Introduction to Computing at SIO: Notes for Fall class, 2018

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Chapter 1

Introduction

This course is intended to help incoming students get up to speed on the various computing tools that will help them with their research and some of the homework assignments for other classes. The perspective is largely that of the Geophysics program at SIO, but we hope that the course is general enough to be useful for other students as well.

All students should have access to a Mac and an account on the IGPP Mac network. Please let me know if you do not already have an account. If you are using your own Mac, you will need to install the following:

1. gfortran
2. nedit (see Macports IGPP Public Help wiki)
3. GMT (see Macports IGPP Public Help wiki)
4. XCode tools and XQuartz/X11 (see IGPP Public Help wiki)
5. ghostscript and gv (see Macports IGPP Public Help wiki)
6. TexShop

There are download instructions on the class website.

We will spend a few classes on UNIX, GMT and other topics, but the bulk of the class will be an introduction to the Fortran90 programming language. If you are already experienced in C or Fortran, you probably don't need to take this class (although you may find some of the other material and the geoscience examples of interest).

1.1 Scientific Computing at SIO

1.1.1 Hardware

Before 2004 or so, computer hardware used at SIO was of two main types:

1. UNIX Workstations (e.g., Sun, HP, Silicon Graphics, etc.)
   (a) Scientific programming
   (b) Data storage
   (c) General research
   (d) (some word processing, graphics)
2. PCs (Windows machines, Macs)
   (a) Word Processing
   (b) Graphics
   (c) Presentations (talks and posters)
   (d) (some programming)

However, these boundaries are now gone because many PCs run Linex[1] (an open source form of UNIX) and Apple has adopted UNIX for their operating system (starting with OS X). This permits these machines to be used for both serious scientific computations and word processing and more traditional PC activities.

Twenty years ago, most geophysics departments had networks of Sun workstations. Today these have largely been replaced with networks of cheap PCs running Linux or with Apple machines. At IGPP we now use Macs for everything except for certain specialized or high-performance computers maintained by individual PIs. For example, David Sandwell's group maintains some Suns because some of their processing software runs only on that platform.

1.1.2 Software

Here is a list of some of the programming languages and software used at IGPP (Items with * will be discussed in this class).

1. Programming
   (a) *FORTRAN (most IGPP faculty use this, large library of existing code)
   (b) C (more widely taught and used by computer scientists)
   (c) C++ (extended version of C)

[1] Linex is pronounced similar to "linen" (see http://www.paul.sladen.org/pronunciation/)

   (d) Java (used a lot for web programming, has portability advantages, but often not fast enough for serious computing)
   (e) Python (lots of buzz, has graphical capabilities, but slower than C and Fortran)
   (f) R (often used for statistics and graphics)
   (g) MatLab (widely used but commercial product, expensive when you are no longer student, IGPP has site license)
   (h) HTML for web sites (most people now don't program in raw html, but use web designer software, such as DreamWeaver)

2. Community Programs

   (a) Bob Parker programs (plotxy, color, contour; now used mainly by older IGPP faculty)
   (b) *GMT for mapping (UNIX based)
   (c) SAC for seismic analysis
   (d) etc.

3. Commercial Programs

   (a) MS Word for word processing
   (b) MS Powerpoint or Apple Keynote for talks, sometimes for posters
   (c) *TeX/LaTex (no single vendor, different implementations available, files are compatible, best option for papers & thesis)
   (d) Adobe Illustrator (for graphics, preparing posters)
   (e) PhotoShop
   (f) Mathematica
   (g) etc.

1.2 Why you should learn a "real" language

Many students arrive at SIO without much experience in FORTRAN or C, the two main scientific programming languages in use today. While it is possible to get by for most class assignments by using Matlab, you will likely be handicapped in your research at some point if you don't learn FORTRAN or C. Matlab is very convenient for quick results but has limited flexibility. Often this means that a simple FORTRAN or C program can be written that will perform a task far more cleanly and efficiently than Matlab, even if a complicated Matlab script can be kludged together to do the same thing. In addition, Matlab is a commercial product that does not have the long-term stability of other languages, including large libraries of existing code that are freely shared among researchers.

Your research may involve processing data using a FORTRAN or C program. If you do not understand the program, you will not be able to modify it to do anything other than what it can already do. This will make it difficult to do anything original in your research. You may resort to elaborate kludges to get the program to do what you want, when a simple modification to the code would be much easier. Worse, you may drive your colleagues crazy by continually requesting that the original authors of the program make changes to accommodate your wishes.

Finally, you will be in a more competitive position to get a job after you graduate if you have real programming experience.

1.3 Learning to program

Learning to program can be intimidating, particularly if you have not previous experience. The worst thing to do is to buy a book on the language and try to read it. There is simply too much material and it seems overwhelming. DO NOT DO THIS! Instead, begin by writing the simplest possible program and get it to work. Then read just enough to add a single additional feature to your program and get that to work. You only really learn when you get your own programs to work, so the idea is to write lots of little programs that do various things and only gradually add in new concepts. There is no need to learn everything that the language will do all at once.

Part of learning to write more complicated programs is to figure out ways to logically divide the problem into smaller pieces. This will come with experience. The final project in this class will be to write a program that plays tic-tac-toe. This is a daunting task if one tries to write it all at once. But we will divide it into smaller parts for separate assignments over the weeks, and only put all the pieces together for the final program at the end.

Also, be aware the most languages have far more features than you actually need. Few of us except professional programmers learn them all. But we do not need to write professional programs—we only need to learn to write practical programs that serve our own needs. For example, I probably only know about 20 UNIX commands. A real computer nerd would laugh at many of the ways that I do things. But it's been enough for me to get by and to do the science that I want to do. (Having said that, it wouldn't hurt for me to learn more and I'm going to look over some of Duncan Agnew's notes from previous classes to find some new tricks)

1.4 FORTRAN vs. C

Some years ago when I (Peter) first started teaching programming in this class, I had to decide whether to teach C or Fortran. Like most SIO faculty of my generation or older, I was experienced in FORTRAN but had little exposure to C. After talking to some people who know both FORTRAN and C, however, I decided to bite the bullet and learn enough C to teach this class. This was motivated in part by the fact that C is now one of the standard languages taught in computer science departments; many of our incoming students have C experience but few have Fortran experience.

Here is my summary of the advantages and disadvantages of either choice:

- FORTRAN
  - Advantages
    * Large amount of existing code
    * Preferred language of most (?) IGPP faculty (most faculty are *old*)
    * Complex numbers are built in
    * Choice of single or double precision math functions
  - Disadvantages
    * Column sensitive format in older versions
    * Dead language in computer science departments
- C
  - Advantages
    * Large amount of existing code
    * Preferred language of incoming students, some younger faculty
    * Free format, not column sensitive
    * More efficient I/O
    * Easier to use pointers
  - Disadvantages
    * Less user-friendly than FORTRAN (I think so, but others may debate this)
    * Fewer built in math functions (but easy to fix)
    * No standard complex numbers (but easy to fix)
    * Easier to use pointers

With reasonable compilers, both languages are equally fast. Ultimately, there are fixes for both languages that permit them to assume the advantages of the other language. For example, you can use pointers in FORTRAN90 and you can define an add-on set of functions to do complex arithmetic in C. However, after learning

enough C to teach the class, I concluded that C is not a very user friendly language for those without programming experience. So I switched to Fortran90, an improved version of Fortran77, that combines the advantages of Fortran and C into a more user-friendly package.

1.5 Python

In several previous years, this class taught Python, sometimes combining it with Fortran90 (too much material for a single class!), This fall, Python is being offered at SIO in a separate class, allowing us to concentrate on F90.

Python is an up-and-coming programming language that is gaining popularity. It is very flexible and combines many of the advantages of traditional programming languages (e.g., C and Fortran) with object-oriented languages (e.g., Java) and with scripting languages (e.g., UNIX shell scripts). It also has more integrated graphics options in its standard library than C or Fortran (which require use of non-standard plotting packages). Indeed it has so many features that it can be daunting for beginning programmers.

Python is free and runs on almost all computers. An interesting feature is that indentation is *required* in the block delimiters used in *if* statements and *do/for* loops. The idea is to enforce good programming style. Python was started in 1989 by Guido van Rossum from the Netherlands, who has been been given the name Benevolent Dictator for Life (BDFL) by the Python community. The name Python comes from the old Monty Python TV series and Monty Python references are common in example code.

Python is a dynamic programming language, which is not *compiled* before it is run (C and Fortran programs are first compiled). Other examples of dynamic languages include BASIC and Matlab. Dynamic languages generally run much slower than compiled languages, which can be a disadvantage for serious data processing and number crunching. However, it is possible to call C or Fortran subroutines from within Python. This provides a way to combine the speed of Fortran with the graphical capabilities of Python.

Chapter 2

UNIX introduction

You will very likely do your scientific computing in a UNIX environment. UNIX is by far the most common operating system for the workstations that dominate today's scientific computing. There are many different versions of UNIX. In this class we will be using OS X on the Macs, which is an Apple version of UNIX. There is also a free version of UNIX, called LINUX (pronounced lynn′ exs), that will run on most PCs.

2.1 Getting started

To use UNIX on the Macs, you will need to bring up a regular text-based window rather than the standard Mac windows. This can be done by running the "Terminal" program, which in normally in Applications/Utilities. We will assume in these notes that you are entering UNIX commands within such a window.

UNIX comes in different flavors, called *shells*. We are going to assume that you are running the "bash" C-shell, which since OS X 10.3 has been the default shell for Macs. Before that, Macs used "tcsh" as the default shell, which is another very common shell and is used by many scientists here at SIO. Unfortunately, many commands that work under tcsh will not work under bash, and vice versa.

To find out what UNIX shell you are running, just look at the top of the Terminal window and it will say. Alternatively, type

```
printenv
```

or simply

```
env
```

within your UNIX shell and it will tell you lots of interesting things, including what your SHELL is. Or type

```
echo $SHELL
```

if you want to just see your shell type.

To make bash your default shell (if it is not already), in the Terminal program go to Preferences/General and make sure you have set that shells open with the default login or with the command "/bin/bash" and then close the Terminal preferences box and restart Terminal.

Within a Terminal window, you can change to bash by typing:

```
/bin/bash
```

or change to tcsh by typing:

```
/bin/tcsh
```

Later we will learn about UNIX scripts, which are wonderful tools to automate operations and procedures on your computer. But typically these scripts will work only under one type of UNIX. So suppose your advisor sends you a complicated script to process some data that she wrote using tcsh commands. You try running it under bash and it crashes. What can you do? You could figure out how to translate the script to bash but that would be a lot of work. You also could temporarily change your terminal to tcsh (see above). But the easiest option is probably to simply add "#!/bin/tcsh" as the very first line of the script (more about this later). This will cause the script to run locally under tcsh and it should work just fine, even though the Terminal is using bash.

To learn more about UNIX shells on the Macs, check out:
http://www.macdevcenter.com/pub/a/mac/2004/02/24/bash.html

I am by no means an expert on UNIX; probably there are several of you here who know much more than I do. I have learned only enough to get by and could benefit from learning more. So I'm just going to outline the basics here for the benefit of those students who have not been exposed much to UNIX.

The UNIX operating system was originally designed to run on mainframe computers where security was a big issue. You don't want users to be able to delete other user's files or do other nasty things. So there are a lot of security features. The first of these is the login and the password. You will be assigned a login name

and password. The first thing that you should do after you login is change your password so that only you know what it is. This normally happens automatically upon your first login. If not, or if you later want to change your password, on the Macs, go to System Preferences and click on Accounts. To change your password on more traditional UNIX machines, use the command:

```
passwd
```

You should choose a password with numbers or special characters as well as letters. Do not choose a common word that can easily be guessed by outside hackers. The NetOps people here are very concerned about security issues and IGPP computers have been attacked many times. Do not write your password down (like on a note next to your computer!) where it can be found. Do not tell other students your password. You can easily give them access to read your files without giving them the password.

Let us assume that you have successfully logged on. Your will now be located in your home directory. UNIX uses a directory tree structure, similar to the "folders" used by PCs but without all the fancy icons. Normally you will have a cursor prompt that tells you what machine you are running on. In my case, this looks like:

```
shearer@koan>
```

Your default prompt is likely to be different from this. If you want to have one like mine, enter

```
PS1='\u\h> '
```

where \u will give your username, \h your machine (host) name (koan is my laptop), and > will just give > and the space provides a little space between the > and what you type. To automatically invoke this for every Terminal window you open, you can put this in your .bashrc file (see below).

2.2 Basic commands

To find out where you are, enter "pwd" which stands for "Print Working Directory." In my case, this will give:

```
shearer@koan> pwd
/Users/shearer
```

This shows that I am located in my home directory (named shearer) in the Users directory on my laptop.

You can list the contents of your current directory with the "ls" command:

```
shearer@koan> ls
```

(I'm not showing you the output because it's too messy in my case!)

UNIX has an online set of manuals that may be accessed with the "man" command. For example, suppose you forgot what "ls" does. You could type "man ls" and you would get a description of the ls command and its many options. One annoying aspect of standard UNIX is that the man command output uses a form of the VI editor rather than the normal window output, which permits scrolling up and down in the window. When you enter "man ls" you will get a page of output on the screen with a colon (:) at the bottom. If you enter the space bar, you will then get the next page of output, etc. But you can't scroll backwards using the window scroll arrows. To go backwards, enter "b" at the colon prompt. When you get to the final page, you will see END at the bottom. To leave the man pages and return to the normal terminal, hit the 'q' key (for quit) at any point.

If you find this too annoying to deal with, you can always save the man pages to another file. To do this, enter:

```
man ls > man.ls
```

The output will now be directed into a file named "man.ls" rather than to the screen. To look at man.ls, use the 'cat' command:

```
cat man.ls
```

The 'cat' command prints a text file to the screen. The advantage in this case is that you can use the scroll bar. Note that if you try to look at man.ls using a text editor, you will likely see all kinds of weird control characters that are used to format the screen output.

Of course, you risk cluttering up your directory with lots of files named "man.whatever" if you do this a lot. If you don't want to worry about deleting them, one solution is to use the name "junk" as a temporary place to store output. If you already have a file named junk, it will just overwrite the old file. This way, you only ever have one "scratch" file in your directory at one time.

Another approach, if you have access to the web, is to simply Google 'unix man ls' to bring up the man pages, nicely formatted!

There usually are options to UNIX commands that can make them more useful for what you want. For example, "ls" simply lists the file names in your directory. If you want to find out how big they are or when they were last modified, then use "ls -l" where the "l" stands for the long output option. In your home directory, you will have a very important file called ".bashrc" (see below). This file will not appear if you just enter "ls". To make it appear, enter "ls -a" where the "a" stands for the "all file" option.

To change your directory, use:

```
cd dirname
```

This will move you to the directory dirname. This directory name must be in your current directory. Or you can give the full path name for dirname, i.e.

```
cd /Users/shearer
```

will get me to my home directory no matter where I am on the system. Alternatively, one can go to one's home directory by entering

```
cd
```

You can also go directly from anywhere to specific subdirectories by entering:

```
cd ~/dir1/dir2
```

This will get you to directory dir2, located in dir1 in your home directory. Naturally this does the same thing as

```
cd
cd dir1
cd dir2
```

You can go back up one level by entering

```
cd ..
```

You can go back up and then down again into a different directory by entering:

```
cd ../dir2
```

To create a new directory, use the "make directory" command:

```
mkdir dir1
```

It is often convenient to use a different naming convention for your directories in order to distinguish them from your files. Some people put .dir after their directories. For awhile I put d. in front of the directory names, which has the advantage of grouping them together when "ls" is entered, since UNIX lists things in alphabetical order. Most recently, I have been using all capital letters for the directory names. This makes them more visible, but has the disadvantage of slowing down typing their names (yes, UNIX is case sensitive!).

If you don't want to use special names for directories or if you find yourself in somebody else's directory where they don't do this, you can use the "ls -F" command:

```
ls -F
```

This will add a / suffix to directory names and a * prefix to executable file names. I like this so much that I have set this up as my default "ls" command by putting an alias into my .bashrc file (more about this later).

2.3 Files and editing

Files can be simple ascii (text) files or they can be binary files, often the executable versions of computer programs. One standard UNIX editor is called vi and is still used by some of the old time programmers at IGPP who will insist that it is remains the best editor. If you know all of its tricks it can be an extremely powerful editor. You can do things, like cut and paste columns of numbers, that most editors can't do. It also has the advantage of running on any terminal so if you log in from home you can still edit files.

If you know vi or decide that you want to learn it—more power to you. You will not lose any points around here. However, vi is not mouse or window friendly and is not favored by most students today. I have forgotten most of the vi that I once knew (I used it to do my thesis back in the late Cretaceous).

Editors on the Mac include:

- TextEdit – You can find this in the applications folder. Be sure to set the format (under Preferences) to Plain text and not Rich text, which will put in control characters that will screw things up. You also will want to turn off "smart quotes" and "smart dashes" to avoid entering non-standard characters not recognized by UNIX.

- nedit – This is supposed to run on all platforms and has more features than textedit.

- emacs – this is a very powerful editor that is used by computing professionals. It can do just about anything but may be somewhat harder to learn at first than simpler editors.

- Xcode – special Mac editor designed for editing programming code

You can use any of these editors to create a new file or edit an existing file. Unix file names are case sensitive. By convention, the type of file is often indicated by .type, for example:

testprog.f for Fortran77 program source code
testprog.f90 for Fortran90 source code
testprog.c for C program source code
testprog.m for a MatLab script
testprog.o for an object file
figure1.ps for a Postscript file
figure1.gif for a GIF file

Be aware that the Mac Finder will hide many of these suffixes when you look at file names within a Mac folder, but they will appear when you type "ls" in a Unix Terminal window.

You may wish to create your own naming convention to keep track of your files. When used with wildcards (see below) this will make it easy to list all files of a particular type.

WARNING: Do not use a slash (/) or the dash character (-) in file names; this may cause all kinds of problems for you. Use . or _ to separate the words. NEVER USE BLANKS IN FILE OR DIRECTORY NAMES USED IN PROGRAMMING!!! (I know this is common on Macs and PCs for document files but you will eventually have big problems reading with your programs any file names with blanks)

2.4 Basic commands, continued

If you want to remove a file use the 'rm' command:

```
rm filename
```

If you want to change the name of a file, use the 'mv' (move) command:

```
mv filename1 filename2
```

If filename2 already exists, this will have the possibly undesired consequent of deleting the original filename2. To guard against this, use the "-i" option:

```
mv -i filename1 filename2
```

Now if filename2 already exists, the computer will ask you first if you want to overwrite this file.

mv can also be used to move files between directories:

```
mv filename dirname
```

will move filename into directory dirname (assuming dirname already exists!) where it will have the same name. Note that this does the same thing as

```
mv filename dirname/filename
```

For convenience, you can leave off the /filename if the file is to keep the same name. A note of caution: In this shortened version, if dirname does not exist as a directory, then the name of filename will be changed to dirname.

The copy command works in a similar way:

```
cp filename1 filename2
```

makes a copy of filename1 called filename2.

```
cp -i filename1 filename2
```

will first ask if you really want to do this if filename2 already exists. You can copy files to different directories in the same way as the mv command works.

Many people so prefer the -i option for mv and cp that they make it the default option by defining an alias in their .bashrc file (see below) so that mv and cp become "mv -i" and "cp -i". I recommend that you do this—it is likely to save you some grief in the future. If you are super cautious, you can also add the -i option for the "rm" command, but I find this annoying because I normally intend to remove the specified file when I use the "rm" command. Note that there is no "undo" command in UNIX. Once a file is gone, it's gone (unless you have a backup somewhere).

To remove a directory, use the "rmdir" command:

```
rmdir dirname
```

The directory must first be empty for this to work. To recursively remove a directory and its contents use:

```
rm -r dirname
```

Use this with extreme caution to avoid accidentally deleting more than you intended!

2.4.1 Wildcards

UNIX commands become much more powerful when they are used with the wildcard character * which can take on any ascii string[1].

