (idim=180, jdim=360)
6 7	с		integer real	i , j gasconst
9 10 11		1	real ,	pressure(idim,jdim), mol_den (idim,jdim) temp (idim,jdim)
12 13			external	calcp , calcd
14 15	с		data	gasconst / 8.3147 /
	С		call calcd (do 20 j=1,jdin do 10 i=1,io	

Given that variable arrays **pressure** and **mol_den** are computed by subroutines **calcp** and **calcd** respectively (lines 18 and 19), line 22 calculates the temperature for each (i,j). Note that arrays can be passed as subroutine arguments as well; the only stipulation is that in **calcp**, the variable **pressure**, or whatever it is called there, must be of the same type (real) and have the same dimensions (idim,jdim) as in the calling routine. As in lines 18 and 19, the array dimensions may be passed to the subroutine in the calling list.

This example also illustrates the use of the **parameter** statement (line 4). Like variables, parameters may have any type (integer, logical, real, character which must be declared in an **implicit none** environment) and may be passed as subroutine arguments and used in the right hand side of assignment statements just as constants are used. However, parameters differ from variables in that they may not be arrays, and once assigned by a parameter statement, they may not be re-assigned a value by a regular assignment statement in the program (*i.e.*, they may not appear on the left-hand side of an assignment statement). The nice thing about parameters is that integer parameters may be used to dimension arrays. Thus, should I want to redo this problem but at twice the resolution, I need only change the value of **idim** and **jdim** once in the parameter statement (line 4), and not everywhere they may appear in the declarations (lines 9 and 10).

4.4 Variable Assignments

In the body of the program, variables are assigned values using the "equals sign", and the syntax of the constants depends on the variable type. Examples of such assignments are included in the program "snippet" below.

```
(
                                                               5)
 1
           integer
                          ivar
                                    , i
                                                iarray
 2
           character*12
                          filename
 3
           logical
                          lvar
 4
                                                              5)
           real
                          rvar
                                     r_one
                                                rarray
                                                          (
 5
          real*8
                                                              5)
                                                          (
                          dvar
                                     d_one
                                                darray
 6
  С
 7
   C-
 8 c
 9
                           = 12
           ivar
10
                           = 'output.data
                                                 ,
           filename
11
           filename(8:11) = 'text'
12
                           = .true.
           lvar
13
           rvar
                           = 1.3807e-23
14
           r_one
                           = 1.0
15
                           = 6.6261d - 34
           dvar
16
                           = 1.0d0
           d_one
17
           do 10 i=1,5
18
             iarray(i)
                           = 2 * i
19
             rarray(i)
                           = 2.0 * real ( i ) - 1.0
                             2.0d0 * dble ( i ) - 1.0d0
20
             darrav(i)
21 10
           continue
```

Lines 1 through 5 declare the variables and lines 9–16 assign values to each of the variables. Note that double precision variables use the letter d (*e.g.*, line 15) rather than e (*e.g.*, line 13) to designate the exponent. Line 14 shows that when the exponent is zero, it is not necessary to include it as part of the expression for a single precision (real) value. However, as shown in line 16, the exponent must be included when assigning double precision (real*8) variables, even if it is zero, so that they are distinguishable from single precision (real) values. Note that 1.0 is a single precision value, while 1.0d0 is a double precision value. Thus, the statement d_one = 1.0 when d_one is real*8 is technically mismatched, and on some compilers may cause error messages or worse, unpredictable results elsewhere in the program.

Lines 18, 19, and 20 show simple integer, real, and real*8 arithmetic to assign the five elements in the integer array **iarray** to the even integers up to 10, and the five elements of the real array **rarray** and real*8 array **darray** to the real equivalents of the odd integers up to 9. Note the use of the intrinsic functions **real** and **dble** to convert the integer **i** to real and real*8 respectively, to prevent mixed variable type arithmetic in the assignment statements. The intrinsic function **real** will also accept a real*8 argument and convert it to real, while the intrinsic function **dble** will accept a real argument and convert it to real*8. Finally, note that both constants in line 19 end in .0 (so that they are real and thus avoid mixed variable type arithmetic, while the constants in line 20 end in .0d0 for the same reason.