For example, suppose you wanted to list all files ending with .f the suffix used to identify Fortran source code. Simply enter:

```
ls *.f
```

You could move all of these programs in a subdirectory called source.dir by entering:

```
mv *.f source.dir
```

You might have a bunch of plot files called mypost1, mypost2, etc. You could delete all of these at once by entering:

[1]The question mark (?) can also be used as a wildcard and in most cases will work the same as *. However, * is preferred because it will avoid files with an initial . and thus you will not accidentally delete your .bashrc file by entering something like "rm *rc".

```
rm mypost*
```

For obvious reasons, be very careful when using * with the rm command. For example, suppose you wanted to delete all files in your current directory that end in %, which some text editors use to store the original version of edited files. To do this, enter:

```
rm *%
```

Suppose, however, that you are careless when you type this and enter instead:

```
rm * %
```

This will delete everything in your current directory! So always look carefully at what you have typed before hitting the return key when you are deleting files using wildcards.

2.4.2 The .bashrc and .bash_profile files

In your home directory, you can have files that are executed automatically under certain conditions. These files begin with a '.' and do not appear with the 'ls' command without the '-a' option. They also do not appear in the Mac Finder, as they are considered for advanced users only.

These files are useful for defining and customizing your environment. Typically you will want them executed whenever you open a new Terminal window. Under bash, this file is normally the .bashrc file. You may already have a default .bashrc file set up by NetOps for your account, but you can modify this file to do what you want.

For example, you can put aliases in your .bashrc file for the mv and cp commands so that you don't accidentally overwrite files:

```
alias cp='cp -i'
alias mv='mv -i'
```

I also recommend that you make "ls -F" your default to make it easier to tell the difference between directories and files:

```
alias ls='ls -F'
```

If your want, you can also define a custom prompt:

```
PS1='\u@\h> '
```

Programs in the Mac applications folder can be conveniently run from within a UNIX window by including suitable aliases in your .bashrc file, e.g.,

```
alias tedit='open -a /Applications/TextEdit.app/'
alias xcode='open -a /Applications/Xcode.app/'
```

in which case you can just type tedit filename or xcode filename to open filename in the desired editor.

One of the most important things in the .bashrc file is defining your *path*. This lists all the directories that the computer should look in when you try to run a program. For example, if you type "matlab" the computer needs to know where to look to find the matlab program. If you get a "Command not found" message, then you don't have the right paths set in your .bashrc file.

Here is an example of how to define your path:

```
PATH=$PATH:/usr/local/gfortran/bin:/opt/local:/opt/igpp:/usr/local/bin
PATH=$PATH:/Applications:/Applications/Utilities:/Developer/Applications
```

Note the use of the colon to append additional paths to the current set of paths.

In the past, I recommended that students include the current directory in their path, i.e.,

```
PATH=$PATH:.
```

This has the advantage that you can run programs in the current directory simply by typing their name, i.e., if you have a program called compspec, you can run it by typing 'compspec' on the command line. However, NetOps recently convinced me that this is a security risk because bad people could put malevolent programs into your directories, with the same name as common UNIX commands (e.g., ls), which would be executed when you innocently typed them. This means that to execute compspec within the current directory, you must type './compspec' on the command line (which really is not *that* much more work).

You can always look at other people's .bashrc files if you have trouble with yours. If you make any changes to your .bashrc file, they won't take place until you open another Terminal window. Alternatively you can enter:

```
source .bashrc
```

to make the changes immediately. But you will have to do this separately for each window that you have open.

For reasons that I don't completely understand, sometimes when you open a new Terminal, your computer will execute a file called .bash_profile instead of .bashrc. Thus to make sure that your .bashrc file is always executed, you should have a .bash_profile file in your home directory that contains the following:

```
if [ -f ~/.bashrc ]; then
   source ~/.bashrc
fi
```

which ensures that .bashrc is sourced, assuming it exists.

2.5 Scripts

One of the most powerful ways to use UNIX is to write scripts to run your programs. This is an easy way to keep track of the input and output parameters and to make changes without having to enter everything in again. For example, suppose you have a program called mapfocal that asks you a bunch of questions like this:

```
shearer@koan> ./mapfocal
 reading cmt file...
 nev =        24584
 Enter output file name
globalcmtmap.ps
 Enter fill level, line thickness for conts
0.93 1
 Enter line thickness for plate boundaries
5
 Enter line thickness for beachballs
1
 Enter minimum magnitude
0
 Enter circle radius for beach balls (neg. for M0 scale)
0.08
 (1) complete plot  or  (2) outline for test
1
 Creating psplot postscript file : globalcmtmap.ps
 nplot =          415
shearer@koan 17>
```

After running this program, you decide that you would like to change the continent line thickness to 2. This is tedious if you have to type in everything again. Instead you can write a script to run the program called 'do.mapfocal' that looks like this:

```
./mapfocal << !
globalcmtmap.ps
0.93 1                !fill level, line thickness for continents
5                     !line thickness for plate boundaries
1                     !line thickness for beach balls
0                     !mininum magnitude
0.08                  !circle radius for beach balls (neg for mom scale, 0.08 looks nice)
1                     !1=complete plot or 2=outline for test
!
```

This is just an ascii file that you write with your favorite text editor. The comments following the numbered input (e.g., !min,max quake magnitude) are convenient if the program that you are running is robust enough to ignore additional characters on lines that follow the numbers that are actually input into the program.

To run the script, simply enter:

```
./do.mapfocal
```

You may get a message which says:

```
do.mapfocal: Permission denied
```

This means that you don't have execute permission on this file. To see what the permissions are, use the 'ls -l' command:

```
shearer@koan> ls -l do.mapfocal
-rw-r-xr-x  1 shearer  669  419 Oct  3  2012 do.mapfocal*
```

The '-rw-r–r–' shows what the permissions are for the file. Columns 2-4 (rw-) are your permissions as owner of the file. Columns 5-7 and 8-10 give the permissions for your group and all others, respectively. The r means read permission, the w means write permission and x means execute permission. In this case our problem is that we have 'rw-' instead of 'rwx' To fix this, use the 'chmod' command:

```
chmod 755 do.mapfocal
```

This will give you rwx permission of file do.mapquake and will give everyone else rx permission but not w permission. This is probably the most common set of permissions you will want to set, assuming you are OK with others looking at your code and running your programs, as long as they are not allowed to make changes. Because the default permission for files created by most text editors does not give

execute permission for newly created scripts, I commonly have to use chmod before I can run the scripts. To save time, I have created an alias in my .bashrc file called fix:

```
alias fix='chmod 755'
```

so that I can just enter 'fix filename' to correct the permissions for filename.

If you don't want anyone else to be able to see your file, set

```
chmod 700 do.mapfocal
```

The three digits following chmod define the permissions for you, your group, and everyone else respectively. As shown by the above examples, the most common to assign are:

7 = read, write, and execute permission

5 = read and execute permission, but no write permission

0 = no permission

For more details see the chmod manual. You can also check and/or change permissions within the Mac Finder environment by clicking on a file or directory name and then entering Command-i for information. This will show the sharing and permission status.

The do.mapfocal script will run the mapfocal program and enter all of the required inputs. Notice that in this case I have added helpful comments to the numerical input lines. You can do this with most programs and it will not affect the input (at least for FORTRAN, I'm not so sure about C). You usually cannot, however, add comments to the character inputs (e.g., globalcmtmap.ps in this example) because it will consider them part of the name.

Now it's easy to keep track of the inputs and to make changes without having to re-enter everything. You can also put scripts together to run the program many times:

```
./mapfocal << !
globalcmtmap1.ps
0.93 1               !fill level, line thickness for continents
5                    !line thickness for plate boundaries
1                    !line thickness for beach balls
0                    !mininum magnitude
0.08                   !circle radius for beach balls (neg for mom scale, 0.08 looks nice)
1                     !1=complete plot or 2=outline for test
```

```
!

./mapfocal << !
globalcmtmap2.ps
0.93 2                !fill level, line thickness for continents
5                     !line thickness for plate boundaries
1                     !line thickness for beach balls
0                     !mininum magnitude
1.1                    !circle radius for beach balls (neg for mom scale, 0.08 looks nice)
1                      !1=complete plot or 2=outline for test
!
```

In this case, you can make two different plots from the same script.

2.6 File transfer and compression

You often will want to get files from another computer. There are various ways to do this. Today often files can simply be accessed via the web through a web browser, or by directly mounting the disk of the other computer. An old fashioned method of file transfer is the ftp (file transfer protocol) command, which is still used quite a bit.

2.6.1 FTP command

One classic method of UNIX file transfer is the ftp command. For many public sites and data centers this is done with anonymous ftp. You simply enter:

```
ftp othercomputer
```

where 'othercomputer' is the name (or IP address) of the other computer. When you are asked to login, just enter 'anonymous' and then your e-mail address as a password. Of course, if you have login permission on the other computer then you can ftp to the machine even if it is not set up for anonymous ftp.

Once within ftp, you will get a ftp prompt. You then can use the 'cd' command to get to the directory that you want and 'ls' to see the file names on the remote computer. Finally use 'get' to bring the desired file to your own computer and then 'quit' to exit ftp. If you want to get all of the files in the directory, use the command 'mget *' and you will be prompted for each file name. If you don't want to be prompted, you can turn off the interactive mode by entering

```
ftp -i othercomputer
```

when you first invoke ftp. If you are getting binary files (rather than simple text files), you should enter

```
type binary
```

at the FTP prompt before getting the files. Because 'type binary' will work with all types of files, including ascii, it is a good practice to always enter 'type binary' as soon as you enter ftp. The default for the Suns is 'type ascii' which does not work with binary files.

If the remote computer objects to regular ftp for security reasons, you might try 'sftp' which is the secure ftp command.

If you have just a few files to transfer, you may want to use the secure copy command:

```
scp filename *.ps shearer@rock.ucsd.edu:./TRANSFER
```

will copy filename and all files ending with .ps from the current directory to the TRANSFER directory in shearer's account on rock.ucsd.edu (after first prompting for the password). If you want to copy a directory, you need to use the -r (recursive) option, i.e.,

```
scp -r dirname shearer@rock.ucsd.edu:./TRANSFER
```

Note that one can also copy files from the remote computer to the current directory, i.e.

```
scp -r shearer@rock.ucsd.edu:/net/moray2/scratch/dirname dirname_local
```

In this case the remote directory was on the /net/moray2 disk; notice how we specified the complete path name.

2.6.2 File compression

Often the files that you retrieve will be compressed. Files can be compressed using the UNIX 'compress' command:

```
compress filename
```

This will change the name to filename.Z which tells you that it is compressed. This is useful to save disk space when you will not be using the file for awhile. To get back to the original file, use uncompress:

```
uncompress filename
```

You can compress a whole bunch of files by using wildcards:

```
compress *.ps
```

will compress all of your Postscript files, assuming you use the .ps suffix convention for these files. These can be uncompressed with 'uncompress *.ps' as you would expect.

An alternative compression method (not standard UNIX but usually available) is invoked with the gzip command:

```
gzip filename
```

This changes the name to filename.gz with the reverse operation:

```
gunzip filename
```

The gunzip command will also decompress .Z files (but the uncompress command will not decompress .gz files).

Note: On Macs, most compressed file formats can be uncompressed by simply double-clicking on them.

You may find it useful to use compression yourself by compressing files that you do not use very often in order to save space. I often do this when I want to get some disk space but am too nervous to delete the files and too lazy to write them to long-term backup.

2.6.3 Using the tar command

Often you may want to save or retrieve an entire directory of files. This is most easily done using the 'tar' command. If you are within the directory containing the files that you wish to save, then enter:

```
tar -cvf ../archive.tar .
```

The arguments are as follows:

```
-c              create tar archive
-v              verify by printing file names to screen
-f              output file name will follow
../archive.tar  name for tar file (../ to put in next level up)
.               tar every file in current directory
```

Alternatively you can save the entire directory and its contents from the level above the directory:

```
tar -cvf programs.tar programs.dir
```

The tar file can then be FTPed to another machine. For even more efficiency you may wish to compress the tar file first. The files can be retrieved as follows:

```
tar -xvf archive.tar
```

which will put all of the files in the archive into the current directory.

The tar command was originally written largely to write and retrieve backups, etc., onto tape, in which case the file name (e.g, ../archive, programs.tar, etc.) in the above examples is replaced with the name for the tape device. Today hardly anyone uses tape drives because large capacity hard drives have gotten so cheap. The Exabyte and DAT tape drives we used to have in the IGPP Barnyard have been retired. If your advisor hands you an old data tape, you might check with NetOps to see if they can read it, as they still have a few old tape readers.

2.6.4 Remote logins and job control

Often you will want to run on a different machine than the one that you are sitting at. The other machine may be faster, have more memory, be connected to a large hard drive with data, etc. To do this enter:

```
ssh machinename
```

and you can login and run remotely on this machine. Of course this will slow the machine down for anyone else using it, so exercise some courtesy in doing this. One option is to start your job with the 'nice' command:

```
nice do.bigjob
```

where do.bigjob is the script that runs your program. The "nice" command lowers the priority of your job so that it will not interfere with others using the machine. You still may be unpopular, however, it you use a lot of memory on the machine.

Niceness levels range from 1 (highest) to 19 (lowest). The default for the nice command is niceness 4 or 10 (depending upon which UNIX shell you are running). To set the niceness to a specific value, you can specify a number, e.g.,

```
nice +15 do.bigjob
```

will run do.bigjob at niceness 15.

As a word of caution, most people don't like to have other people run jobs on their 'personal' machines (the ones in their offices) without permission, even if the jobs are set to run at large niceness values.

To find out what jobs are running on your machine, you can use the 'top' command to list the most active jobs:

```
top
```

This will take over your window and update the results continuously until you enter q for quit. The Process ID (PID) is listed, together with the username, the niceness, the fraction of the CPU being used and other useful information. top is interactive and you can input various commands (? for help, u to see only one user, etc.). You can stop (kill) jobs from within the top program, or at the command line using the "kill" command (see below).

If you did not originally use nice when you started a job you can 'renice' the job from within top by entering 'r' Alternatively, if you know the job number you can change the niceness at the command level, e.g.,

```
rock> renice +15 1132
```

where 1132 is the PID number (get from top program). You can renice more than once, but only to raise the niceness level— you can never lower the niceless level once it is set.

On the Macs, the "Activity Monitor" program (in Applications/Utilities) provides a convenient alternative to the UNIX top command.

2.7 Miscellaneous commands

Unix keeps track of your previous commands. To see them, enter

```
history
```

for history and it will list your last 30 commands. To repeat a past command, enter ! followed by line number in the 'h' list **or simply the first few letters of the command**. To repeat the very last command, enter !!

Want to see what just the beginning or end of a big file looks like? Use the head or tail command:

```
head filename          ---lists the first 10 lines of the file
tail filename          ---lists the last 10 lines of the file
```

To see a file one page at a time, use the 'more' command:

```
more filename
```

and then hit the space bar to advance one page at a time.

Want to see how many lines and words are in a text file? Use the word count ('wc') command:

```
wc filename
```

This will list the number of lines, words, and bytes in the file. Often I just want to know the number of lines, in which case it will run faster to use the -l option for line:

```
wc -l filename
```

Lose track of where a file is? You can use the 'find' command:

```
find . -name filename -print
```

This will look in the current directory (that's what the . is for) and below for the file named 'filename' and then print where it is. What if you only know some of the characters of the file? You can use a wildcard:

```
find . -name 'map*' -print
```

This will find all files that begin with 'map' and print them on your screen. Note that you MUST enclose 'map*' in apostrophes for this to work. Of course, most computers now have built in search programs (e.g., Mac Spotlight) to locate files, which may be more useful in many cases.

Unix has many powerful utility programs. One of these is the 'sort' command to sort files in alphabetical or numerical order. Example:

```
sort +4 -n -b -r file1 -o file2
```

This sorts file1 and outputs the results to file2. The following options are used in this example:

```
+4  skip first 4 fields (leave out to use beginning of line)
-n  numerical order (default is alphabetical order)
-b  ignore leading blanks
-r  reverse order (leave out for standard order)
```

NOTE: The +4 option no longer seems to work in Mac UNIX. Instead you set the field number (normally the column number) using the -k option, i.e.

```
sort -k 5 -n -b -r file1 -o file2
```

should do the same thing as +4, i.e., skip 4 columns and sort on the 5th column.

To find out how much disk space is available use df (disk free):

```
df
```

This will not list all the disks on the system unless they have been mounted. Just go to the disk that you are interested in and retry 'df' if it does not appear the first time.

To see how much space you are using, the best command is

```
du -ks *
```

This will list the disk usage of each of your subdirectories. It is a good idea to go through your directories once a month or so to delete unnecessary files and/or compress large files that you don't use very often.

To check for misspelled words in a file, use:

```
spell filename
```

This will list all words not found in a dictionary (which one?). Use the -b option for the British spelling if you are submitting a paper to Nature. (NOTE: unfortunately spell does not seem to work in Mac UNIX)

To reformat a text file to a uniform maximum line length of 72 characters, use:

```
fmt file1 > file2
```

This assumes that blank lines separate paragraphs. Line feeds within a paragraph are removed and added as necessary to make the lines of approximately equal length. This command is a useful feature if you use regular unix mail and create your outgoing messages with a text editor. It is helpful when you want to change a line in the middle of a paragraph because you don't have to redo all the following lines in order to make things look nice.

To preview a postscript file on the screen use:

```
gv filename.ps
```

which is an abbreviation for the old ghostview program.

2.7.1 Common sense

This should go without saying, but you never know. Do not download pornography, hate literature, etc., on UCSD computers. You may get into BIG trouble (worse, you could get your advisor into trouble!). You also should not illegally download copyrighted material (musics, movies, etc.).

You should not consider UCSD e-mail to be completely private. Even deleted e-mail is usually still on the computer system somewhere, often on daily and weekly backup tapes. Be very careful when you reply to messages sent to a group of people that you do not send your message to everyone on the list (unless that is your intention).

Attempts at sarcasm and irony usually misfire in e-mails. It's best to err on the side of professionalism in your communications with your colleagues.

2.8 Advanced UNIX

This writeup so far contains most of what I have ever done with UNIX. You can go pretty far with only 20 commands or so. However there are much more powerful

things you can do. If you really want to be a UNIX guru, try reading up on pipes, grep, awk, sed, etc. Then you will be able to write custom scripts to do all kinds of neat things. Here are some examples:

```
grep dziewonski filename
```

This will print every line from file filename that contains the string Dziewonski.

```
grep -v dziewonski filename
```

This will print every line from file filename that does NOT contain the string Dziewonski.

```
grep dziewonski filename > dz.lines
```

This works as above except the lines containing dziewonski are written to the file dz.lines rather than printed to the screen.

```
grep dziewonski *
```

This lists lines containing dziewonski from ALL files within your current directory. However, you may really want just the file names of the files that contain the string dziewonski, in which case the following command will work better:

```
grep -l dziewonski *
```

This lists the file names of the files that contain the string dziewonski

```
grep ezxplot $(find . -name Makefile -print)
```

This is one that recently saved me when I could not find a program that I knew I had written, but I did not know its name or which directory it was in. I knew, however, that the program was compiled with a Makefile that would contain ezxplot because this is necessary to make the program work. The grep command searches for ezxplot in a list of file names returned by the find command. Note that the find command must be enclosed with $(....).

```
ps -eaf
```

This lists all processes that are running on your machine

```
ps -eaf | grep shearer
```

This lists all of the processes that contain the string shearer in the output lines of ps. In this case, the vertical line is a 'pipe' that directs the output of the first command, ps, into the input of the second command, grep.

```
ps -eaf | grep shearer > junk
```

As above, but writes the output into file junk rather than to the screen.

```
kill PID
```

This kills a job with process ID number PID (obtained from the tops or ps command). This is useful for runaway jobs. For stubborn jobs, use the -9 option:

```
kill -9 PID
```

You can compare two files using the diff command:

```
diff file1 file2
```

This lists all differences between file1 and file2. This is useful if you have made some changes to a file but cannot remember exactly what they are.