Many novice programmers will forget to include the conversions (e.g., real) explicitly, or even to put the .0 at the end of real numbers. For example, one might be tempted to write line 19 as:

19 rarray(i) = 2 * i - 1

Indeed, you *may* be able to get away with this, as many compilers will perform the conversions automatically, but this is both careless and dangerous. The conversion rules may not be exactly as you expect, or the compiler may do something entirely stupid like interpret **rarray** as an integer from this point on, yielding unpredictable consequences later on in the computation. If you're doing floating arithmetic, then do floating arithmetic; anything else is sloppy. In line 19, this means using 2.0, not 2; real(i), not i; and 1.0, not 1.

V COMMON FORTRAN STATEMENTS

In this glossary, only the most commonly used FORTRAN statements are described. For each statement listed, a generic example of its usage in a FORTRAN context is given, followed by a description of the program element, as appropriate. In the generic example, key words that are to be used as shown are written in typewriter font. Items appearing in *italics* are intended to be substituted for whatever is needed at that place in the program. Items appearing between square brackets, [], are optional items which, if left out, will invoke sensible defaults.

5.1 do

1do n i=ibeg,iend,[iint]2FORTRAN statement(s)3 ncontinue

where n (the target) is an integer between 1 and 99999 which must appear immediately after the key word do (separated by at least one blank), as well as in the first five columns of the last line of the do-loop, normally a continue statement. The continue statement is a "no-op" (performs no operation), and is used in FORTRAN primarily as targets.

i is an integer variable set by the internal counter of the do-loop, and may not be assigned a value by any statement or operation inside the do-loop itself. It may be *used* inside the do-loop (*i.e.*, it may appear on the right hand side of an assignment statement), but not on the left hand side where variables are assigned. Outside the do-loop, you may treat i as any other variable.

During the first pass of the do-loop, the value of i is *ibeg* and during the last pass, *iend*. At each pass, i is incremented by *iint* which, if left out, is assumed to be 1. For *iint* > 0, *iend* must be > *ibeg* and for *iint* < 0, *iend* must be < *ibeg*. Otherwise the compiler will generate an error message.

The target need not be a **continue** statement; instead, one could place n somewhere in the first five columns of the last *FORTRAN statement* in the loop. This line would then perform its intended function *plus* act as the target for the do-loop.

One may dispense with the need of a target statement altogether by replacing the docontinue structure with the do-enddo structure (non-standard FORTRAN77, but standard FORTRAN90). Thus, the following example is identical to the preceding example should your F77 compiler support do-enddo:

1	do <i>i=ibeg,iend</i> ,[<i>iint</i>]
2	FORTRAN statement(s)
3	enddo

Sticking with standard FORTRAN77, I shall use the "targeted do statements" from now on,

and use continue statements for all targets.

Do-loops may be nested as needed, so long as the "target paths" don't cross. Thus,

1	do 20 j=jbeg,jend
2	do 10 i=ibeg,iend
3	FORTRAN statement(s)
4 10	continue
5 20	continue

is correct syntax, as is

1	do 10 j=jbeg,jend
2	do 10 i=ibeg,iend
3	FORTRAN statement(s)
4 10	continue

where both loops end at the same statement. However

1		do 20 j=jbeg,jend
2		do 10 i=ibeg,iend
3		FORTRAN statement(s)
4	20	continue
5	10	continue

is illegal, since the paths of the loops cross. Loop 10 begins inside loop 20, but ends outside, which makes no sense logically. Finally, both following

1	do 20 j=jbeg,jend
2	do 10 j=j1,j2
3	FORTRAN statement(s)
4 10	continue
5 20	continue

and

```
      1
      do 20 j=jbeg,jend

      2
      do 10 i=ibeg,iend

      3
      j = i + 1

      4
      FORTRAN statement(s)

      5 10
      continue

      6 20
      continue
```

are illegal, since the value of j is reset inside loop 20 which uses j as its counter. However,

1	do 20 j=jbeg,jend
2	i = j + 1
3	do 10 i=ibeg,iend
4	FORTRAN $statement(s)$
5 10	continue
6 20	continue

is perfectly OK, since line 2 assigns a value to i *outside* loop 10.

$5.2 \, if$

1 if (logical expression) single executable statement

where the *single executable statement* is executed only if the *logical expression* is true. The *single executable statement* can be any legal FORTRAN statement that only requires one line (possibly with one or more continuations) to execute. This includes an assignment statement, a read statement, a call to a subroutine, *etc.* It could not be a do-statement, since the do will require a target line (or an enddo), and other statements in between. Thus, do-loops require the use of the if-then-else-endif structures described next.

The *logical expression* consists of a left hand side, a right hand side, and a comparator (.eq., .ne., .lt., .le., .gt., or .ge.). More complicated logical expressions can be built up from smaller ones by use of the logical connectors .or. and .and.. Parentheses should be used to group simpler logical expressions where there may be ambiguity. Thus, examples of legal logical expressions include:

5.3 if-then-else-endif

1	if (logical expression)	then
2	instruction set 1		
3[else		
4	instruction set 2]		
5	endif		

The syntax for the *logical expression* is identical to that described in the *if* section.

Line 2 represents as many FORTRAN statements (executables, comments, no-ops, *etc.*) as needed, and represent logic that is to be executed provided the *logical expression* in line 1 is true.

Lines 3 and 4 are optional, and are omitted if there is nothing to do in the event the *logical* expression is false. Otherwise, line 4 represents as many FORTRAN statements as may be needed in the event that the *logical expression* in line 1 is false.

Line 5 is a no-op that closes off the if-then-else-endif structure.

5.4 go to; goto

1 go to n 2 FORTRAN statement(s) 3 n continue where n (the target) is an integer between 1 and 99999 which must appear immediately after the key word to (separated by at least one blank), as well as somewhere in the first five columns of the intended target line (*e.g.*, a continue statement). The go to (goto is equivalent) statement then redirects execution to the indicated target. A go to statement can redirect execution to a line *after* it (as in the example above), or *before* it (as in the example below). However, go to statements cannot redirect execution outside the program module (*i.e.*, to another subroutine).

If a go to statement is performed *unconditionally*, then if execution is redirected after the go to statement, the coding in between the go to and its target will never be executed (as in the example above). On the other hand, if execution is redirected before the go to statement, the coding in between the go to and its target will be repeated over and over again without break, forming what is called an *infinite loop*. To avoid either of these scenarios, go to statements are normally used in conjunction with if statements, as in the following example.

Line 5 will cause the execution to return to line 2 (target 10) so long as i remains less than or equal to imax. Once i exceeds imax (as it will eventually by virtue of line 4), execution skips on to line 6 and then on to whatever follows. Notice that without the if-test in line 5, this would be an infinite loop, with nothing in the logic to break the cycle.

Note also that the above example is logically equivalent to the following do-loop:

1	do 10 i=1,imax
2	$FORTRAN \ statement(s)$
3 10	continue

1

Indeed, most uses of the go to statement can be replaced with other, better structured FORTRAN such as do-loops and if-then-else-endif structures. Because go to statements can make the code difficult to read and the logic difficult to follow, they should be avoided where ever possible. Still, there are times when a go to statement is unavoidable.

For the more advanced programmer, there is a *computed* go to statement, which allows execution to be directed to one of many places depending on which of many values a variable may have. *Computed* if statements also exist, and the interested reader should consult a comprehensive FORTRAN manual for their descriptions. These structures can truly lead to "spaghetti code", and should be avoided in all but the most extenuating of circumstances.

5.5 **open**

open (lunit, file='filename', status='filestat'[, err=target])

The open statement opens a disc file and connects it to the logical unit *lunit* (an integer)

which is specified as the first argument in the open parameter list. The name of the file *filename* is known only to the open statement; from this point on, the program will know this file only by its unit number *lunit*, and all reads, writes, rewinds, *etc.*, will be done to unit *lunit*. *filename* should be the complete name typed exactly as you would if you were to access the file from the directory in which the program was launched. Thus, if the name of the file is output, and it exists or is to be created in the same directory in which the program is started, *filename* should be set to output. However, if the file output actually exists or is to be created in one directory up from where the program is launched, then *filename* should be set to .../output. Thus, directory paths, as complicated as they need to be, may be included as part of *filename*.