2.8.1 Some sed and awk examples

```
cat file1 | sed -n '1,1p' > file2
  Copy first line only of file1 to file2.  Note that -n
  indicates that a line number range will follow, the p
  is to print the lines.

cat file1 | sed -n '5,10p' > file2
  Copy lines five to ten of file1 to file2.

cat file1 | sed -n '2,$p' > file2
  Copy all but the first line of file1 to file2. Note that
  $ indicates the last line.

cat file1 | sed 's/Peter/Paul/' > file2
  Copy file1 to file2, substituting "Paul" for the first "Peter"
  on each line.

cat file1 | sed 's/Peter/Paul/g' > file2
  Copy file1 to file2, substituting "Paul" for the every "Peter"
  on each line (note the "g" flag for global substitution).
```

```
cat file1 | sed 's/^/Paul says /' > file2
  Insert the prefix "Paul says " at the beginning of each line.
  Note that "^" means start of line

cat file1 | awk '{print $5,$3,$1}' > file2
  Assuming file1 has 5 columns of figures, this copies columns
  5, 3, and 1 to file2, in that order, omitting the 2nd and
  4th columns.

cat file1 | awk '{print $2, $1*(-10)}' > file2
  Switch columns 1 and 2 and multiply original 1st column
  numbers by -10.

cat file1 | awk '{print substr($0,1,10) substr($0,31,10) substr($0,21,10)
                  substr($0,11,10) substr($0,41,length($0)-40)}' > file2
  This copies file1 to file2, swapping the contents of columns 11-20
  and columns 31-40.  $0 is the line, substr takes a chunk of it, the
  last part prints the remainder of the line.

cat file1 | awk '{print "Columns 11 to 20 are " substr($0,11,20)}' > file2
   Start the beginning of each line with "Columns 11 to 20 are " and then
   list the contents of those columns in the input file.
```

Variations on the last few examples can be used to reformat ascii data files, including those that do not have spaces between fields.

To learn more about sed and awk, please see Duncan Agnew's notes on the class website.

2.9 Example of UNIX script to process data

By combining UNIX commands into a script, it is possible to create very powerful tools for processing data. Consider a simple example where we have a number of data files contained in a data directory:

```
rock> cd data.dir
rock> ls
data1 data2 data3
```

We have written a program to process the data in these files and write new data files which we might want to call data1.proc, etc. The program is called procdata and prompts the user for an input file name and an output file name, and, in this simple example, a multiplier factor to scale the data. If the program is one level up from the data directory, then:

```
rock> ../procdata
Enter input file name
data1
Enter output file name
data1.proc
Enter multiplier factor
3
rock>
```

To process all of the files in the directory, we could run the program for each file, manually entering the file names. However, clearly this would get very tedious if we had lots of files to process. We could modify the program to accept a list of file names, but perhaps it is a complicated program that someone else wrote that we don't want to mess with. Another approach is to write a UNIX script to run the program for all of the files in the directory. Here is one way to do this, using the command file do.proc, which looks like this:

```
#!/bin/bash

\rm data.dir/*.proc

ls data.dir > filelist
cd data.dir

# loop over data file names
for filename in $(cat ../filelist)
do

echo "processing file:" $filename

../procdata << !
$filename
$filename.proc
200
!

done

cd ..
\rm filelist
```

Note that we start with

```
#!/bin/bash
```

to make sure we are in the bash environment. In general, scripts written for tcsh will not work under bash, and vice versa.

This script is designed to be located in the same directory as the program, one level up from the data directory. Note that within the script, we use 'backslash rm' instead of 'rm' so that any aliases that might require interactive verification of the deletions are not performed. Otherwise the computer might prompt us to see if we really want to delete the files and the script would not be prepared to handle this.

Next, we remove any existing processed files in the data.dir directory, using a wildcard and assuming that the file names end in .proc

Next, we write a list of the data file names within data.dir into the file filelist.

Then we go into data.dir where we loop over the filenames contained in filelist, using the lines

```
for filename in $(cat ../filelist)
do
```

which assigns the variable filename sequentially to each line in filelist, each time executing the lines in the script between 'do' and 'done' which terminates the loop. $(....) is bash for "execute the UNIX command inside the parentheses." In a simple case in which the file names are always data1, data2, and data3, this line could have been written as

```
for filename in data1 data2 data3
```

but this is not a very versatile way to write the script.

Note that comment lines start with #, i.e.,

```
# loop over data file names
```

is just to make the script easier to understand.

We use the echo command to output to the screen each file name that is being processed. Note that we must include $ in front of the variable filename when it is referred to after its definition.

We then run the procdata program (one level up, so we need the ../). The procdata program is terminated within the script with the ! symbol.

Following the 'done' statement that completes the loop over the files, we go back to the directory containing the program and delete filelist, as it is no longer needed.

The power of this script is that it can be run on a directory containing thousands of files, just as easily as for a smaller number of files.

Now let's explore some possible changes to this script. Perhaps we don't want all the program i/o lines to print on our screen. To write these to an external file, we could write the following:

```
#!/bin/bash

\rm procdata.log
\rm data.dir/*.proc

ls data.dir > filelist
cd data.dir

# loop over data file names
for filename in $(cat ../filelist)
do

echo "processing file:" $filename

../procdata >> ../procdata.log << !
$filename
$filename.proc
200
!

done

cd ..
\rm filelist
```

Now, the screen output from the program (all of the 'Enter input file name', etc., lines) are directed to a file called procdata.log, so the first thing we do is remove any old versions of this file, if it exists.

In this example, we really did not need to generate the file filelist because we eventually deleted it. Thus, we could have written the script as:

```
#!/bin/bash

\rm procdata.log
\rm data.dir/*.proc

cd data.dir

# loop over data file names
for filename in $(ls)
do

echo "processing file:" $filename
```

```
../procdata >> ../procdata.log << !
$filename
$filename.proc
200
!

done

cd ..
```

We won't have time in this class to go into the details of all of the different things one can do in scripts like this. There are lots of books and websites on UNIX that one can consult for this purpose, but most of us just pick up stuff as we need it. The main point that I want to get across is that if you are spending lots of time running programs manually, then you are wasting your time. Spend some of that time learning how to write a UNIX script and you will be far better off in the long run. Your work will be better documented and it will be much easier for you (and others) to reproduce your work.

For example, geophysics students often write elaborate scripts to request data from a data center, convert it to a more desirable format, perform quality control, and then execute a series of processing steps that may involve a mixture of different programs.

2.10 Common UNIX command summary

```
cat filename    print filename on your screen

cd dirname      change directory to dirname
cd ..           go back up one level
cd             go to home directory
cd ~/dirname    go to directory dirname in home directory
cd ~otheruser   go to home directory of otheruser

cp file1 file2  copy file1 to file2
cp -i f1 f2     copy f1 to f2 but ask before overwriting f2

df              list disk space on the different disks
du -ks *        list disk usage for files/dirs in current directory

lpr -P silo filename  send filename to printer silo

ls              list files in directory
ls -l           list
ls -a           list all files including those starting with .
```

```
ls -F           flag directories by adding slash to their name
ls *.f          list all files with ending with ".f"

mkdir dirname   make directory dirname

mv file1 file2  change name of file1 to file2
mv -i f1 f2     change name of f1 to f2 but ask before overwriting existing f2
mv *.f src      move all files ending in '.f' into existing directory src

pwd             print working directory

rm filename     remove filename
rmdir dirname   remove directory dirname (directory must be empty)

wc filename     count words in file
wc -l filename  count lines in file
```

Chapter 3

A GMT Tutorial

Generic Mapping Tools, almost always called simply GMT, is a set of UNIX tools for making map and plots written by Paul Wessel and Walter Smith. This software is in the public domain and is still maintained by Wessel and Smith.

If you have an IGPP laptop, GMT should already be installed. If you need to install it on your own Mac, I recommend that you follow the NetOps Macports instructions at: https://igppwiki.ucsd.edu/wiki/pages/A0i460e/Installing_Macports.html

To learn about GMT, there is a website at http://gmt.soest.hawaii.edu/ that contains links to documentation, a GMT tutorial, and a number of examples. Often the best strategy for figuring things out is to look through the examples and find something close to what you want and use that as a starting point. If you Google "GMT tutorial" you will find a number of useful sites.

Once you have learned a little bit about how to use GMT, it's helpful to use the online help documents as your primary reference. You can access these at the UNIX command level by simply entering: man gmt pscoast or even just gmt pscoast, although the latter option does not produce text as nicely formatted as the former. But be warned, GMT is not very "user friendly". If you are unfamiliar with some of the features of the UNIX environment like piping output, etc., you may find it fairly intimidating at first. However, it is extremely powerful in the number of things that it can do and the time spent learning how it works will not be wasted as you will become familiar with many useful UNIX tools. GMT is capable of producing very nice maps and plots and is pretty much the industry standard for Earth Science map making.

We begin with an example using the tool pscoast. You will ALWAYS want to run GMT as a UNIX script (see Chapter 2). Here is one called do.gmt1:

```
#!/bin/csh
gmt pscoast -R0/360/-90/90  -JQ180/6i  -B60g30  -P  -Dc  -G150  >! map.ps
gv map.ps
```

The first line, #!/bin/csh, invokes the C-shell environment. The script will run without this, but it is probably safest to always go into the C-shell because most example GMT scripts do this. Presumably in some cases it may make a difference.

Next we encounter gmt pscoast which invokes the GMT program that draws coastlines. Note that older versions of GMT than GMT5 will leave out the "gmt" and start the command with "pscoast" alone. Older GMT scripts will not work under GMT5 unless you modify them by adding "gmt" in front of all the commands (there are other changes as well, but this is the biggest one).

GMT programs have a lot of options that, in UNIX style, are invoked with a dash and a letter on the same line (e.g. -P, -Dc, etc.). The output of the program is directed to the Postscript file map.ps. Note that we use >! instead of > to avoid getting an error message if map.ps already exists; but beware, you will overwrite any existing map.ps file.

To get a full list of options, simply type man gmt pscoast. But for now, let us examine the arguments in our example:

```
-R0/360/-90/90
```

This sets the map limits of longitude (lon1=0, lon2=360), and latitude (lat1 = −90, lat2 = 90). Note that we could have written this with a space between the "R" and the zero ("0") immediately following. Most people leave this space out to more easily separate the different commands.

```
-JQ180/6i
```

This specifies the map projection to be cylindrical equidistant (a simple linear scaling of lat/lon). The center meridian is set to 180 degrees; the plot width is set to 6 inches (the "i" means inches). A very large number of different map projections are available!

```
-B60g30
```

This sets the labeled lat/lon lines to 60 degree intervals and the unlabeled lines to 30 degree intervals

`-P`

Specifies "portrait" mode so that the plot is not rotated by 90 degrees as in "landscape" mode (default).

`-Dc`

Sets the resolution of the coastline to "c" for crude. This is all that is required for a small map of the whole globe. For larger maps or closeups, higher resolution will be required. The available options are: (f)ull, (h)igh, (i)ntermediate, (l)ow and (c)rude. Note that the full resolution files require over 55Mb of data and provide great detail, which would be wasted in this case. For efficiency in generating and storing the plots, you should only use as much resolution as you need and thus -Df should be reserved for extreme closeups. The default is (l)ow resolution.

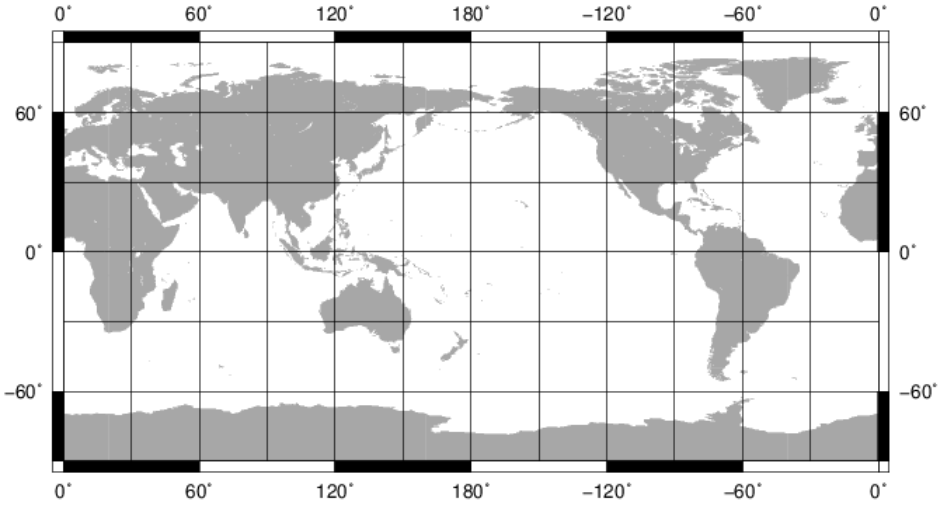
`-G150`

Specifies the grayshade level for the continent shading from 0 (black) to 255 (white). These nonintuitive units are a Postscript convention!

The GMT part of the script is entirely the "gmt pscoast" command and we could stop there. Running the script would creates the map.ps file, which could examine after the script is finished. However, it's convenient to display the result immediately, so we add a line to preview the Postscript file:

```
gv map.ps
```

After running the script do.gmt1, you should get a Postscript plot that looks like this:



If you open the file in gv, you will notice that there is a lot of white space around the plot and it is not centered on the page. The white space is not a big problem, as you can remove the space if you want by opening the .ps file in Preview and then saving it as a .eps or pdf file. You can also import .ps files directly into Adobe Illustrator for resizing, adding labels, etc. However, if you generate a plot larger than the page size, GMT will truncate it. To give yourself more room, set the media type to ArchE, which is poster size, using gmtset PAPER_MEDIA ArchE.

The plot is not centered on the page because the default position for the lower left corner is at x=1inch, y=1inch. We can change this by specifying the x and y positions directly:

```
-X1.2i -Y4i
```

This sets the lower left corner to 1.2 inches from the left edge and 4 inches from the bottom.

You may also decide that you don't want grid lines drawn on the plot so we remove the "g30" from the -B command:

```
-B60
```

This puts a label on the latitudes and longitudes every 60°, but doesn't draw the grid.

You may prefer a smaller font. This can be set with GMTSET before calling pscoast:

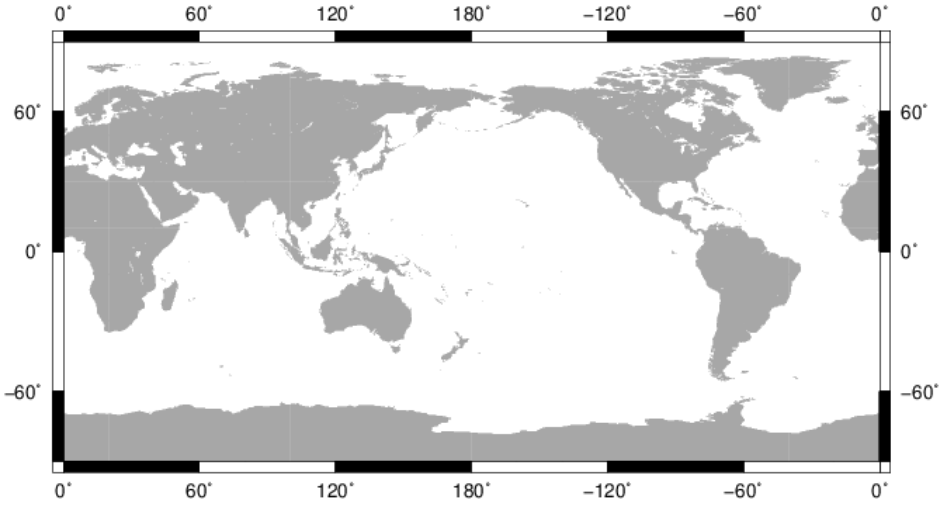
```
gmt gmtset FONT_ANNOT_PRIMARY 10
```

The resulting script (do.gmt2) is:

```
#!/bin/csh
gmt gmtset FONT_ANNOT_PRIMARY 10
gmt pscoast -R0/360/-90/90  -JQ180/6i  -B60  -P  -Dc  -G150 \
        -X1.2i -Y4i >! map.ps
gv map.ps
```

Note that we used a backslash to indicate that the line continues to the next line. In this way we can avoid making our lines too long.

This script produces:



After running the do.gmt2 script, if we run the do.gmt1 script again, we will be surprised to see that the font size is the same as we just got using the do.gmt2 script. In other words, do.gmt1 is not working exactly the same as it did before. What is going on? The answer is contained in a file called gmt.conf that GMT creates (or updates) in your current directory. It contains all of your "custom" settings, like font size, that you specify when running gmt. If you look at this file, you will see that the font size is what you specified in do.gmt2. When you run GMT, it looks to see if you have a gmt.conf file and will take parameter values from this file if it exists. This is a way to customize GMT to your own preferences. These might vary from project to project, in which case you can maintain different gmt.conf files in different directories for each project. If you don't want to read from a gmt.conf file

when you run your script, just rename the gmt.conf file to something else before running the script.

Next, suppose you have a file containing the coordinates of some seismic stations which we wish to plot on this map. The file is called station.list and its first five lines are:

```
   9.02920   38.76560 2442 AAE
  42.63900   74.49400 1645 AAK
  37.93040   58.11890  678 ABKT
  51.88370 -176.68440  116 ADK
 -13.90930 -171.77730  706 AFI
```

Here is a script (do.gmt3) that will plot these points on our map:

```
#!/bin/csh
gmt gmtset FONT_ANNOT_PRIMARY 10
gmt pscoast -R0/360/-90/90  -JQ180/6i  -B60  -P  -Dc  -G150 \
        -X1.2i -Y4i -K >! map.ps
gmt psxy -O  -R  -JQ180/6i  -St0.06i  -G0 -: station.list  >> map.ps
gv map.ps
```

The first part of the script is the same as before, except that the -K is necessary to tell GMT to keep the Postscript file open (i.e., don't put a "showpage" at the end of the file) so that more can be added to the file.

Next, we use gmt psxy to read and plot the x-y points from file station.list. We use >> to append the output onto the end of the map.ps file. Note that > or >! would not work here because it would overwrite the file instead of adding to it.

WARNING: It appears that psxy sometimes will not work if the numbers start in the first column of the input file. If you are having trouble getting psxy to work, try adding a blank character to the start of each line.

The arguments of psxy are as follows:

`-O`

Indicates that this is an overlay onto an existing Postscript file to avoid the initializations at the beginning of the file. VERY IMPORTANT: Every GMT command but the first should have -O, every GMT command but the last should have -K.

`-R`

Sets the plot boundaries (defaults to those set by pscoast)

`-JQ180/6i`

Sets the map projection (according to the manual, just saying -JQ should automatically match the previous projection (i.e., you don't need the 180/6i) but I have not always found this to be true. Try it and see what happens with your version of GMT!).

`-St0.06i`

Plots xy points as (t)riangles of 0.06 inch width. Other options are (c)ircle, (d)iamond, (s)quare, (i)nverted triangle, (x)cross, and (v)ector. In the case of the vector, the direction and length are also read from the file (see manual).

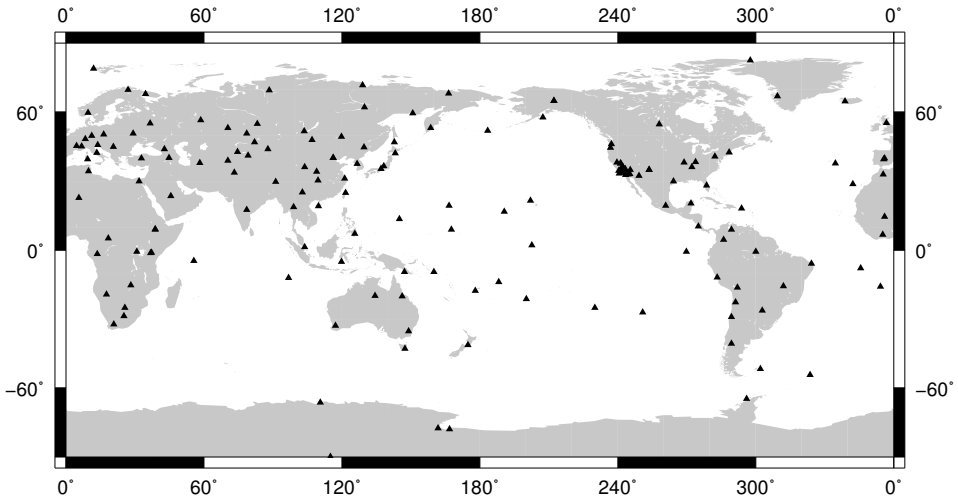
`-G0`

Set fill parameter to 0 (black). This will fill in the triangles.

`-:`

This tells the program that the data are to be read as y-x pairs. The default is x-y, or (lon, lat) in our case. For seismology this option is very useful because coordinates are usually given as lat, lon rather than the other way around.