The status of the file, *filestat*, can be one of **new**, **old**, or **unknown**, and one of these three words must be enclosed in quotes as indicated. Status **new** means no file of name *filename* should already exist. If one does, an error message is generated and if no *target* is specified for **err**, execution is aborted. Status **old** means the file *filename* should already exist on disc, and you wish to open it for modification. If no such file is found, an error code is generated, and again, if no *target* is specified for **err**, execution is aborted. Finally, status **unknown** means the file *filename* may not already exist, in which case a new one is created, or it may exist, in which case the old one is opened.

Finally, the parameter **err** allows you to redirect execution elsewhere in case an error message is generated. You may want to allow for the possibility that a file does not already exist without having to create a new one (as **unknown** would do). In this case, if you specify the target to some other line in the code (just as a **go to** or a **do**-loop would), then you could carry on execution without having to open up a new file should the one you tried to open not already exist. Note that the **err** parameter is optional; you can omit it altogether as many examples in this primer have done.

There are numerous other, less-used parameters associated with the **open** statement, and the interested reader is referred to any comprehensive FORTRAN manual for details.

5.6 close

1 close (*lunit*)

The **close** statement closes the file attached to the logical unit *lunit* (an integer) by an earlier **open** statement. If you forget to close a file, the compiler closes it for you upon completion of the program. **close** statements are really only needed if you should want to try to re-open an existing file later on. Should it be still open, it can't be re-opened, and attempting to do so would generate an error message.

Like **open**, there are a variety of parameters you could set besides *lunit*, but these are rarely used.

5.7 write/format

1 write (lunit, wformat) [varlist]

The write statement writes text and/or the values of the variables listed in *varlist* to the device specified by the "logical unit" *lunit* (which could be the terminal screen, a disc file, a printer, even a character variable). How the text is written is specified by *wformat*, which can be an asterisk (*) meaning "unformatted" text, or an integer between 1 and 99999 which targets a format statement elsewhere in the program module. It is important to realise that the write statement converts everything to character strings before writing it to the output device. By writing the value of a real number, for example, you never actually see the real variable itself, but instead a character representation of that real number. To examine the actual real number would mean you would be looking at bits (0's and 1's).

If *lunit* is 6, output is directed to the computer terminal (often referred to as "standard output"). The statement:

```
1 write ( 6, * ) 'Hello!'
```

will write the exclamation Hello! (which must be enclosed by quotes in the write statement) so that the compiler knows that Hello! is a character string and not a variable name) to the computer screen by virtue of the integer 6 appearing in the slot where the logical unit goes. The asterisk implies the write statement is "unformatted", which really means that some default formatting that depends on what is being output (in this case, the word Hello!) is invoked.

If *lunit* is an integer other than 5 or 6, the write statement will direct its output to the disc file to which the logical unit has been attached by a previous open statement.

```
1 open ( 10, file='output', status='unknown' )
2 FORTRAN statements
3 write ( 10, * ) 'Hello!'
```

In this example, the exclamation Hello! is written to the next line of the opened disc file output, which was attached to logical unit 10 by virtue of the open statement (§5.5) in line 1.

Finally for *lunit*, if *lunit* is a declared character variable instead of an integer, the write statement will direct its output to the variable named. In this way, a real variable can be converted to a character variable, should such a conversion be required. The short program **testwr** below illustrates this feature.

```
1
          program testwr
2 c
3
          character*10
                         cvar
4
          real
                         rvar
5 c
6 c
      Boltzmann's constant...
7 c
          rvar = 1.3807e-23
8
          write ( cvar, 2010 ) rvar
9
                     6, 2020 ) rvar, cvar
          write (
10
```

```
11 c

12 2010 format ( 1pg10.4 )

13 2020 format ( 'rvar=', 1pg10.4, ', cvar=', a10)

14 c

15 stop

16 end
```

Line 9 writes the character representation of the real variable **rvar** to the character variable **cvar** according to the format specified in format statement 2010 (line 12). The format code 1pg10.4 means the number will be written with ten characters (including the sign, mantissa, decimal point, the character **e** to herald the exponent, the sign for the exponent, and two digits for the exponent) with four digits appearing to the right of the decimal point (*i.e.*, four decimal places). The 1p portion of the format code indicates that one non-zero digit will appear to the left of the decimal place.

Line 10 then writes both variables to the screen so the reader can see that the conversion has been performed correctly. Since cvar is a character variable, it requires a different format code to write than the real variable rvar. Thus, in format statement 2020 (line 13), the real variable is written with the same format code (1pg10.4) as in format statement 2010, whereas the character variable cvar is written with the format code a10. The a means ASCII text, the 10 means ten characters. As given, the screen output as determined by line 13 looks like:

rvar=1.3807E-23, cvar=1.3807E-23

If we dropped the 1p from the format code in line 13 (but kept it in line 12), the output would change to:

rvar=0.1381E-22, cvar=1.3807E-23

Finally, if the format code 1pg9.4 were used in line 13 rather than 1pg10.4, the output would look like:

```
rvar=*******, cvar=1.3807E-23
```

since 9 characters in total is not enough to display 1.3807E-23. In fact, ten characters would not be enough if rvar were negative, since the negative sign would require an eleventh character. Thus, as a rule of thumb, I always specify 7 more characters in total than the number of decimal places you want. Thus, 1pg11.4 will always have enough characters to display the full real number with four decimal places. If you want five decimal places, specify 1pg12.5, *etc.*

As we've seen, the **format** statement dictates how the output appears by use of various format codes enclosed by parenthesis after the keyword **format**. Format codes may be snippits of text to be written between the variables, or special codes which dictate how the variables listed in the *varlist* of the targeting **write** statement are to appear. All format codes listed in a **format** statement must be separated by commas. Extra spaces are optional. The following is a more comprehensive example of a **write** and **format** statement combination.

If i=5, j=12, k=110, den(i,j,k)=0.1025, eks(5)=0.5, why(12)=1.2, and zed(k)=11.0, these lines of FORTRAN would write to your screen the output:

5 d(5,12,**) = 1.02500e-01 6 measured at (x,y,z) = 0.50000 1.20000 11.0000 7 c===+====1====+====2===+====4====+====5====+====6====+===7==

Line 7 (a number line) has been added so you can count columns better. It is not part of the output.

Lines 1 and 3 illustrate that text can be specified in the *varlist* of the write statement (e.g., `measured at (x,y,z) = `), or directly in the format statement (e.g., `d(`). If given in the *varlist*, there must be a corresponding character format code in the format statement (in this case, a22) which indicates 22 characters (the number of characters in 'measured at (x,y,z) = ', including all blanks) will be written.

In this example, the *varlist* consists of three integers, followed by one real, one character string, and three reals in the continuation line. Thus, the format codes in the format statement must be given in the same order, namely three integers codes (i2 appearing three times), one real code (1pg12.5), one character code (a22), and finally three real codes (1p3g12.5, where the 3 appearing between the p and g indicates that this code is to be applied three times). In between each format code, you are free to insert whatever text and spacing codes you like. Thus, the format statement in line 3 will lead the first three integers with d(, then place commas between each integer, closing the three integers with) =, giving the very readable output d(5,12,**) = 1.02500e-01 in line 5.

Note that the format code i2 was given for each of the three integers. Now, the first integer is 5, requiring only one character. Since i2 allows for two characters, a blank is inserted before the digit 5 in the output (line 5). If you wanted to have two *bone fide* digits rather than a blank and one digit, you could use the code i2.2, which forces two digits to be printed (the integer after the dot is the number of forced digits). This would then generate the output d(05,12,**) rather than d(5,12,**). The second integer is 12, which uses up all two characters assigned to this field by the code i2. The third integer is 110, which cannot be accommodated by two digits, thus generating ** in the output. To correct this you would have to replace the third i2 with i3.