Note that the program automatically converts the longitude convention of the data points (-180 to 180) to the longitude convention of the map (0 to 360). This is a nice feature of GMT.



Now let's try a different map projection, plot the points in red, and add a title in a script called do.gmt4:

```
#!/bin/csh
gmt gmtset FONT_ANNOT_PRIMARY 10
gmt pscoast -R-180/180/-90/90  -JH0/6i  -Bg0:."IRIS FARM stations": \
        -P  -Dc  -G150 -X1.2i -Y4i -K >! map.ps
gmt psxy -O  -R  -JH  -St0.06i  -G255/0/0 -: station.list  >> map.ps
gv map.ps
```

The changed commands are as follows:

```
-JH0/6i
```

Invokes the equal-area Hammer projection with 6 inch width

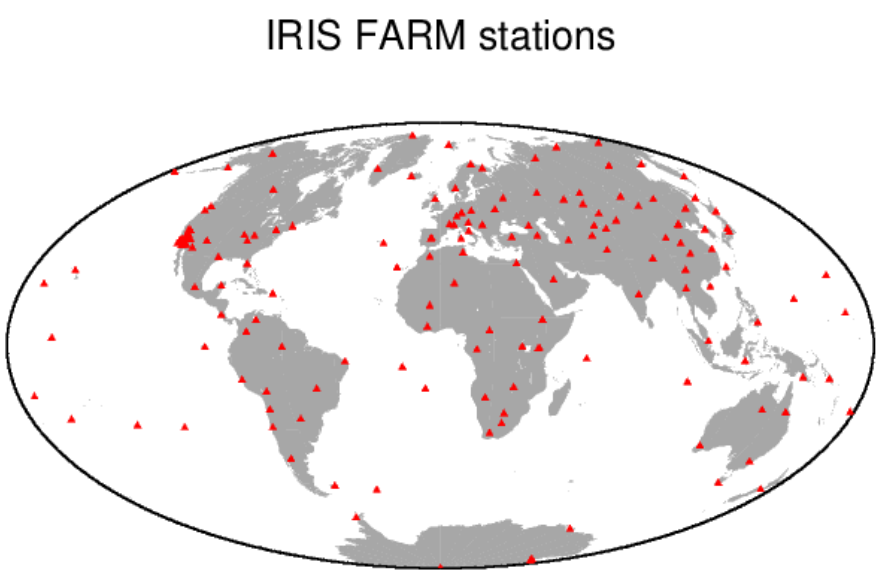
```
-Bg0:."IRIS FARM stations":
```

The 0 results in no grid lines or labels The title is set off with :." and ": (weird!)

```
-G255/0/0
```

Define the fill for the xy plot as red=255, green=0, blue=0

The result is:



To my taste, the title is way too big. This can be changed using the gmtset HEADER_FONT_SIZE command (see below).

Next, let's look at a closeup of these stations in southern California with the script do.gmt5:

```
#!/bin/csh
gmt gmtset FONT_ANNOT_PRIMARY 10p FONT_TITLE 20p
gmt pscoast -R-121/-114/32/37  -JM6i  -B1g1:."IRIS FARM stations": \
        -P  -Di -I1 -I2 -I3 -N1 -N2 -G255/200/200 -X1.2i -Y4i -K >! map.ps
gmt psxy -O  -R  -JM  -St0.06i  -G0 -: station.list  >> map.ps
gv map.ps
```

Changes are:

```
gmtset HEADER_FONT_SIZE 20
```

Set font size for title to 20

```
-R-121/-114/32/37
```

Set lon1,lon2,lat1,lat2 to S. California

```
-JM6i
```

Use Mercator projection, width = 6 inches

`-B1g1:."IRIS FARM stations":`

Label and draw grid lines every 1 degree and use same title

`-I1 -I2 -I3`

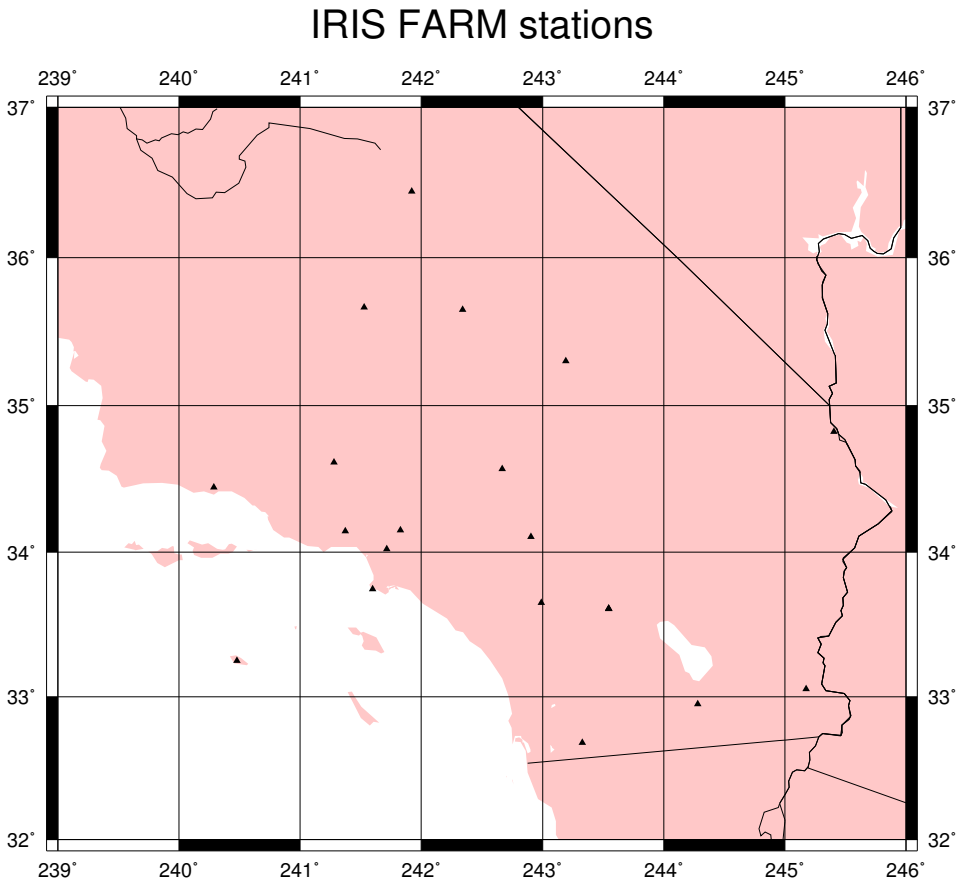
Plot permanent major rivers, additional major rivers, and additional rivers, respectively

`-N1 -N2`

Plot nation boundaries and state boundaries, respectively

`-G255/200/200`

Fill land areas with red=255, green=200, blue=200 — an unsightly shade of pink:



Next, let's add lines that show the traces of mapped faults in southern California. For this, we use a file called calif.flts that has the following format:

```
370.0000 99.0000
-115.5496 32.9312
-115.5419 32.9142
-115.5358 32.9029
-115.5276 32.8890
370.0000 99.0000
-115.9218 32.9916
-115.9096 32.9849
-115.8936 32.9745
-115.8729 32.9655
-115.8398 32.9498
-115.8216 32.9410
-115.7983 32.9295
-115.7796 32.9228
370.0000 99.0000
-115.8391 33.0127
-115.8205 33.0069
-115.8017 33.0015
-115.7892 32.9973
etc.
```

The faults are defined as (lon, lat) pairs. The creator of this file used a value of (370, 99) to separate the different faults because 370 is off the map (longitude only goes to 360). However, as we will describe below, GMT allows us to explicitly define any string we want to separate the line segments that GMT draws on the map.

To plot these faults on our map of the southern California stations, we can use the psxy command a second time in the script do.gmt6:

```
#!/bin/csh
gmt gmtset FONT_ANNOT_PRIMARY 10p FONT_TITLE 20p
gmt gmtset IO_SEGMENT_MARKER '370'
gmt pscoast -R-121/-114/32/37  -JM6i  -B1:."IRIS FARM stations": \
        -P  -Di -I1 -I2 -I3 -N1 -N2 -G255/200/200 -X1.2i -Y4i -K >! map.ps
gmt psxy -O  -R  -JM  -W1p,255/0/0 calif.flts -K >> map.ps
gmt psxy -O  -R  -JM  -St0.15i  -G0/0/255 -: station.list >> map.ps
gv map.ps
```

Changes are:

```
-B1:."IRIS FARM stations":
```

We removed the g0 so we don't plot grid lines which might get confused with the faults.

We plot the faults using:

```
psxy -O  -R  -JM -W1p,255/0/0 calif.flts -K >> map.ps
```

In the fault file, lines that start with '370' mark the segment boundaries, i.e., they separate the series of points that defines each individual fault. Without these separators, the program would draw lines between the end of one fault and the beginning of the next fault and the plot would look like a mess. In GMT, the default separator is the character '>' but we define our own separator using

```
gmt gmtset IO_SEGMENT_MARKER '370'
```

In GMT4, this could have been done using:

```
psxy -O  -R  -JM  -M'370' calif.flts -K >> map.ps            ****DON'T USE IN GMT5
```

but the '-M ' option has been removed (deprecated) from psxy in GMT5 in favor of IO_SEGMENT_MARKER.

WARNING: The quotes around 370 (or whatever string you want to use as a separator) MUST be the apostrophe character and not any kind of "smart quotes" that your text editor may want to use. If you are using the Mac TextEdit program, go to Preferences and turn off the Smart Quotes.

We control the width and color of the fault lines using

```
-W1p,255/0/0
```

This draws the line with linewidth=1p (one point) and color red=255, green=0, blue=0

Note that we do not need the -: option because the points are already given as (lon, lat).

We plot the stations last so that they will go on top of the faults. We change the symbol size and the color:

```
-St0.15i
```

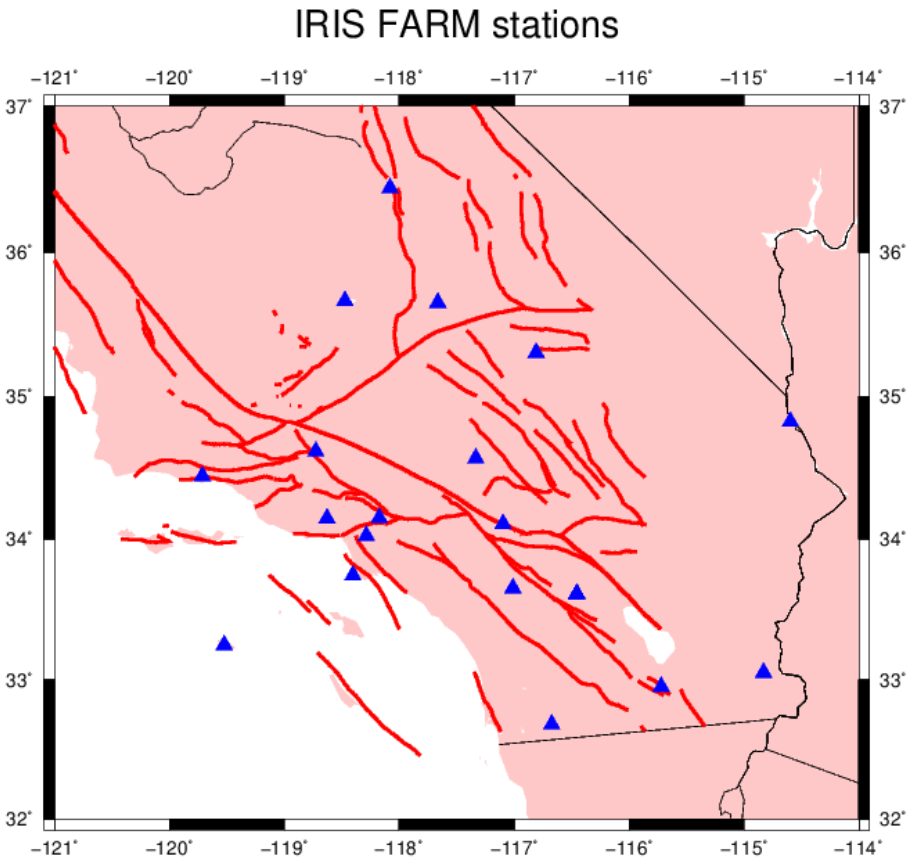
plot triangles 0.15 inches high

```
-G0/0/255
```

plot with red=0, green=0, blue=255

Note that -K is needed on every command except the last; -O is needed on every command except the first. (***THIS IS KEY TO GETTING GMT SCRIPTS TO WORK PROPERLY!!! CHECK THIS FIRST WHEN YOU HAVE PROBLEMS.***)

The script do.gmt6 results in the plot:



(Are there really no faults in eastern southern California?)

We often will want to include labels on our plot. The following script do.gmt7 adds four labels to our map using the pstext command:

```
#!/bin/csh
gmt gmtset FONT_ANNOT_PRIMARY 10p FONT_TITLE 20p
gmt gmtset IO_SEGMENT_MARKER '370'
gmt pscoast -R-121/-114/32/37  -JM6i  -B1:."IRIS FARM stations": \
        -P  -Di -I1 -I2 -I3 -N1 -N2 -G255/200/200 -X1.2i -Y4i -K >! map.ps
```

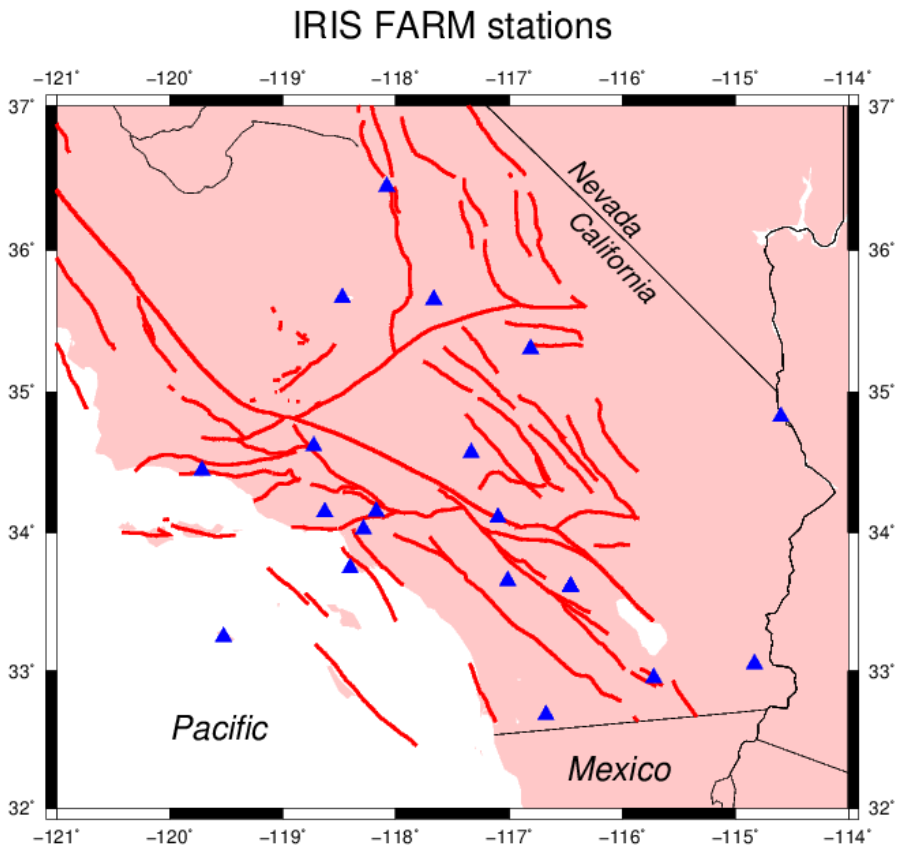
```
gmt psxy -O  -R  -JM  -W1p,255/0/0 calif.flts -K >> map.ps
gmt psxy -O  -R  -JM  -St0.15i  -G0/0/255 -: station.list -K >> map.ps
echo "-120 32.5 18 0 2 BL Pacific" | gmt pstext -O -R -JM  -K >> map.ps
echo "-116.5 32.2 18 0 2 BL Mexico" | gmt pstext -O -R -JM  -K >> map.ps
echo "-116.5 36.2 15 -45 2 BL California" | gmt pstext -O -R -JM  -K >> map.ps
echo "-116.5 36.55 15 -45 2 BL Nevada" | gmt pstext -O -R -JM   >> map.ps
gv map.ps
```

The pstext command expects to read from a file containing a list of labels in a certain format. However, in this case we avoid the need for a separate input file with the labels by using the UNIX echo command to pipe the required inputs into pstext one line at a time. For example,

```
echo "-120 32.5 18 0 2 BL Pacific" | pstext -O -R -JM  -K >> map.ps
```

adds the label "Pacific" to the plot at the (lon, lat) position (-120, 32.5) using font size 18, at an angle of 0 degrees (measured CCW from horizontal), using font number 2 (try different numbers and see what you get!), and positioned so that the reference lon/lat is at the BottomLeft of the label (L, C, R = left, center, right; T, M, B = top, middle, bottom).

The resulting plot is:



Using echo with pstext is convenient for adding just a few labels, but becomes tedious when you have a large number of labels. In the latter case, you should use a separate file for the labels, i.e., if you have the file "labels.gmt" containing

```
-120 32.5 18 0 2 BL Pacific
-116.5 32.2 18 0 2 BL Mexico
-116.5 36.2 15 -45 2 BL California
-116.5 36.55 15 -45 2 BL Nevada
```

then your gmt script can be simply:

```
#!/bin/csh
gmt gmtset FONT_ANNOT_PRIMARY 10p FONT_TITLE 20p
gmt gmtset IO_SEGMENT_MARKER '370'
gmt pscoast -R-121/-114/32/37  -JM6i  -B1:."IRIS FARM stations": \
        -P  -Di -I1 -I2 -I3 -N1 -N2 -G255/200/200 -X1.2i -Y4i -K >! map.ps
gmt psxy -O  -R  -JM  -W1p,255/0/0 calif.flts -K >> map.ps
gmt psxy -O  -R  -JM  -St0.15i  -G0/0/255 -: station.list -K >> map.ps
gmt pstext labels.gmt -O -R -JM   >> map.ps
```

```
gv map.ps
```

To my taste, the California and Nevada labels should be moved a bit down the CA/NV border to the lower right. However, there are limits to how much "fine tuning" of plots should be done using GMT because getting everything exactly right for a publication quality plot can be tedious. Precise adjustment of labels and other plots details can be done far more easily using interactive WYSIWYG programs like Adobe Illustrator. Thus, despite what I said in the class introduction about how you should use scripts to ensure the reproducibility of your results, I generally make an exception when preparing plots for publication. The distinction is between what you need to do to see the science results and what you do at the very end when you are preparing plots for talks, papers, posters, etc. The important thing is to wait to use Illustrator until you are certain that you have the final version of a plot. Before that point, script-generated working versions of your plots should be adequate.

3.0.1 Setting default values

After you have used GMT for awhile, you may find that all your scripts have many of the same lines, i.e., you always want to be in Portrait mode, or change the header font size, etc. For convenience, GMT provides a way to customize your GMT environment, i.e., to change the default parameter values. To do this, all you have to do is edit your gmt.conf file, which should be in the same directory as your scripts. If the file does not already exist, GMT automatically generates this file when you first run GMT. It will have the standard default values, except for any values that you explicitly change when you run GMT.

There are a large number of parameter choices in this file. As you gain experience with GMT, you will likely want to set many of these to reflect your own preferences for how things should look. Once they are in your gmt.conf file, then you don't need to set them each time in your GMT scripts.

Chapter 4

LaTeX

Someday you will want to publish the results of your research. IGPP scientists typically use either Word or Latex for this purpose. Most of you probably already know how to use Word. It is very easy to use (WYSIWYG) and is the "standard" word processor of choice in many institutions. It is not, however, ideal for writing scientific articles. It has particular difficulty handling equations and specialized typesetting requirements. A far better choice is LaTeX. Guess what these notes are written in!

Advantages of LaTeX:

1. It is in the public domain so you are not supporting the Evil Empire.
2. You can run it on Macs, PCs or UNIX machines.
3. By using macros, it is a far more powerful and versatile system than all the pull down menu stuff you find in most commercial word processors.
4. AGU uses LaTeX for its electronic submission of articles and abstracts. They provide macros to match the style of their journals so that preparing camera-ready copy is trivial.
5. You can produce beautiful looking equations much more easily than with programs like Word.