The 1pg12.5 code has been explained above, as has the a22. The forward slash (/) forces a line break in the output. The code 10x forces ten blank spaces.

Formatted I/O (Input/Output) is one of the trickier things to get used to in FORTRAN, and is one of the perennial complaints about the language. Often error messages resulting from incorrect formatting are cryptic at best and finding the cause of the error message can be frustrating. Taking some defensive measures such as adding a blank after each format code in the **format** statement (as has been done in lines 3 and 4) will help you to scan the format statement by eye for syntax errors. Correct whatever errors you find regardless of

what you think the error message may be telling you, and the error message may well go away.

For example, which line is easier to read: lines 3 and 4 above, or the following:

8 2010 format ('d(',i2,',',i2,',',i2,') = ',1pg12.5,/,10x,a22,1p3g12.5)

Both give identical output, but line 8, with all blanks between format codes and character strings removed, is now a sea of commas and quotes, and it is hard to tell which commas separate format codes and which are meant to be part of the text in the output.

5.8 read/format

```
1 read ( lunit, rformat ) [varlist]
```

The **read** statement is similar to the **write** statement, and reads the values of the variables listed in *varlist* from the device linked to logical unit *lunit* in the format specified by *rformat*.

Read statements can be formatted or unformatted. If a read is used to initialise a variable from the terminal screen, *lunit* should be 5 (often referred to as "standard input"), and *rformat* should be *, *i.e.*, an "unformatted read". When execution encounters a read from the screen, execution is paused until the user has typed the desired value, and hit the Enter or Return key. Thus, before any read from the screen, it is wise to use a write to the screen to prompt the user for the desired value, as in the following example:

```
1 write ( 6, 2010 )
2 2010 format('Enter a real value for the radius.')
3 read ( 5, * ) radius
```

Without the prompt, execution may remain paused for a very long time as the user wonders what is taking the program so long to execute, possibly unaware that the program is waiting for the user!

Reads may be formatted, in the same fashion write statements are formatted (§5.7), but this is usually reserved for reads from disc files, in which the exact format of the file is known. If the format rules in the format statement don't match *exactly* the format in the disc file from which the data are read, your data entry can go terribly wrong. For example, the following program reads the values of three variables: ivar, an integer; rvar, a real; and date, a character string (ten characters) from the discfile indata.

```
1
            program testread
 2 c
 3
            character*10 date
 4
            integer
                            ivar
 5
            real
                            rvar
 6 c
 7
                   ( 10, file='indata', status='unknown' )
            open
            read ( 10, 1010 ) i, rvar, date
write ( 6, 2040 ) i, rvar, date
 8
9
            close (10)
10
11 c
```

```
12 1010 format( i4, 1pg12.5, a10 )

13 2040 format('i=', i4, ', rvar=', 1pg12.5, ', date=', a10 )

14

15 stop

16 end
```

The read statement in line 8 refers to format statement 1010 (line 12) which specifies that the first 4 characters (character 1 through 4) on the input line shall contain the integer variable, the next 12 characters (characters 5 through 16) shall contain the real variable, and the last 10 characters (characters 17 through 26) shall contain the character string. Thus, if indata were a disc file with the single line:

100 1.25000e-03November 1

then the output from the program testread would look like:

```
i= 100, rvar= 1.25000E-03, date=November 1
```

and everything is fine. However, just one slightest glitch in indata such as putting two spaces between the 100 and the 1.25 instead of one space:

100 1.25000e-03November 1

can corrupt the output from the program testread completely:

```
i= 100, rvar= 1.2500 , date=3November
```

This is because the formatted **read** was expecting characters 5 through 16 to contain the real number. With the real shifted over by one character, the last digit of the exponent (3) is now the 17th character, and is not read as the last character of the real number (which is therefore reported as 1.2500), but instead as the first character of the character string, which now loses its last intended character, the digit 1.