LaTeX takes a little while to learn at first, but you will find it well worth your effort. I will describe running LaTeX from the UNIX command line although I am actually most familiar with using it on my Mac using a fancy implementation (TexShop), which you can download from:

http://pages.uoregon.edu/koch/texshop/

4.1 A simple example

Use your favorite text editor to create the file samp1.tex (an example from the Latex book, Kopka and Daly, A Guide to Latex2e):

```
\documentclass{article}
\begin{document}
Today (\today) the rate of exchange between the British pound
and the American dollar is \pounds 1 = \$1.63, an increase of
1\% over yesterday.
\end{document}
```

which will produce:

Today (September 24, 2018) the rate of exchange between the British pound and the American dollar is £1 = $1.63, an increase of 1% over yesterday.

The document must first define a document class. Options are book, report, article, or letter. The guts of the document are then enclosed between the \begin{document} and \end{document} commands.

This example highlights some of the special characters and macros in Latex. The following characters are normally interpreted as Latex commands:

```
$  &  %  #  _  {  }
```

To print these out in your text, you must precede them with a backslash, i.e.,

```
\$  \&  \%  \#  \_  \{  \}
```

In this example, '\today' invokes a macro to print today's date and '\pound' will print the British pound symbol. From this example you can see that Latex is not WYSIWYG! To typeset this document, enter:

```
latex samp1
```

Assuming you have no errors in the input file, this will generate the file samp1.dvi. To preview this file, enter:

```
xdvi samp1
```

To convert the file to a Postscript file, enter:

```
dvips samp1 -o samp1.ps
```

Notice that Latex automatically indented the first line of the paragraph. To avoid this, use the command for the target paragraph:

```
\documentclass{article}
\begin{document}
\noindent
Today (\today) the rate of exchange between the British pound
and the American dollar is \pounds 1 = \$1.63, an increase of
1\% over yesterday.
\end{document}
```

To globally change the paragraph indenting, you can change the default for this directly:

```
\documentclass{article}
\begin{document}
\setlength{\parindent}{0.5in}
Today (\today) the rate of exchange between the British pound
and the American dollar is \pounds 1 = \$1.63, an increase of
1\% over yesterday.
\end{document}
```

This will now indent all paragraphs by 0.5 inches. To remove paragraph indenting, just set this parameter to zero. Latex ignores the carriage returns at the ends of each line in the input file. It also ignores extra blanks; it only considers the first blank. New paragraphs are defined by adding a blank line between blocks of text.

4.2 Example with equations

```
\documentclass{article}
\begin{document}
\setlength{\parindent}{0.0in}

The function $X(p)$ is more nicely behaved than $T(X)$ since it does not
cross itself (there is a single value of $X$ for each value of $p$), but
the inverse function $p(x)$ is multi valued.  An even nicer function is
the combination
\begin{equation}
```

```
\tau(p) = T(p) - pX(p),
\end{equation}
where $\tau$ is called the {\it delay time}.  It can be calculated very
simply:
\begin{equation}
\tau(p) = 2 \int_0^{z_p} \left[ {u^2 \over {(u^2-p^2)^{1/2}}} -
  {p^2 \over {(u^2-p^2)^{1/2}}} \right] \, dz
\end{equation}
or
\begin{eqnarray}
\tau(p) &=& 2 \int_0^{z_p} (u^2-p^2)^{1/2} \, dz \\
        &=& 2 \int_0^{z_p} \eta(z) \, dz
\end{eqnarray}
where $\eta$ is the vertical slowness.

\end{document}
```

which typesets as:

The function $X(p)$ is more nicely behaved than $T(X)$ since it does not cross itself (there is a single value of X for each value of p), but the inverse function $p(x)$ is multi valued. An even nicer function is the combination

$$\tau(p) = T(p) - pX(p), \tag{4.1}$$

where τ is called the *delay time*. It can be calculated very simply:

$$\tau(p) = 2 \int_0^{z_p} \left[\frac{u^2}{(u^2-p^2)^{1/2}} - \frac{p^2}{(u^2-p^2)^{1/2}} \right] dz \tag{4.2}$$

or

$$\begin{aligned} \tau(p) &= 2 \int_0^{z_p} (u^2-p^2)^{1/2} \, dz & (4.3) \\ &= 2 \int_0^{z_p} \eta(z) \, dz & (4.4) \end{aligned}$$

where η is the vertical slowness.

Note that equations within the text are enclosed with $ signs. \begin{equation} and \end{equation} are used to put the equation on a separate line. Variables within the equations are automatically put into italics. Greek letters are defined as \tau, \eta, etc. Equations are automatically numbered (this can be changed if desired). Subscripts are defined with the underscore (_), superscripts with the carat. Fractions are written as, for example, {x \over y}. \int is for the integral symbol; note how the limits are written. Curly brackets are used to separate things—they do not appear in the typeset version.

The \begin{eqnarray} section is used to align the = signs in the two lines of equations. Note that &=& is used to define what it is that is being aligned. Every line except the last line has a carriage return (\\). Although TeX generally does an excellent job of spacing equations, sometimes some fine tuning will help. In this case \, is used to place a tiny amount of space before the dz.

4.3 Changing the default parameters

4.3.1 Font size

There is a standard font size declared for each document class. In most cases this is Roman 10 pt. One easy way to change the size is with the following commands, arranged in increasing order of size:

```
\tiny
\scriptsize
\footnotesize
\small
\normalsize
\large
\Large
\LARGE
\huge
\Huge
```

4.3.2 Font attributes

```
\itshape  =  switch to italics
\slshape  =  switch to slanted font
\upshape  =  switch to upright (normal) font

\bfseries  =  switch to bold
\mdseries  =  switch (back) to regular weight
```

These commands can be invoked in several different ways to put “in situ” in italics and then return to normal font:

```
\itshape in situ \upshape
```

OR

```
{\itshape in situ}
```

OR

```
\begin{itshape}
in situ
\end{itshape}
```

These different options also apply to the font sizes listed above. Here is an example of how these options can be used:

```
\documentclass{article}
\begin{document}

Let's test different ways to say \itshape in situ \upshape
in italics.  There are several different ways to say
{\itshape in situ} in italics; indeed
\begin{itshape}
in situ
\end{itshape}
can be written in italics in at least three different ways.

Next let's experiment with {\large large}, {\Large Large},
and {\LARGE LARGE} type, as well as {\small small},
{\footnotesize footnotesize}, and {\scriptsize scriptsize}
type.

\end{document}
```

which produces:

Let's test different ways to say *in situ* in italics. There are several different ways to say *in situ* in italics; indeed *in situ* can be written in italics in at least three different ways.

Next let's experiment with large, Large, and LARGE type, as well as small, footnotesize, and scriptsize type.

4.3.3 Line spacing

There is a default line spacing created whenever a new font is selected. Here are examples of two different ways that this can be changed:

```
\setlength{\baselineskip}{10pt}   Change line spacing to 10 point
                                  (single spacing for 10pt font).

\renewcommand{\baselinestretch}{2}   Change normal (single) line spacing
                                     by a factor of 2.  This will result
                                     in double spacing.  This must be
                                     called before \begindocument or before
                                     a new font declaration.
```

Here is an example:

```
\documentclass{article}
\begin{document}
\setlength{\baselineskip}{20pt}
Today (\today) the rate of exchange between the British pound
and the American dollar is \pounds 1 = \$1.63, an increase of
1\% over yesterday.  Let's write one more line here so that we
get up to three lines and can see the spacing better.
\end{document}
```

which produces:

Today (September 24, 2018) the rate of exchange between the British pound and the American dollar is £1 = $1.63, an increase of 1% over yesterday. Let's write one more line here so that we get up to three lines and can see the spacing better.

4.4 Including graphics

Postscript, EPS, and PDF files can easily be embedded as figures in a Latex document by including Latex extension packages such as graphics or graphicx. Here is an example that uses graphicx:

```
\documentclass{article}
\usepackage{graphicx}
\begin{document}
\setlength{\baselineskip}{20pt}
We are now going to show how to embed a Postscript file into
a LaTex document using the includegraphics command.

\begin{figure}[h]
\begin{center}
\includegraphics[scale=0.7]{figures/plot_1.pdf}
\end{center}
\caption{Here is the caption for this plot.  This will be automatically
positioned below the plot.}
\end{figure}

And then here is some more text to show where the next block of text
will appear.  Blah, blah, blah...
\end{document}
```

which will produce:

We are now going to show how to embed a Postscript file into a LaTex document using the includegraphics command.

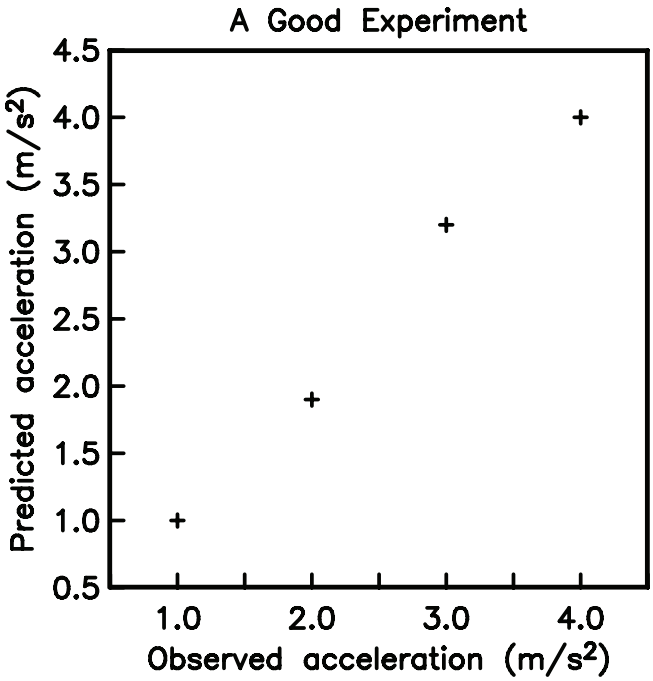


Figure 4.1: Here is the caption for this plot. This will be automatically positioned below the plot.

And then here is some more text to show where the next block of text will appear. Blah, blah, blah...

Note that the graphicx package is loaded with the \usepackage{graphicx} command at the start of the file. The \begin{figure} macro has various options for where the figure will be positioned, including at the present location in the text [h], or at the top [t] or bottom of the page [b]. These options can be combined, i.e., [tb] will position the figure at either then top or bottom of the page. In this example, the figure is scaled to 70% of its original size. Depending upon how the figure is positioned in the PDF file, you also may need to apply a "bounding box" to remove the surrounding white space using the bb= option, e.g.,

```
\includegraphics[bb=2in 4in 7in 9in, scale=0.7]{figues/plot_1.pdf}
```

which specifies exactly what part of the page will be windowed and displayed. This is necessary for PDF figures that appear in only part of an entire page and it can be tedious to find the right bounding box. In my experience, an easier option is to use the Mac Preview program to open Postscript or EPS files (from Adobe Illustrator

or other graphics programs) and then save them within Preview as PDF files. In this case, they are tightly windowed and the bb option is not needed.

Figures are automatically numbered; users have control over the starting figure number.

LATEX ASSIGNMENT

Reproduce the following using Latex (don't worry about the equation numbering):

The standard technique is to *linearize* the problem by considering small perturbations to a target location

$$\mathbf{m} = \mathbf{m}_0 + \Delta\mathbf{m}, \tag{4.5}$$

where $\mathbf{m}_0$ is the current guess as to the best location and $\mathbf{m}$ is a new location a small distance away from $\mathbf{m}_0$. The predicted times at $\mathbf{m}$ may be approximated using the first term in the Taylor series expansion

$$t_i^p(\mathbf{m}) = t_i^p(\mathbf{m}_0) + \frac{\partial t_i^p}{\partial m_j}\Delta m_j. \tag{4.6}$$

The residuals at the new location $\mathbf{m}$ are given by

$$\begin{aligned} r_i(\mathbf{m}) &= t_i - t_i^p(\mathbf{m}) \\ &= t_i - t_i^p(\mathbf{m}_0) - \frac{\partial t_i^p}{\partial m_j}\Delta m_j \\ &= r_i(\mathbf{m}_0) - \frac{\partial t_i^p}{\partial m_j}\Delta m_j. \end{aligned} \tag{4.7}$$

4.5 Want to know more?

There is a huge amount of material about Latex on the web. Check out former IGPP student David McMillan's great Latex example file, ex.tex, which you can find in ~shearer/CLASS/COMP/LATEX. The accompanying files psfig.tex, hobbes.ps, and gnufig.tex are also included.

A good Latex reference book is:

Kopka, H., and P.W. Daly, A Guide to Latex 2e, Addison-Wesley, New York, 1995.

Chapter 5

Fortran

Why learn Fortran? The answer for geophysics students at SIO is obvious—most IGPP faculty program in Fortran. However, let me make a broader pitch for its usefulness. Through the 1970s, Fortran was the language of choice for scientific programming. However C then emerged as a competitor and is much more widely taught to students, perhaps because it is favored by computer science departments (who worry more about writing compilers than how to handle complex numbers). The result is that a visit to the UCSD bookstore will reveal many shelves of books on C and C++, but the few Fortran books, if they can be found at all, will likely be found in the "Miscellaneous Language" section. Of course there are many other popular languages, such as Java and Python, but these are not fast enough to be used for serious number crunching.

Why learn Fortran if you already know C? Several reasons come to mind:

1. You will communicate and exchange software more readily with most IGPP faculty, who are generally proficient in Fortran but rather challenged in C.

2. There is a huge library of existing Fortran subroutines to perform various algorithms, both at IGPP and in the wider scientific community.

3. Complex numbers and double precision are included.

4. It's fun!

Finally, some cranky advice: It is important to become familiar with at least one major programming language. Fortran and C are such languages; Matlab and other application programs are not. In the long run, you will handicap your ability

to do science if you do not take the time to gain experience with a real programming language. In the worst case, you will be one of those annoying people that is forever asking others to write or modify programs for you.

5.1 Fortran history

The name Fortran is derived from IBS Mathematical FORmula TRANslation System. Originally it was spelled in all caps as FORTRAN, but the more modern usage is to only capitalize the first letter. Fortran is one of the oldest computer programming languages and was begun in 1954 by IBM programmers led by John Backus (no relation to George at IGPP). It is updated and "improved" by some committee of computer sciences every ten years or so. Important versions include:

Fortran IV (released in 1972)

Fortran 77 (released in 1980), major revision

Fortran 90 (released in 1991), major revision

Fortran 95 (released in ?), minor revision

Wikipedia also lists Fortran 2003 and 2008, which I don't know anything about. I would not recommend using these at this point in time. Most versions are designed to be fully backward compatible with previous versions. However, Fortran90 departed from the column sensitive format of older Fortran, resulting in a more modern approach that necessitated some slight incompatibilities with older Fortran. I will try to teach this class entirely in Fortran90, but will describe the differences with Fortran77 when they are important because you are likely to need to work with existing Fortran77 code at some point.

5.2 Texts and manuals

This class will be a tutorial on Fortran90 and will not be comprehensive. Thus, I recommend that you buy a textbook that will be serve as a more complete reference. I just checked on Amazon and there are 4 or 5 books out there. One that I have used and recommend is: *Modern Fortran Explained* (Metcalf et al., Oxford Univ. Press, 2011) You may want to check around to see which book you like best.

In class, we will use gfortran, which can be downloaded free for the Macs. To make sure you have it in your path, enter: 'which gfortran' and you should get something like /usr/local/bin/gfortran

I recommend that you add the following to your .bashrc file:

```
alias f90='gfortran'
```

This will allow you to just type f90 instead of gfortran when you want to compile programs. The examples that follow assume that you have done this.

5.3 Compiling and running F90 programs

Fortran90 programs are written as ascii files that end in '.f90'. This is called the source code. Programs in older versions of Fortran end in simply '.f'. Because of the slight incompatibilities between the versions, be sure to use the appropriate suffix so that both you and the compiler know which version to use. It is in fact possible to set things up so that your F90 programs end in .f rather than .f90. I do not recommend this because there is so much existing code around in Fortran77 that confusion is likely to result if you do not explicitly identify your code as F90.

Before the program can be run, it must be compiled using the Fortran90 compiler on your computer, creating the executable file that you use to actually run the program. For example, suppose you have a program called printmess.f90 with contents:

```
! simple Fortran90 test program (printmess.f90)
program printmess
   print *, "test message"
end program printmess
```

To compile this program from my computer (rock when I first wrote these notes), I enter 'f90 printmess.f90 -o printmess' and get the following response:

```
rock% f90 printmess.f90 -o printmess
rock%
```

No news is good news! If there was a syntax or other error detected during the compilation, we would get an error message at this point. This creates an executable version of the program called 'printmess' (you should ALWAYS use name of the program without the ".f90" for the executable) which can then be run simply by entering ./printmess:

```
rock% ./printmess
 test message
rock%
```

Note the because . is not in our path, we need to type ./printmess and not just printmess.

If you are like me, you will quickly tire of typing in the line 'f90 printmess.f90 -o printmess' Thus, I recommend that you create a Makefile (yes, the first character MUST be capitalized) in the same directory as the program. Include in the Makefile the following lines:

```
%:      %.f90
        gfortran $< -o $*
```

Very important: The tricky part of this is that the wide space before the gfortran MUST be entered as a tab, not as a series of spaces.

Once you have set up this Makefile, then you can just enter:

```
make printmess
```

in order to compile the program. Makefiles are very useful to keep track of compiler options and to bind with subroutines. (more about this later).

The difference between source code and excutables is fundamental to languages like FORTRAN and C. It is why they generally run much faster than uncompiled languages like BASIC or Matlab or Python scripts.

5.3.1 The first program explained

OK, now let's examine our simple F90 test program again:

```
! simple Fortran90 test program (printmess.f90)
program printmess
   print *, "test message"
end program printmess
```

The first line is a comment line. Anything following an exclamation mark (!) is a comment. The end of the line terminates the comment. There is no need (as in many languages) to terminate the comment with another flag. We can also use ! to add an inline comment following a statement, e.g.,

```
   print *, "test message"    !print message on screen
```

would be a valid line. The next line is blank. You can put in as many blank lines as you want and they will be ignored by the compiler. Blank lines provide a good way

to improve the readability of longer programs by breaking them up into coherent blocks of code.

The next line is used to name the program. The name printmess is not used by the program at all. This line is optional but is considered good programming style. Good style also suggests that lines in the body of the program are indented, in this case by three spaces:

```
   print *, "test message"
```

print * will output to the screen. The desired output is enclosed in quotes (apostrophes would also work). Finally, all F90 programs must terminate with an 'end' statement. The 'program printmess' is optional, but is considered good programming practice. These style points don't matter much for a short program like this, which would work just as well if were written as:

```
print *, "test message"
end
```

but are helpful for longer programs (hundreds to thousands of lines of code) where the label following the 'end' would remind a reader of which program is actually ending.

ASSIGNMENT F1

Write a F90 program to print your favorite pithy phrase.

5.3.2 How to multiply two integers

Here is a simple F90 program to multiply 2 and 3:

```
program multint
   integer :: a, b, c      !declare variables
   a = 2
   b = 3
   c = a * b
   print *, "Product = ", c
end program multint
```

The program uses three variables, the letters a, b and c. Variable names can be from 1 to 31 characters long. The first character must be a letter. The remaining characters can be any combination of letters, numbers, and underscores (_). Variables in Fortran can be of many types, including real (floating point), integer,

complex, double precision, character and logical. In our case, we want them to be integers so we define them using a 'type statement'

```
integer :: a, b, c      !declare variables
```

Older Fortran programs do not include the :: in these statements; this convention still works under F90 but is discouraged. For the Sun F90 compiler, these are 4-byte integers that can range from -2,147,483,648 to 2,147,483,647. Alternatively, they could have been defined as real numbers:

```
real :: a, b, c
```

in which case they would be floating point (real) variables. For the Sun compiler, real numbers range from 1.175494e-38 to 3.402823e+38)

The lines that follow are pretty self explanatory:

```
a = 2
b = 3
c = a * b
print *, "Product = ", c
```

Note that * is used to indicate multiplication as is true in almost all programming languages. Addition is +, subtraction is -, and division is /. In Fortran, a to the power of b is written as a**b where a and b can both be real, another Fortran advantage over standard C.

IMPORTANT: You must declare all your variables BEFORE any other statements in your program. That is,

```
integer :: a, b, c      !declare variables
```

must come before any of the lines in

```
a = 2
b = 3
c = a * b
print *, "Product = ", c
```

When writing long Fortran programs you may find it useful to use an editor with a split screen, so that you can see and/or change the variable declarations at the start of your program at the same time that you work with the variables in the body of the code.

5.4 Why you should always use 'implicit none'

It is not required that variables be declared in Fortran. If they are not declared, then the compiler assigns them as integer or real, depending upon their first letter. Variable names beginning with i through n (INteger, get it?) are assumed to be integers; all others are assumed to be real. Many, if not most, older Fortran programs adopt this convention. Often they only declare variables when the rule is broken, for example when it is desired that the variable 'year' be an integer. A prominent example of this type of Fortran programming may be found in the first edition (1986) of Numerical Recipes (but by the time of the second edition in 1992, the authors had been shamed into declaring all variables).

Such undeclared variables are said to be declared implicitly based upon their first letter. An 'implicit' statement can be used to modify the default rules, for example

```
implicit real (a-z)
```

will make all undeclared variables real. However, modifications such as this will only lead to more confusing code. Modern programming practice is to explicitly declare ALL variables and to have the compiler warn us when variables are not declared. This can be done by including the statement

```
implicit none
```

at the beginning of every Fortran program. I will admit that, as a long time Fortran programmer, I do not always follow this practice. I must concede, however, that it is a good idea and is likely to save more time in the long run (by eliminating program bugs that are often caused by undeclared variables) than is lost while writing the program.

Example 1: Suppose you should have the following line in your program:

```
x2 = a1 + a2*sin(theta)*scale1/scale2
```

but you accidentally type:

```
x2 = a1 + a2*sin(theta)*scalc1/scale2
```

If you don't follow the practice of declaring all of your variables, then the error will not be detected during compilation. The program will run and assign zero (or whatever happens to be sitting in the computer memory) to the otherwise unused variable *scalc1* and you will get wrong answers. On the other hand, if you use 'implicit none' and declare your variables, the compiler will flag *scalc1* as an undeclared variable and you can fix it before it causes any more trouble.

Example 2: Suppose you have the following lines in your code:

```
kmdeg = 111.19
dist = (delta2 - delta1)*kmdeg
```

but you have not declared *kmdeg* explicitly. Because the letter k is between i and n, the program will declare *kmdeg* as an integer. The value 111.19 will be truncated to 111 and you will get values for *dist* that are slightly, but not obviously, wrong (the worst kind of program bug to have).

To save you from these embarrassments and to encourage good programming habits, we will declare all variables for the programs in this class and I will dock you points if you fail to do so in assignments.

ASSIGNMENT F2

Copy the program multint but leave out the integer :: a, b, c statement. What happens when you run the program? Why?

ASSIGNMENT F3

Cut and paste the following defective program onto your computer:

```
program longjump
   beamon_long = 8.90    !distance in meters
   powell_long = 8.95
   dif_inch = (powell_long - beamon_1ong) * 39.37
   print *,"Powell jumped ",dif_inch," inches more than Beamon"
end program longjump
```

Compile and run the program. Then explain why it gives the wrong answer.

5.4.1 Alternate coding options

There are always lots of ways to write the same program. Here is another way to write the multint.f90 code:

```
program multint2
   implicit none
   integer :: a=2, b=3, c      !declare variables
   c = a * b; print *, "Product = ", c
end program multint2
```

First, notice that variables can be assigned values when they are declared (OK in F90, don't try this in F77). Second, notice that more than one command can be included on a line if the commands are separated by a semicolon (again, only OK in F90). Both of these changes make the code more similar to C. The variable assigning option is a reasonable convenience, but the multiple command option is certainly misused in this case because it makes the code much harder to read. Unless you have a really good reason to put more than one command on a line (saving space is NOT a good reason!), I suggest that you never use semicolons in this way.

5.5 Making a formatted trig table using a do loop

Any reasonable programming language must provide a way to loop over a series of values for a variable. In C, this is most naturally implemented with the 'for' statement. In FORTRAN this is done with the 'do loop'.

Here is an example program that generates a table of trig functions:

```
program trigtable
   implicit none
   integer :: itheta
   real :: theta, stheta, ctheta, ttheta, degrad
   degrad = 180./3.1415927
   do itheta = 0, 89, 1
      theta = real(itheta)
      ctheta = cos(theta/degrad)
      stheta = sin(theta/degrad)
      ttheta = tan(theta/degrad)
      print "(f5.1,1x,f6.4,1x,f6.4,1x,f7.4)", theta, ctheta, stheta, ttheta
   enddo
end program trigtable
```

Fortran (like C and Matlab) uses radians (not degrees) as the arguments of the trig functions. Thus, following the definitions of the variables as real, we assign degrad to 180/pi so that we can easily make this conversion.

```
   do itheta = 0, 89, 1
```

This begins the do loop which must eventually be closed with the enddo statement. For clarity, we indent the inside of the loop. This is a loop over values of theta from a starting value of 0, incremented by 1 each time, until theta is greater than 89. The 1 is actually optional as it is the default increment. Thus theta will assume the values (0, 1, 2, ..., 88, 89) inside the loop. Notice that we use an integer for the do loop. Older versions of Fortran (e.g., F77) permitted the use of real variables in do loops. This is not recommended and roundoff peculiarities mean that the do loop would need to be written in the form:

```
do theta = 0.0, 89.1, 1.0              !****WON'T WORK IN F95!
```

Note that we use 89.1 rather than 89.0 as the ending value to avoid the possibility that roundoff error might cause the desired ending value (computed by successively adding 1.0 to theta) to slightly exceed 89 and thus be excluded from the loop. I have a lot of old code of this form, but I'm going to slowly try to get rid of it.

Inside the do loop we first convert from the integer theta to the real theta using:

```
theta = real(itheta)
```

We then compute the cosine, sine and tangent of theta, after converting from degrees to radians by dividing by degrad (anybody see how we could make the program slightly more efficient?). To make the output look nice, we do not use

```
print *, theta, ctheta, stheta, ttheta
```

which would space the numbers irregularly among the columns. Instead, we explicitly specify the output format using a format specification:

```
print "(f5.1,1x,f6.4,1x,f6.4,1x,f7.4)", theta, ctheta, stheta, ttheta
```

where f5.1 specifies that theta will be output as a real number into 5 total spaces, with 1 digit to the right of the decimal place. Similarly, f6.4 specifies that ctheta is output into spaces with 4 digits to the right of the decimal place. The numbers will be right justified, with leading blanks used as necessary. The 1x specifies that one blank character will be output between each of the numbers.

An alternative way to write this:

```
print "( f5.1,   f7.4,   f7.4,   f8.4)", &
       theta, ctheta, stheta, ttheta
```

Here we have used the continuation character & to split the statement into two lines. Blanks are ignored so we can space things out neatly to line up the variables with their formats. Notice that we have removed the need for the 1x between formats by adding an additional column to the appropriate formats (i.e., writing f7.4 rather than f6.4). Because the numbers are right justified, this will add an additional space to the left of each number. Aligning things this neatly is probably more trouble than it's worth, but it certainly makes the code easier to understand.

Notice that in this case the f7.4 appears twice in a row. Often programmers will write this more compactly as:

```
print "(f5.1, 2f7.4, f8.4)", theta, ctheta, stheta, ttheta
```

since Fortran allows this syntax.

Older Fortran programs usually put the format specifier into a separate numbered line, i.e.

```
      print 117, theta, ctheta, stheta, ttheta
117   format (f5.1, 2f7.4, f8.4)
```

This convention is still allowed in F90 but should not be used unless you want to use the format statement more than once, e.g.,

```
      print 117, theta1, ctheta1, stheta1, ttheta1
      print 117, theta2, ctheta2, stheta2, ttheta2
117   format (f5.1, 2f7.4, f8.4)
```

117 is termed a line label and must consist of digits. It is best not to refer to it as a line number (the old usage) because it normally has nothing to do with the line numbers and the labels need not be sequential (more about this later). Note that the format line need not immediately follow the print line(s); it can come before. Many older programs put all of the format statements at the end of the code.

An alternative way in F90 to use the same format specification more than once is to define it as a character variable, i.e.,

```
      character (len = 30) :: fmt

      fmt = "(f5.1, 2f7.4, f8.4)"
      print fmt, theta1, ctheta1, stheta1, ttheta1
      print fmt, theta2, ctheta2, stheta2, ttheta2
```

but we are getting ahead of ourselves because we have not yet shown how to use character variables.

5.5.1 Fortran mathematical functions

We used the Fortran sine, cosine and tangent function in the trigtable program. Here is a complete list of math functions:

```
acos(x)       arccosine
asin(x)       arcsine
atan(x)       arctangent
atan2(y,x)    arctangent of y/x in correct quadrant (***very useful!)
cos(x)        cosine
cosh(x)       hyperbolic cosine
exp(x)        exponential
log(x)        natural logarithm
log10(x)      base 10 log
sin(x)        sine
sinh(x)       hyperbolic sine
sqrt(x)       square root
tan(x)        tangent
tanh(x)       hyperbolic tangent
```

5.5.2 Possible integer vs. real problems

As an aside, note that the trigtable program uses:

```
degrad = 180./3.1415927
```

rather than simply

```
degrad = 180/3.1415927
```

The reason is to make completely sure that the program will compute a real quotient and not an integer quotient. In fact, this caution is not needed in this case, as the following program demonstrates:

```
program testfrac
   implicit none
   real c
   c = 2/3
   print *,'2/3 = ', c
   c = 2/3.
   print *,'2/3. = ', c
   c = 2./3
   print *,'2./3 = ', c
   c = 2./3.
   print *,'2./3. = ', c
end program testfrac
```

Running the program yields:

```
 2/3 =  0.0E+0
 2/3. =  0.6666667
 2./3 =  0.6666667
 2./3. =  0.6666667
```

As long as one part of the fraction is real, the program will compute a real quotient. It is only when both numbers are written as integers that the result is truncated. However, I have gotten into the habit of always including the decimal point in real expressions to avoid someday accidentally writing something like:

```
a = sin(phi/degrad) + (2/3) * cos(theta/degrad)**2
```

which will definitely produce the wrong answer!

5.5.3 More about formats

There are many different formats that can specified. Here are some common examples:

```
i5   =  integer, 5 spaces, right justified
i5.4 =  as above but pad with zeros to 4 spaces (88 becomes 0088)
f8.3 =  real, 8 spaces, 3 to right of decimal place
e12.4 = real output with exponent, 4 places to right of decimal
        e.g., b-0.2342E+02 where "b" is blank
        (useful for big or small numbers or when you are not
         sure what size they will be and want to be sure you
         have enough room to output them)
        (cranky aside:  why always start with "0." which wastes
         a space?  -2.342E+01 would be more compact)
'product is ' = print the string "product is "  (ONLY ALLOWED FOR OUTPUT)
                note that any string can be output in this way
```

If a number does not fit into the allocated spaces, it will appear as a series of asterisks (*****)

```
a8  =  character output, 8 spaces, right justified
       (if the length of the string is greater than 8,
       then the leftmost 8 characters will appear)
2x  =  output two blanks
tn  =  tab to position n
tln =  tab left n spaces
trn =  tab right n spaces (tr2 is the same as 2x)
/   =  start a new line
```

ASSIGNMENT F4

Write a F90 program to print a table of x, sinh(x), and cosh(x) (the hyperbolic sine and cosine, these are built-in functions in Fortran) for values of x ranging from 0.0 to 6.0 at increments of 0.5 (use these x values directly in sinh(x) and cosh(x), do not convert them to radians). Use a suitable format to make nicely aligned columns of numbers.

5.6 Input using the keyboard

So far all of our example programs have run without prompting the user for any information. To expand our abilities, let's learn how to input data from the keyboard. In most programs, we will want to first prompt the user to input the data, so here is an example of how to input two numbers:

```
   print *, "Enter two integers"
   read *, a, b
```

Pretty easy, isn't it? (Compare this section with the corresponding input section in my C or Python notes and you will see why I think Fortran is more user friendly than C or Python)

Here is an example of a complete program that multiplies two numbers:

```
program usermult
   implicit none
   integer :: a, b, c
   print *, "Enter two integers"
   read *, a, b
   c = a * b
   print *, "Product = ", c
end program usermult
```

Running this program, we have:

```
rock% usermult
 Enter two integers
2 5
 Product =  10
```

The program will also accept the input on two lines:

```
rock% usermult
 Enter two integers
2
5
 Product =  10
```

Often in cases like this I will forget that I'm supposed to input more than one number. When the program just sits there, I then realize that I need to input more numbers (or I wonder why it's taking so long to finish!).

What happens if we make a mistake and try entering a real number? Let's check:

```
rock% usermult
 Enter two integers
3.1 15

 ******  FORTRAN RUN-TIME SYSTEM  ******
 Error 1083:  unexpected character in integer value
 Location:  the READ statement at line 4 of "usermult.f90"
 Unit:  *
 File:  standard input
 Input:  3.1
          ^
Abort
rock%
```

This is what happens on my old Sun computer, but most Fortran compilers will produce a similar message. The error message in this case is quite informative and tells us exactly what the problem is. This is better than performing the computation and returning the wrong answer (the default in C for this example unless you are quite careful).

5.7 If statements

Next, let's modify this program so that it will allow the user to continue entering numbers until she/he wants to stop:

```
program usermult2
   implicit none
   integer :: a, b, c
   do
      print *, "Enter two integers (zeros to stop)"
      read *, a, b
      if (a == 0 .and. b == 0) exit
      c = a * b
      print *, "Product = ", c
   enddo
end program usermult2
```

Here the do loop has no arguments and the block of code inside the do loop will be repeatedly executed until an 'exit' command is executed. 'Exit' (a new feature

in F90) means to leave the do loop entirely and go to the next line after the 'enddo' statement. As in our previous example, we indent the block inside the do loop to make the code easier to read.

The program will allow the user to continuing entering numbers to be multiplied. When the user wishes to stop the program (in a more elegant way than hitting CNTRL-C), he/she enters zeros for both arguments. The if statement checks for this and exits the do loop in this case:

```
if (a == 0 .and. b == 0) exit
```

A list of the relational (comparison) operators in different languages is as follows:

FORTRAN 77	FORTRAN 90	C	PYTHON	MATLAB	meaning
.eq.	==	==	==	==	equals
.ne.	/=	!=	!=	~=	does not equal
.lt.	<	<	<	<	less than
.le.	<=	<=	<=	<=	less than or equal to
.gt.	>	>	>	>	greater than
.ge.	>=	>=	>=	>=	greater than or equal to
.and.	.and.	&&	and	&	and
.or.	.or.	||	or	|	or
.not.	.not.	!	not	~	not

The F77 syntax will still work under F90 and you are likely to see this in many of the older programs, e.g.,

```
if (a .eq. 0 .and. b .eq. 0) exit
```

will also work. These operators can be combined to make complex tests, e.g.,

```
if ( (a > b .and. c <= 0) .or. d == 0) z = a
```

There is, of course, an order of operations for these things which I can't remember very well. Look it up in a book if you are unsure or, better, just put in enough parenthesis to make it completely clear to anyone reading your code.

One nice aspect of Fortran compared to C is that if you make a mistake and type, for example,

```
if (a = 0) exit
```

you will get an error message during compilation. In C this is a valid statement with a completely different meaning than is intended!

5.7.1 If, then, else constructs

In the above example, a single statement is executed when the if condition is true. A more versatile form is as follows:

```
if (logical expression) then
   (block of code)
else if (logical expression) then
   (block of code)
else if (logical expression) then
   (block of code)
.
.
else
   (block of code)
end if
```

The blocks of code can contain many lines if desired. As many 'else if' statements as required can be used. At most, one block of code will be executed (once one of the 'if' tests is satisfied, it does not check the others). The final 'else' will be executed if none of the preceding if statements is true. The final 'else' is optional.

Here is a demonstration program that repeatedly prompt the user for a positive real number. If it is negative, ask the user to try again. If it is positive, it computes and displays the square root using the sqrt() function. If the user enters zero, the program stops.

```
program usersqrt
   implicit none
   real :: a, b
   do
      print *, 'Enter positive real number (0 to stop)'
      read *, a
      if (a < 0) then
         print *,'This number is negative!'
         cycle
      else if (a == 0) then
         exit
      else
         b = sqrt(a)
         print *, 'sqrt = ', b
      end if
   end do
end program usersqrt
```

Notice the use of the 'cycle' command (also new in F90), which directs the program to the next iteration of the do loop. In contrast, the 'exit' command exits

the do loop entirely. The 'cycle' and 'exit' commands permit code to be written that is free of the 'go to' statements that would likely have been present in a F77 version of this program ('go to' statements are considered mortal sins by the programming style police).

ASSIGNMENT F5

Write a program to repeatedly ask the user for the constants a, b, and c in the quadratic equation $ax^2 + bx + c = 0$. Using the quadratic formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

have the program identify and compute any real roots. Output the number of real roots and their values. Stop the program if the user enters zeros for all three values. HINT: You will need to check if $b^2 - 4ac$ is negative, zero, or positive, and do different things in each case. Test your program for some simple examples to make sure it is working correctly ($a = 1, b = 2, c = -3$ should return -3 and 1; $a = 1, b = 2, c = 3$ should state there are no real roots; $a = 1, b = -4, c = 4$ should return a single root of 2).

5.8 Greatest common factor example

Here is an example program that uses some of the concepts that we have just learned:

```
! compute the greatest common factor of two integers
program gcf
   implicit none
   integer :: a, b, i, imax
   do
      print *, 'Enter two integers (zeros to stop)'
      read *, a, b
      if (a == 0 .and. b == 0) then
         exit
      else
         do i = 1, min(a, b)
            if (mod(a, i) == 0 .and. mod(b, i) == 0) imax=i
         end do
         print *, "Greatest common factor = ", imax
      end if
   enddo
end program gcf
```

This is not a particularly efficient algorithm, but it runs plenty fast for small numbers. There are some new things here:

1. min(a,b) computes the minimum of a and b using the intrinsic Fortran 'min' function. Naturally there is also a 'max' function. min and max can have more than 2 arguments if desired.

2. mod(a,i) computes the remainder of a divided by i (this is called the modulus). If mod(a,i) is zero, then a is evenly divisible by i. If non-zero, then mod(a,i) has the sign of a.

Here are some more useful Fortran functions:

```
abs(a)      absolute value
sign(a, b)  abs(a) with sign of b

real(a)     conversion to real (F77 float(a) still works)
int(a)      conversion to integer
nint(a)     nearest integer
ceiling(a)  least integer greater than or equal to number
floor(a)    greatest integer less than or equal to number
```

ASSIGNMENT F6

Modify gfc.f90 to compute the least common multiple of two integers.

5.9 User defined functions and subroutines

As the length and complexity of a computer program grows, it is a good strategy to break the problem down into smaller pieces by defining functions or subroutines to perform smaller tasks. This provides several advantages:

1. You can test these pieces individually to see if they work before trying to get the complete program to work.

2. Your code is more modular and easier to understand.

3. It is easier to use parts of the program in a different program.

To illustrate how to define your own function, here again is the greatest common factor program:

```
program gcf2
   implicit none
   integer :: a, b, gcf
   integer, external :: getgcf
```

```
   do
      print *, 'Enter two integers (zeros to stop)'
      read *, a, b
      if (a == 0 .and. b == 0) then
         exit
      else
         gcf = getgcf(a,b)
         print *, "Greatest common factor = ", gcf
      end if
   enddo
end program gcf2


integer function getgcf(x, y)
   implicit none
   integer :: x, y, i, z
   do i = 1, min(x,y)
      if (mod(x,i) == 0 .and. mod(y,i) == 0) getgcf = i
   end do
end function getgcf
```

We now perform the gcf calculation in the function getgcf. The variables a and b in the main program are the function arguments. They are passed to the function in the statement:

```
gcf = getgcf(a, b)
```

The function getgcf definition begins with:

```
integer function getgcf(x, y)
```

The variables x and y in the function will assume the values passed to the function by the main program. These arguments must match in number and type (real vs. integer, etc.) with the variables in the main program. Note, however, that they do not need to have the same names.