But things could be much worse. Look what happens if the blank in front of the 100 is omitted, causing the field for the real number (characters 5 through 16) to include was was intended as the first letter of the character string (N). Thus, if indata is this:

100 1.25000e-03November 1

the program aborts, giving the most cryptic output:

```
dofio: [1015] read unexpected character
logical unit 10, named 'indata'
lately: reading sequential formatted external IO
part of last data: .25000e-03No|vembe
Abort
```

All that is obvious to me is the last line: Abort. The rest is gobbledigook, except maybe to more "seasoned" programmers.

You may have already come to the conclusion that formatted read statements are completely impractical for large quantities of data entry, particularly if those data are to be typed in by a human. Should another computer program generate the data, fine, but if a human has to type in hundreds of exact numbers in precise fields, forget formatted reads. For most beginning programmers, unformatted reads from the computer screen are likely the best way to input data to start off a program run. But even this can get unwieldy if the program evolves to one which requires dozens of input parameters for each run. In this case, the more advanced programmer may want to look into the **namelist** feature, which is supported by many FORTRAN77 compilers, and is standard to FORTRAN90, but beyond the scope of this primer.

Finally, as write statements can be used to convert a real variable to a character string, a read statement can be used to convert a character string to real. Thus, line 4 in the following example

1	character*10	cvar		
2	real	rvar		
3	cvar = '1.38	07e-23'		
4	read (cvar,	*) rvar		

assigns to rvar the real value equivalent to the character string assigned to cvar in line 3.

5.9 Intrinsic Functions

Intrinsic functions are keywords recognised by the FORTRAN compiler when included as part of the right hand side of an assignment statement that invoke mathematical operations. With the exception of the double asterisk (§5.9.1), intrinsic functions have the format

function (parameter list)

where, for the most part, the parameter list consists of just one variable, constant, or arithmetic expression.

5.9.1 ** y = x**n

raises x to the nth power, and assigns that value to y. Both x and y must be declared to have the same data type (integer, real, or double precision), otherwise a type mismatch error will occur. If x and y are integer, n must be integer too. To raise an integer to a real power, you must first convert all integers to real. If x and y are real (double precision), n may be integer or real (double precision).

If n is a positive integer, the compiler interprets the above expression as

 $y = x \times x \times \ldots \times x$ (where x appears n times)

If n is a negative integer, the compiler computes

 $y = \frac{1}{x \times x \times \dots \times x}$ (where x appears n times)

Finally, if n is real, the compiler computes

$$y = e^{n \ln x}$$

Thus, numerically, $\mathbf{x}**2$ ($x \times x$) and $\mathbf{x}**2.0$ ($e^{2\ln x}$) may give slightly different results because of "round-off errors". Since raising a real number by a real power invokes the log and exponentiation functions, it is considerably more costly in computer time than simply multiplying a number by itself n times. Thus, it is always more desirable to do $\mathbf{x}**n$ than $\mathbf{x}**n.0$ when n is an integer. However, when n is real, there is no way of avoiding the invocation of the log-exponentiation algorithm.

5.9.2 sqrt

$$y = sqrt(x)$$

assigns to y the square root of x, and may be used for both single and double precision variables. x and y must be declared with the same data type, otherwise a type mismatch error will result.

Square roots are expensive computationally, and should be avoided where possible. The following is an example of where you might think a square root is necessary, but in fact can be avoided. Suppose you want to perform one set of calculations inside a sphere of radius r_0 , and another set outside that radius. If you are doing the calculation in 3-D Cartesian coordinates, the distance r between the origin (centre of the sphere) and a point (x, y, z) is given by $r = \sqrt{x^2 + y^2 + z^2}$, and thus the relevant snippet of coding might look like:

```
1
           do 30 k=1,kmax
 2
             zsq = zed(k) * 2
 З
             do 20 j=1, jmax
               ysq = why(j) **2
 4
               do 10 i=1, imax
 5
 6
7
                  radius = sqrt ( eks(i)**2 + ysq + zsq )
                  if ( radius .gt. r0 ) then
 8
                    instruction set 1
 9
                  else
10
                    instruction set 2
11
                  endif
12 10
               continue
13 20
             continue
14 30
           continue
```

First, note that we can avoid doing many of the squares by computing z^2 once per loop on k (line 2), and y^2 once per loop on j (line 4). Note that the square root on line 6 can be omitted altogether if we just do the if-test on radius**2 rather than on radius. Thus, by replacing lines 6 and 7 with:

6 radsq = eks(i)**2 + ysq + zsq 7 if (radsq .gt. r0sq) then (where the line r0sq = r0**2 needs to be inserted somewhere before do-loop 30 starts) causes a logically-equivalent if-test to be performed, but without the sqrt function.

5.9.3 exp

y = exp(x)

performs an exponentiation $(y = e^x)$, and may be used for both single and double precision variables. x and y must be declared with the same data type, otherwise a type mismatch error will result.

5.9.4 log

 $y = \log(x)$

performs a natural logarithm $(y = \ln x)$, and may be used for both single and double precision variables. x and y must be declared with the same data type, otherwise a type mismatch error will result.

5.9.5 log10

y = log10 (x)

performs a logarithm to the base 10 ($y = \log_{10} x$), and may be used for both single and double precision variables. x and y must be declared with the same data type, otherwise a type mismatch error will result.

 $5.9.6 \sin$

y = sin (x)

performs the function $y = \sin x$, where x is assumed to be in radians. This function may be used for both single and double precision variables. x and y must be declared with the same data type, otherwise a type mismatch error will result.

 $5.9.7 \cos$

 $y = \cos(x)$

performs the function $y = \cos x$, where x is assumed to be in radians. This function may be used for both single and double precision variables. x and y must be declared with the same data type, otherwise a type mismatch error will result.

The tangent function tan, and all hyperbolic trigonometric functions (sinh, cosh, tanh) exist as well and are used the same way as sin and cos. Inverse trig functions (asin, acos,

atan) and inverse hypertrig functions (asinh, acosh, atanh) may exist as extensions of your compiler, but are not part of ANSI standard FORTRAN77.

5.9.8 min y = min (x1, x2[, x3, ..., xn])

sets y to the minimum value among those listed in the argument list. The argument list must have at least two elements in it, and each element must have the same type (*i.e.*, all integer, all real, or all double precision). y must be the same type (integer, real, or double precision) as the elements in the argument list (x1, x2, etc.). If any one of y, x1, etc. have a different type from any of the others, a type mismatch error will occur.

 $5.9.9 \mathrm{max}$

y = max (x1, x2[, x3, ..., xn])

sets y to the maximum value among those listed in the argument list. The argument list must have at least two elements in it, and each element must have the same type (*i.e.*, all integer, all real, or all double precision). y must be the same type (integer, real, or double precision) as the elements in the argument list (x1, x2, etc.). If any one of y, x1, etc. have a different type from any of the others, a type mismatch error will occur.

5.9.10 abs

y = abs (x)

sets y to the absolute value of x (by setting the first bit of the number to 1, *i.e.*, positive). This function may be used for integer, real, and double precision variables. x and y must be declared with the same data type, otherwise a type mismatch error will result.

5.9.11 sign

y = sign (x1, x2)

(transfer of sign) sets y to x1 if x2 is greater than or equal to zero, and to -x1 if x2 is less than zero. This function may be used for integer, real, and double precision variables, but all variables must have the same type, otherwise a type mismatch error will occur. Thus, if x1 and x2 are real, y must be declared real, *etc.*

5.9.12 int

i = int (x)

converts a real or double precision value (x) to an integer by truncation, and assigns that integer to i. If i is not declared to be an integer, a type mismatch error will occur.

Truncation means that the decimal portion of the real number is simply cut off. Thus, 1.2 is truncated to 1; 3.993 is truncated to 3, -5.27 is truncated to -5, and -12.75 is truncated to -12.

5.9.13 real

y = real (x)

converts an integer or double precision variable (x) to real, and assigns that value to y. If y is not declared real, a type mismatch error will occur.

5.9.14 dble

y = dble (x)

converts an integer or real variable (x) to double precision, and assigns that value to y. If y is not declared double precision, a type mismatch error will occur.