Notice that we must declare getgcf in the calling program:

```
integer, external :: getgcf
```

This is the preferred F90 syntax, although the following will also work:

```
integer :: getgcf
```

The name of the function is by default the value that will be passed back to the main program. In some cases involving recursive functions (a more complicated topic that we may cover later), it may desirable to have the value returned to the main program be specified by a different variable name. To do this, we can use the optional 'result' specifier in the subroutine name:

```
function getgcf(x, y) result(z)
   implicit none
   integer :: x, y, i, z
   do i = 1, min(x, y)
      if (mod(x, i) == 0 .and. mod(y, i) == 0) z = i
   end do
end function getgcf
```

The result(z) indicates that the result will be passed back to the calling program as the variable z. Thus, gcf in the calling program will assume the value of z in the function.

ASSIGNMENT F7

Modify your program from F6 to compute the least-common multiple as a user-defined function.

5.9.1 Subroutines

Functions are limited in their usefulness because they are designed to pass only one value back to the calling program. A more general construct is the Fortran subroutine, which allows unlimited numbers of values to be passed to and from the calling program.

Here is our first geophysically useful example, a subroutine to compute the distance and azimuth between any two points on the Earth's surface:

```
program userdist
   implicit none
   real lat1, lon1, lat2, lon2, del, azi
   do
      print *, 'Enter 1st point lat, lon'
      read *, lat1, lon1
      print *, 'Enter 2nd point lat, lon'
      read *, lat2, lon2
      call SPH_AZI(lat1, lon1, lat2, lon2, del, azi)
      print *,'del, azi = ', del, azi
   end do
end program userdist
```

```
! SPH_AZI computes distance and azimuth between two points on sphere
!
! Inputs:  flat1  =  latitude of first point (degrees)
!          flon2  =  longitude of first point (degrees)
!          flat2  =  latitude of second point (degrees)
!          flon2  =  longitude of second point (degrees)
! Returns: del    =  angular separation between points (degrees)
!          azi    =  azimuth at 1st point to 2nd point, from N (deg.)
!
! Notes:
!
! (1) applies to geocentric not geographic lat,lon on Earth
!
! (2) This routine is inaccurate for del less than about 0.5 degrees.
!     For greater accuracy, use double precision or perform a separate
!     calculation for close ranges using Cartesian geometry.
!
subroutine SPH_AZI(flat1, flon1, flat2, flon2, del, azi)
   implicit none
   real :: flat1,flon1,flat2,flon2,del,azi,pi,raddeg,theta1,theta2,  &
           phi1,phi2,stheta1,stheta2,ctheta1,ctheta2,                &
           sang,cang,ang,caz,saz,az
   if ( (flat1 == flat2 .and. flon1 == flon2) .or.     &
        (flat1 ==  90.  .and. flat2 ==  90.)  .or.     &
        (flat1 == -90.  .and. flat2 == -90.) )  then
      del=0.
      azi=0.
      return
   end if
   pi=3.141592654
   raddeg=pi/180.
   theta1=(90.-flat1)*raddeg
   theta2=(90.-flat2)*raddeg
   phi1=flon1*raddeg
   phi2=flon2*raddeg
   stheta1=sin(theta1)
   stheta2=sin(theta2)
   ctheta1=cos(theta1)
   ctheta2=cos(theta2)
   cang=stheta1*stheta2*cos(phi2-phi1)+ctheta1*ctheta2
   ang=acos(cang)
   del=ang/raddeg
   sang=sqrt(1.-cang*cang)
   caz=(ctheta2-ctheta1*cang)/(sang*stheta1)
   saz=-stheta2*sin(phi1-phi2)/sang
   az=atan2(saz,caz)
   azi=az/raddeg
   if (azi.lt.0.) azi=azi+360.
end subroutine SPH_AZI
```

The subroutine is called with the statement:

```
call SPH_AZI(lat1, lon1, lat2, lon2, del, azi)
```

In this case, the lat/lon values are passed to the subroutine while del and azi are passed back to the main program. However, note that if flat1, etc., were changed in the subroutine, then the corresponding variable would also be changed in the main program as well. lat1 in the main program and flat1 in the subroutine point to the same memory location. If one is changed, the other automatically changes as well.

Fortran is not case-sensitive so sph_azi and SPH_AZI have the same meaning. I like to put subroutine names in all caps so they are more visible. Note that sph_azi does not have to be declared in the main program.

The subroutine is well-documented in this case, explaining exactly what is going into the subroutine and what is going out, as well as some of the limitations of the routine. This may seem like overkill, but documenting your subroutines as completely as possible is likely to save you considerable time later if you ever want to use the routine again. It is good to document the routine well enough that you, or someone else, can use it correctly without having to study the code itself. Clarity is important—I have seen versions of this routine that do not make clear whether the azimuth is measured at the first point to the second point, or vice versa. Listing the limits of the subroutine may help prevent future misuse of the routine, in this example it may prevent the naive user from assuming that the distance returned is accurate when used with geographic latitude and longitude on the Earth. The routine is also designed to be robust with respect to pathological inputs, such as when the two points have the same coordinates.

ASSIGNMENT F8

Write a single subroutine that computes the volume, surface area, and circumference of a sphere, given its radius, together with a main program that inputs different values for the radius from the keyboard and prints the results. Allow the user to terminate the program by entering zero for the radius. E-mail me the source code in a single file containing both the main program and the subroutine.

5.9.2 Linking to subroutines during compilation

A powerful aspect of subroutines is that one can link to compiled versions of existing subroutines without having to recompile them. This means that you only have to

maintain one version of a subroutine; it need not be listed along with the source code of the main program. For example, the SPH_AZI subroutine is also part of a F77 package of spherical geometry subroutines contained in:

```
~shearer/PROG/SUBS/sphere_subs.f
```

Our main program could simply consist of:

```
program userdist2
   implicit none
   real flat1,flon1,flat2,flon2,del,azi
   do
      print *,'Enter 1st point lat,lon'
      read *,flat1,flon1
      print *,'Enter 2nd point lat,lon'
      read *,flat2,flon2
      call SPH_AZI(flat1,flon1,flat2,flon2,del,azi)
      print *,'del, azi = ', del, azi
   end do
end program userdist2
```

When we compile this program, we need to indicate where the SPH_AZI subroutine can be found. We want to link with what is called an 'object file' for the subroutines. Object files end in .o and there is a sphere_subs_f90.o file in the same directory (shearer/PROG/SUBS) as the source file sphere_subs.f.

You must link with object files that have been compiled using the same Fortran compiler as you use for the main program. When I switched to using gfortran from g77 a year or two ago, I had to recompile my subroutines in order for them to link properly with gfortran compiled code. I still occasionally run into this problem when I link to a subroutine I have not used in awhile.

To create a F90 object file, enter, for example:

```
gfortran -c someprogram.f90 -o someprogram.o
```

You can also create a F90 object file from F77 source code:

```
gfortran -c anotherprogram.f -o anotherprogram.o
```

This will work on native F77 code that includes non-F90 compatible features (e.g., comment lines starting with C), because the F90 compiler sees that the source file ends in .f rather than .f90.

To compile userdist2 and link to sphere_subs.o, we enter:

```
gfortran userdist2.f90 /home/shearer/PROG/SUBS/sphere_subs.o -o userdist2
```

This quickly becomes cumbersome to write so you will find it convenient to set up a Makefile to keep track of all this for you. Here is part of a Makefile that does this for this program:

```
OBJS1=  /home/shearer/PROG/SUBS/sphere_subs_f90.o

userdist2: Makefile userdist2.f90 $(OBJS1)
       gfortran userdist2.f90 $(OBJS1) -o userdist2
```

Note that you MUST use a tab to generate the spaces before 'gfortran' for the Makefile to work correctly! This is a leading source of confusion for novice Makefile users.

You can list the full path names for any number of subroutine object files in this way. To compile the program, simply enter:

```
make userdist2
```

ASSIGNMENT F9

Study the SPH_MID subroutine contained in sphere_subs.f (in ~shearer/PROG/SUBS). Write a program that uses this subroutine to compute the midpoint between two (lat,lon) points input by the user. Print out the latitude and longitude of this point. Do not attempt to copy the SPH_MID source code, just link to the sphere_subs_f90.o object file. Make sure that the argument list for SPH_MID in your program matches the subroutine arguments. E-mail me the source code and also tell me where the working executable version of the program is located. Be sure to give me execute permission so that I can try running your program. (Remember: 'ls -l' shows the current permissions, 'chmod' is how you change the permissions, 'man chmod' will explain this.) If you are at sea (!), then you may have to copy the sphere_subs.f routines to your local machine. You can make an object file from them using gfortran -c sphere_subs.f -o sphere_subs.o

5.10 Internal procedures

The functions and subroutines that we discussed above are called 'external' because are located outside of the main program. With external procedures all of the values

that are to passed into and out of the procedure must be part of the argument list. All other variables are local to the procedure or to the main program, even if they have the same name as a variable in a different procedure. External procedures are the only kind of procedure allowed in F77 and are what you will find in books like Numerical Recipes or in the subroutine libraries maintained by various scientists at SIO. Their great advantage is their portability—everything you need to know about what they do is contained in their argument list.

However, in some cases it may be more convenient to use an 'internal' subroutine or function, a method that is new to F90. Internal procedures are listed immediately BEFORE the end statement in the main program. All variable names are shared within internal procedures; thus argument lists are not necessarily required for them to work.

Here is an example adapted from the Brainard text that illustrates how internal subroutines work:

```
program sort3
   implicit none
   real :: a1, a2, a3
   call read_numbers
   call sort_numbers
   call print_numbers

contains

subroutine read_numbers
   print *,'Enter three numbers'
   read *, a1, a2, a3
end subroutine read_numbers

subroutine sort_numbers
   if (a1 > a2) call swap(a1,a2)
   if (a1 > a3) call swap(a1,a3)
   if (a2 > a3) call swap(a2,a3)
end subroutine sort_numbers

subroutine print_numbers
   print *,'The sorted numbers are: '
   print *, a1, a2, a3
end subroutine print_numbers

subroutine swap(x,y)
   real :: x, y, temp
   temp = x
   x = y
   y = temp
```

```
end subroutine swap

end program sort3
```

Internal procedures are listed following a 'contains' statement and before the end statement for the main program. Variables already declared in the main program need not be declared in the internal procedure. Arguments are optional; they are used here in the swap routine to permit it to be used for different pairs from a1, a2 and a3. Note that the procedures are not nested (e.g., one might have tried to put swap internal to sort_numbers); internal procedures may not contain other internal procedures. Note also that variables declared within a subroutine are purely local to the subroutine. For example, the value for temp (in swap) is not available in the main program. Even if temp were declared in the main program, its value will not correspond to the value of temp in the swap subroutine (try it!).

The use of internal subroutines is rather pointless in this case because the code would probably be clearer without them. However, for longer programs they may well be useful for making the code more structured. If you write a program and notice that you are using the same block of code over and over again, this would a situation where using a subroutine would make sense. The advantage of an internal subroutine is that you don't have to match the argument lists and declare all of the variables. External subroutines can become cumbersome when they involve a large number of variables. Often common blocks are used to avoid long argument lists in this case (more about this later). In many case, internal subroutines may provide a neater way to handle this situation.

5.11 Extended precision

By default, Fortran stores real variables using 4 bytes, providing a precision of about 6 to 7 significant figures over a range from (on the Suns) 1.175494e-38 to 3.402823e+38. If this is insufficient precision, then variables can be defined in double precision. In F77, this was done by declaring them as 'double precision' or 'real*8' variables. This syntax will still work, although F90 has introduced a new concept—the 'kind' specifier for variables. All of these methods are demonstrated in this program:

```
program testdouble
   implicit none
```

```
   character (len = 30) :: fmt = "(a5,f44.40)"
   real a4
   real*8 a8
   double precision aa
   real (kind=4) :: k4
   real (kind=8) :: k8
   real (kind=16) :: k16    !only include if using 64-bit machine + compiler

   a4 = 8.9
   print fmt, 'a4 = ', a4

   a8 = 8.9d0
   print fmt, 'a8 = ', a8

   aa = 8.9d0
   print fmt, 'aa = ', aa

   k4 = 8.9
   print fmt, 'k4 = ', k4

   k8 = 8.9_8
   print fmt, 'k8 = ', k8

   k16 = 8.9_16              !only include if using 64-bit machine + compiler
   print fmt, 'k16= ', k16   !only include if using 64-bit machine + compiler
end program testdouble
```

which produced the following output on my old Sun computer:

```
a4 =   8.8999996185302734375000000000000000000000
a8 =   8.9000000000000003552713678800500929355621
aa =   8.9000000000000003552713678800500929355621
k4 =   8.8999996185302734375000000000000000000000
k8 =   8.9000000000000003552713678800500929355621
k16=   8.9000000000000000000000000000000000308148
```

and which produces the following output on my Mac running 32-bit gfortran:

```
a4 =   8.8999996185302734375000000000000000000000
a8 =   8.9000000000000003552714000000000000000000
aa =   8.9000000000000003552714000000000000000000
k4 =   8.8999996185302734375000000000000000000000
k8 =   8.9000000000000003552714000000000000000000
```

after I comment out the k16 lines.

Note that a4 and k4 are regular real*4 variables and approximate 8.9 as 8.999996. Much greater precision is obtained with a8, aa, and k8, which are all real*8 (double precision) variables. k16 is a real*16 variable (quadruple precision). k16 is not

supported on all computers. Newer Macs are 64-bit machines and should accept k16 when you compile using fortran.

On most computers, kind=4 is for single precision (4-byte real), kind=8 is for double precision (real*8), and kind=16 is for 16-byte real. Note that the precision of numbers may be specified by appending them with an underscore and the kind value. Thus we write 8.9_8 to indicate that 8.9 is to represented as an 8-byte real number.

The use of 'kind' is intended to give you greater control over the degree of precision in your programs and ultimately make codes that are less platform dependent in their behavior. I'm not sure if this has been achieved! It appears that F90 also allows complex variables to be declared as double precision, something not allowed in F77. We will check if this is actually true later when we consider complex variables.

IMPORTANT NOTE: You must define the extra-precision variables using numbers with the appropriate precision. If you write:

```
a8 = 8.9    !***Not correct if a8 is real*8
```

you will get single precision accuracy. Even the 'dble' operator (which works in F77, at least on the Suns) will not work in F90 in assigning variables:

```
a8 = dble(8.9)     !***Not correct if a8 is real*8
```

will assign a8 only at single precision accuracy. The key is to write:

```
a8 = 8.9d0         !correct way to set double precision variables
```

or

```
k8 = 8.9_8
```

Note that the 0 following the d is the power of 10, thus 1.23d3 is 1230, 0.84d-2 is 0.0084, etc.

To get the full 16-byte precision (only on the Suns or 64-bit Macs), you must say

```
k16 = 8.9_16
```

rather than k16=8.9d0 or k16=8.9_8, which will assign k16 only to double precision accuracy.

Many of my existing F77 routines use dble( ) to define double precision numbers. These will not work correctly if they are changed to F90, unless all of the dble( ) commands are rewritten. They are fine, however, if they continue to be compiled using F77. I don't know if this is a bug in some F90 compilers, or if the use of dble( ) in this way is non-standard Fortran.

ASSIGNMENT F10

Examine the datetime.f source code in ~shearer/PROG/SUBS (also see class website) and write a F90 program to compute the number of seconds that have elapsed since noon on your birth date (or the exact time if you know it) until a user-specified date and time. Have the program print out this number of seconds. You will want to use the DT_TIMEDIF subroutine. Make sure that all of the variables match and are of the same type (integer, real, and real*8 for timdif, the final argument). You should also be aware that & in column 6 of F77 code is how lines are continued, that is:

```
      subroutine DT_TIMEDIF(iyr1,imon1,idy1,ihr1,imn1,sc1,
     &                      iyr2,imon2,idy2,ihr2,imn2,sc2,timdif)
```

is actually all one line.

Because the datetime subroutines are written in older Fortran (hence the .f rather than .f90), do not try to paste these routines into the source code for your .f90 program. Instead, you should compile the routines into object code (with a .o suffix) and then link to the routines when you compile your program, i.e.,

```
gfortran -c datetime.f -o datetime.o
gfortran compsec.f90 datetime.o -o compsec
```

E-mail me the source code of your program. You don't need to include any of the datetime subroutines, as those should be kept separate.

Extra credit: Determine the date and time when you will be (or were) exactly one billion seconds old. This will require using one of the other subroutines in datetime.f Mark your calendar for a party!

5.11.1 Integer sizes

Just as you can set aside fixed numbers of bytes for real numbers, you can do the same to store integers of varying sizes. The standard is 4-byte integers, which have 32 bits and thus will go (approximately) from -2^{31} to 2^{31}. However, 2-byte and 8-byte integers are also allowed. These are sometimes called short and long integers, respectively. The following example program shows how this works, using two different ways to define the integers:

```
program testinteger
   implicit none
   integer*2 i2
   integer i4
   integer*8 i8
   integer (kind=2) :: k2
   integer (kind=4) :: k4
   integer (kind=8) :: k8

   i8 = 32000
   i4 = i8
   i2 = i8
   print *, i2, i4, i8

   i8 = 32000**2
   i4 = i8
   i2 = i8
   print *, i2, i4, i8

   i8 = 32000
   i8 = i8**4
   i4 = i8
   i2 = i8
   print *, i2, i4, i8

end program testinteger
```

This will produce the output:

```
  32000       32000                32000
      0  1024000000           1024000000
      0           0  1048576000000000000
```

The zero fields in the output are incorrect and indicate that the number was too large to be stored in the given variable type. Note that k2, k4 and k8 (defined using the kind statement) will give the same results, even though they are not explicitly tested in the program.

Regular integers suffice for most purposes. Short integers are useful to save space for data sets that don't require bigger numbers (i.e., beyond about ±32000).

5.12 Arrays

Arrays are defined in F90 as in this example

```
real, dimension(100) :: a, b
integer, dimension(50,2) :: index
```

which defines a and b as 100 element arrays (a(1) to a(100)) and *index* as a 50x2 element array (index(1,1) to index(50,2)). Note that the default starting array number is 1 (not 0 as in C). Also note that array elements are written using parentheses, not brackets as in C.

Older Fortran programs would define the same arrays as follows:

```
real a(100), b(100)
integer index(50,2)
```

This syntax will still work and is easier to read for short programs. The new standard has the advantage, however, of being able to easily define many arrays with identical dimensions.

A nice feature of Fortran is that we can specify the lower and upper array boundaries explicitly in the declaration, e.g.,

```
real, dimension(-100:100) :: a, b
integer, dimension(0:50, 2) :: index
```

In this case there are 201 values for a and b (from a(-100) to a(100)) and 102 values for index (from index(0,1) to index(50,2)).

Array values can be assigned one element at a time, or can be assigned in single statements as in this F90 example:

```
program testarray
   implicit none
   integer, dimension(3) :: x = (/ 1, 2, 3 /), y = 1
   print *, x
   x = (/ 15, 30, 40 /)
   print *, x
   print *, y
   y = 2
   print *, y
end program testarray
```

and its output:

```
 1 2 3
 15 30 40
 1 1 1
 2 2 2
```

Note that when an array is set to a scalar, every array element is set to the value of the scalar, i.e., y =2 sets all y values to 2. The individual elements can be specified if they are listed between '(/' and '/)' (Warning: Don't put a space between the / and the parenthesis!!). The number of values must match the dimension of the vector. We will discuss this more later when we consider two-dimensional arrays in detail.

5.12.1 Program to check user input for day of month

Here is a short example program that uses an array to store the number of days in each month, which it then uses to test whether the user has correctly entered a date:

```
program readdate
   implicit none
   integer :: year, month, day
   integer, dimension(12) :: ndaymon

   ndaymon = (/31, 28, 31, 30, 31, 30, 31, 31, 30, 31, 30, 31/)

   do
      print *, 'Enter year, month, day'
      read *, year, month, day
      if (month < 1 .or. month > 12) then
         print *, 'Month is out of bounds. Please try again.'
         cycle
      endif
      if (day > ndaymon(month)) then
         print *, 'Too many days for that month! Please try again.'
         cycle
      else
         print *, 'Nice input!'
      endif
   enddo
```

Note that the code is only completely correct for non-leap years, as it assumes February has 28 days. The code checks for a valid month *before* testing for the number of days to avoid run-time errors associated with out-of-bounds indices for

the array ndaymon. Providing out-of-bounds indices to an array is one of the most common ways for programs to "crash" (more about this later).

This program provides no graceful way to exit and will run forever until manually terminated (usually by entering Control-C).

5.12.2 Program to compute prime numbers

Here is a more complicated program that uses an array to compute prime numbers less than 100:

```
program prime
   implicit none
   integer, parameter :: maxnum=100
   integer :: i, j, max_i, max_j, nprime=0
   integer, dimension(maxnum) :: prod

   do i = 1, maxnum
      prod(i) = 0
   enddo

   max_i = floor(sqrt(real(maxnum)))
   do i = 2, max_i
      if (prod(i) == 0) then
         max_j = maxnum/i
         do j = 2, max_j
            prod(i*j) = 1
         enddo
      end if
   end do

   do i = 2, maxnum
      if (prod(i) == 0) then
         nprime = nprime + 1
         print "(i4)", i
      end if
   enddo

   print *, 'Number of primes found = ',nprime
end program prime
```

The method is sometimes called the sieve of Eratosthenes, named after a Greek mathematician from the 3rd century BC. We start with a list of numbers from 2 to 100 and consider them all possible primes. In the program, this list is the array prod. We initialize the array by setting its values to zero. The strategy is to then flag numbers that are not prime by setting the corresponding array values to one.

We then start with the number 2 and eliminate all multiples of 2 up to the maximum value of 1000. We then move to 3 and eliminate (i.e., set prod to 1) all multiples of 3. We can skip 4 because 4 and all its multiples were already eliminated. We need check numbers, i, only up to sqrt(100) because larger factors would already have been eliminated.

When we are finished, we simply print out all numbers that were not eliminated. In our case, this is all i such that prod(i) = 0. We count the number of primes using the counter variable nprime.

A new aspect of this program is the defining of maxnum as a parameter:

```
integer, parameter :: maxnum=100
```

This tells the program to set maxnum to 100 and that this value will never be changed during the program. It also allows the array dimension for prod (in the next line) to be set by maxnum. This makes it easy for us to change the size of our prime search by changing the value of maxnum without having to change anything else in the program.

Note that in the statement

```
max_i = floor(sqrt(real(maxnum)))
```

it is necessary to convert maxnum to a real number before taking the square root. This is because the argument to the Fortran sqrt function must be real; if we had written sqrt(maxnum) we would have gotten an error during compilation.

This program lists the prime numbers with one number per output line and thus will become cumbersome for larger values of maxnum. Let's modify the program to list 10 primes per line. To to this, we save the prime numbers in a separate array called pnum. Here is the code:

```
program prime2
   implicit none
   integer, parameter :: maxnum=1000
   integer, dimension(maxnum) :: prod=0, pnum
   integer :: i, j, max_i, max_j, nprime=0

   max_i = floor(sqrt(real(maxnum)))
   do i = 2, max_i
      if (prod(i) == 0) then
         max_j = maxnum/i
         do j = 2, max_j
```

```
            prod(i*j) = 1
         enddo
      end if
   end do

   do i = 2, maxnum
      if (prod(i) == 0) then
         nprime = nprime + 1
         pnum(nprime) = i
      end if
   enddo
   print *, 'Number of primes found = ', nprime

   print "(10i5)", (pnum(i), i = 1, nprime)

end program prime2
```

Note that we have shortened the beginning of the code by taking advantage of the fact that we can set array values when they are declared, i.e., we write

```
integer, dimension(maxnum) :: prod=0, pnum
```

rather than wasting the three lines we used in the earlier version of the the code to set all elements in prod to zero.

The program is pretty self-explanatory, but we do introduce a new concept in the output line:

```
print "(10i5)", (pnum(i), i = 1, nprime)
```

This is termed an implicit do loop and is very useful in input/output (I/O) statements. Note that the format specifier 10i5 applies to the first 10 numbers and then is reused for the next 10, etc. The parentheses around (pnum, i=1,nprime) are required. More complicated expressions are also possible, e.g.,

```
print "(5(i4,i4,2x))", (i, pnum(i), i = 1, nprime)
```

will print the primes to the right of their count.

There are some cases when we would prefer not to advance to the next line following a print statement. Instead, we would like to have output continue on the same line. Here is an example of how this can be used to print 10 prime numbers per line without having to store the prime numbers in a separate array:

```
program prime3
   implicit none
   integer, parameter :: maxnum=1000
   integer :: i, j, prod(maxnum)=0, max_i, max_j, nprime=0

   max_i = floor(sqrt(real(maxnum)))
   do i = 2, max_i
      if (prod(i) == 0) then
         max_j = maxnum/i
         do j = 2, max_j
            prod(i*j) = 1
         enddo
      end if
   end do

   do i = 2, maxnum
      if (prod(i) == 0) then
         nprime = nprime + 1
         if (mod(nprime,10) /= 0) then
            write (*,"(i4)", advance='no') i
         else
            write (*,"(i4)") i
         end if
      end if
   enddo
   print *

   print *, 'Number of primes found = ',nprime
end program prime3
```

The statement

```
write (*, "(i4)") i
```

works exactly the same as the print statement we used previously. ('print' only goes to the screen, 'write' can go to the screen or to a file. The * in the above write statement means standard output, not free format).

The statement

```
write (*, "(i4)",advance='no') i
```

does the same thing, except that it does not advance to the next line. The program checks to see if the prime count (nprime) is divisible by 10; if not then the output does not advance. Following the enddo, a print * statement is needed to be sure that the final output (Number of primes found) is on a separate line.

NOTE: With most Fortran compilers, the carriage return (advancement to next line) can also be suppressed simply by adding a $ to the format statement. Thus the above line could be replaced with

```
print "(i4,$)", i
```

and the result would be the same. However, I'm not sure this is standard Fortran so you may get into trouble at some point with this convention.

5.12.3 Checking for problems with the -fcheck=bounds option

Suppose when writing the prime number program, we made the mistake of writing:

```
max_j = maxnum
```

rather than

```
max_j = maxnum/i
```

When the program is run, at some point the product i*j in the line

```
prod(i*j) = 1
```

will exceed the array dimensions of prod (maxnum). The program will then start overwriting adjacent memory locations and disaster will result. Most commonly the program will crash with the following kind of message:

```
Bus error
```

or

```
Segmentation Fault
```

These types of errors result from exceeding array boundaries or mismatched subroutine arguments. These are not very helpful error messages because they do not tell you where in the program the problem occurred. However, there is usually a compiler option you can set that will provide more useful diagnostics. For gfortran, it is the -fcheck=bounds option and can be invoked either by compiling prime4 with:

```
gfortran -fcheck=bounds prime4.f90 -o prime4
```

or changing the Makefile to:

```
%:      %.f90
       gfortran -fcheck=bounds $< -o $*
```

(remember the tab before gfortran!) If you have compiled your program with this option, then the computer will check to see if your array indices exceed their boundaries and tell you where the problem occurs:

```
shearer@katmai 324> ./prime4
At line 11 of file prime4.f90
Fortran runtime error: Array reference out of bounds for array 'prod',
   upper bound of dimension 1 exceeded (1002 > 1000)
```

This is so helpful, and will save you so much time in debugging your programs, that I recommend that you ALWAYS use this option when you are first getting your programs to work. It does slow the code somewhat, so for programs where run time is a factor, you should then recompile without -fcheck=bounds for the final working version. (in these cases, you may also want to experiment with the -O compiler to make your code run faster, see below).

ASSIGNMENT F11

Fortran 90 includes a built in random number subroutine (called 'random_number'). Here is an example program that prints out 20 random values from between 0 and 1.

```
program listrand
   integer :: i
   real :: xran
   do i = 1, 20
      call random_number(xran)
      print *, xran
   enddo
end program listrand
```

Write a simple F90 program to generate 10000 random numbers between 0 and 1. Test the randomness by counting the number of these that fall in each of 10 evenly spaced bins between 0 and 1 (i.e., 0 to 0.1, 0.1 to 0.2, etc.). Print these counts to the screen. Here is an example of what your output might look like:

```
0 1009
1 1048
2 1001
```

```
3 1038
4 1008
5 959
6 993
7 925
8 1017
9 1002
```

HINT: Set up an integer array with 10 elements and initialize all the values to zero. For each random number generated, then add one to the appropriate array element to keep track of how many of the numbers are in that bin.

5.12.4 More about random numbers

To learn more about random number generators, please consult the book Numerical Recipes, which has a discussion about good algorithms and bad algorithms. I have not tested the built-in F90 random number generator to see how well it measures up, but it seems pretty good for most purposes.

You may notice that if you use random_number in a program that you will get the same numbers every time you run the program. This is desirable in many cases. For example, if you are debugging a program, you want any problems to be completely reproducible. But in other cases, you will want to get different results each time. One simple way to achieve this would be to ask the user to input an integer and then compute that many random numbers before continuing to the main program. But this requires the user to think of different input numbers. To avoid this, we can randomize the start of the random number generator itself by using some number that will always be different, for example from the system clock on the computer. This turns out to be annoyingly hard to do in F90. Here is an example program:

```
program listrandseed
   implicit none
   integer :: i, count, count_rate, count_max, narg
   integer, dimension(8) :: idate
   integer, dimension(12) :: seed
   real :: xran

! randomize start of random numbers
   call date_and_time(VALUES=idate)
   print *, 'idate = ', idate
   call system_clock(count, count_rate, count_max)
   seed(1) = count
   seed(2:9) = idate(8:1:-1)
   seed(10:12) = idate(6:8)
```

```
   print *, 'seed = ', seed
   call random_seed(SIZE=narg)
   print *, 'narg = ', narg
   call random_seed(PUT=seed)

   do i = 1, 20
      call random_number(xran)
      print *, xran
   enddo

end program listrandseed
```

Once you have this working, you may want to remove the print statements in the random seed part. But before doing so, make sure that seed is dimensioned to narg. When I recently changed computers, narg changed from 8 to 12 and I had to rewrite this little program.

5.12.5 Arrays as subroutine arguments

Suppose we have defined an array x as:

```
integer :: x(100)
```

If we use x in the argument list for a subroutine, e.g.,

```
call SUMTOT(x,n,y)
```

we include x without any parentheses. The subroutine argument list must also include a matching array of the same size. All array values are passed to and from the subroutine. We will discuss later how to write subroutines that will work for arrays of differing size in the calling program.

5.13 Character strings

A character string may be declared in F90 as follows:

```
character (len = 20) :: name
```

declares the variable "name" to be a character string of length 20. One can also define an array of character strings:

```
character (len = 20), dimension(100) :: name_array
```

The old F77 ways to define these strings will still work in F90:

```
character name*20, name_array(100)*20
```

or

```
character*20 name, name_array(100)
```

A string variable can be assigned as, e.g.,

```
name = "Bill Clinton"
```

The quotes (apostrophes will also work) are required. If name in this case was declared as 20 characters long, then trailing blanks are added so name actually is "Bill Clinton " If, on the other hand, name was declared as 10 characters long, then name would contain "Bill Clint" as the extra letters would be cut off (no error results).

The length of a character string may be obtained with the len function:

```
len("Bill") will give 4
len("  ") will give 2
len(name) will give 20 if name was declared as 20 characters
          long, regardless of any trailing blanks
```

Substrings may be obtained as follows for name = "Bill Clinton":

```
name(1:4) is "Bill"
name(6:12) is "Clinton"
name(6:6) is "C"
```

Thus, we could change the last name as follows:

```
name = "Bill Clinton"
name(6:12) = "Jones  "
```

Note that the trailing blanks are necessary to overwrite the "on"

The following moves the string one character to the right:

```
name(2:13) = name(1:12)
```

This was not allowed in F77 (because of the overlap) but is OK in F90.

Often one wants to know the length of a string without any trailing blanks. This can be done with the built in function len_trim. Another built in function is called trim which gives the string without any trailing blanks.

To find the position of a substring within a string, the built in funtion index can be used:

```
index("Clinton", "in") returns 3
index("Clinton", "on") returns 6
index("Clinton", "no") returns 0 (indicates string not found)
```

To append one string onto the end of another (concatenation), the // operator can be used:

```
text1 = "Bill Clinton"  // " was elected in 1992."
```

sets text1 to the complete sentence (text1 must have been already declared of sufficient length). Note the blank before "was" is necessary for there to be a space between the word.

When trailing blanks are present, the trim function is very useful. For example, if name is declared as 20 characters long, then

```
name = "Bill Clinton"
text1 = name // " was elected in 1992"
```

sets text1 to:

```
 Bill Clinton         was elected in 1992
```

while

```
text1 = trim(name) // " was elected in 1992"
```

will produce the correct result.

When leading blanks are present, the ADJUSTL function will remove them. For example, if stname and stname2 are declared as 4 characters long, then

```
stname = " PAS"
stname2 = ADJUSTL(stname)
```

will left-justify PAS within stname2.

Here is an example program that illustrates how to input a string:

```
program vote
   implicit none
   character (len = 80) :: name
   print *, 'Who did you vote for in 1992?'
   read "(a)", name
   if (index(name,'ill') /= 0 .or.index(name,'lin') /= 0) then
      print *, "Then you are likely a Democrat."
   else if (index(name,'eor') /= 0 .or.index(name,'ush') /= 0) then
      print *,"Then you are likely a Republican."
   else
      print *,"Then you are likely an independent voter."
   end if
end program vote
```

Note the format for the read statement:

```
read "(a)", name
```

does not need to use a80, although that would also work. The free format read statement:

```
read *, name
```

is not recommended in this case because it will only read until the first blank. Thus Bill Clinton would be read in as "Bill" (unless the full name were enclosed in quotes, but who wants to make the user do that?).

ASSIGNMENT F12

Write a simple version of the famous 1960s program, Eliza, that simulates a psychologist talking to a patient. A humorous fictional account of such a program is contained in "Small World," the David Lodge satire of academia. There is an online version of the original program at: http://chayden.net/eliza/Eliza.html

Programs of this type are now called "bots" and examples can be found at alicebot.org.

Begin your program by asking the patient:

```
"How are you?"
```

Then use the index function to input a line from the user/patient. Search this line for various key words that you can then use to guide the computer's response. Design the program so that it will continue this "conversation" between doctor and patient.

Some suggestions:

```
If the input string contains a "?", then respond:
  "Let me ask the questions.  Why is it important to you?"

If the string contains "!", then respond:
  "You seem pretty upset.  What is really bothering you?"

If the string contains "mother" then respond:
  "Tell me more about your mother."

If the string contains any swear words, respond:
  "There is no need for that kind of language."

If you identify no key words on your list, then respond
with something generic like:
  "Go on."  or  "Tell me more about it."
```

Be creative but don't spend an infinite amount of time on this assignment. Your program will be more realistic if you use random numbers (see above) to randomly select from a series of possible responses so that the computer does not keep saying the same thing.

5.14 I/O with files

So far, all off our examples have involved input from the keyboard and output to the screen. Now let us see how to open files, read from them, and write data to them. Here is a program that reads pairs of numbers from an input file, computes their product, and outputs the original numbers and their product to an output file.

```
program fileinout
   implicit none
   character (len=100) :: infile, outfile
   integer :: i, ios
   real :: x, y, z

   print *, 'Enter input file name'
   read "(a)", infile
   open (11, file=infile, status='old')

   print *, 'Enter output file name'
   read "(a)", outfile
   open (12, file=outfile)

   do i = 1, 999999999           !more lines than any likely input file
      read (11,*, iostat = ios) x, y
      if (ios < 0) then
         exit
```

```
      else if (ios > 0) then
         print *, '***Warning, read error on line: ', i
         cycle
      endif
      z = x * y
      write (12,*) x, y, z
   enddo

   close (11)
   close (12)
end program fileinout
```

We open the input file with the statement:

```
   open (11, file=infile, status='old')
```

Files must be assigned "unit numbers" for I/O. This statement opens the file with unit 11. On most systems, unit 5 is defined as the default standard (keyboard) input and unit 6 is defined as the default standard (monitor) output, so these numbers should always be avoided as unit numbers. I have gotten into the habit of using units 11, 12 and 13 for most of my I/O.

file=infile is what provides the filename. Note that we could "hardwire" a file name here by writing:

```
   open (11, file="file1", status='old')
```

The status='old' is optional, but I recommend always using it for opening files which should already exist. When you say status='old' and the file does not exist, then the program will terminate and print an error condition. If you have not set status='old' then the program will create a new file and when you try to read from it, you will reach the end of the file immediately and the program will terminate without any obvious errors (except that you will now have zero length files in your directory!). Another value for status is:

```
status='new'   file must not already exist (useful to avoid
                  overwriting existing files)
```

However, in this example we choose to simply write:

```
   open (12,file=outfile)
```

so that we can overwrite existing file names. This assigns unit 12 to the output file (the input and output file unit numbers must be different!).

We read data from the input file with the statement:

```
read (11, *, iostat = ios) x, y
```

This does a free-format read from unit 11 (for a fixed format, the * is replaced with a format specifier such as "(i2, 2f6.2)" etc.). Because we do not know, a priori, how long the input file is, we need some way to recognize when we have reached the end of the file (EOF). The "iostat = ios" specifier does this by assigning the local variable ios (which we must declare as an integer) that is zero for a normal read, positive if there is an error during the read, and negative if the end of the file is reached. Note that we are free to choose any name for ios that we want as long as it is declared as an integer.

Once ios has been set, we check its values to see if there is an EOF or error condition:

```
if (ios < 0) then
   exit
else if (ios > 0) then
   print *, '***Warning, read error on line: ', i
   cycle
endif
```

For ios < 0, we exit the do loop because there are no more lines to read. For ios $>$ 0, we print a warning message and specify the line number. Being able to print the line number is useful because otherwise we would not know where to look for the problem in a big input file. This is why we use "i" in the do loop. Following the warning message, we use "cycle" to skip this line and read the next line. Without the "cycle", the program would write an output line using the same values of x and y used for the previous line, the result being an erroneous duplicate line in the output file.

We should note at this point that older Fortran programs do not use this method of testing for the end of the file. Rather, they will say something like:

```
read (11, *, end = 123) x, y
```

where 123 is a statement label that the program will branch to when the end of file is reached. This method still works in F90 but you lose style points for having to use

a statement label. However, despite this there is one aspect in which the old way of doing things is better than the new way. Suppose there is an error in the input file, for example a stray character in one of the input lines instead of two numbers. In the old way of doing things, the program will crash on the faulty input. In the new approach, using the iostat= convention, any read errors are ignored. **You never want to ignore errors without at least being aware of them.** So if you use iostat= then you always should explicitly look for errors. In other words, you should never write code like this:

```
! example of what NOT to do!
   do
      read (11,*, iostat = ios) x, y
      if (ios < 0) exit
      z = x * y
      write (12,*) x, y, z
   enddo
```

In this case, any input error would be flagged by assigning a positive number to ios. But this code does not check for this and will therefore continue running, retaining the previous values for x and y. The result will be that the output file will repeat the results from the previous line. This is not good, because we have introduced an error into the output that might not be immediately obvious. In the old way of doing things, however, the program crashes on the faulty input.

Continuing to examine the program fileinout.f90, we write the original numbers and their product using a free format write to unit 12:

```
      write (12,*) x, y, z
```

Note that x and y will probably not be in the same format as in the input file.

Finally, after the EOF but before we end the program it is good practice to close the files:

```
   close (11)
   close (12)
```

although the files will be closed automatically anyway when the program ends.

ASSIGNMENT F13

Write a program that reads from a text file containing 5 numbers per line. Compute the mean of the 5 numbers and then subtract the mean from each of the 5

original numbers. Output the 5 "demeaned" numbers to an output file. Allow the user to specify the input and output file names.

For example, if the input file contains:

```
10 20 30 40 50
1 2 3 4 5
2 4 6 8 10
5 5 5 5 5
```

your program should write to the output file:

```
 -20.000  -10.000    0.000   10.000   20.000
  -2.000   -1.000    0.000    1.000    2.000
  -4.000   -2.000    0.000    2.000    4.000
   0.000    0.000    0.000    0.000    0.000
```

Hint: Use the "fileinout.f90" program listed above as a template for the file handling part of your code.

5.15 More about multi-dimensional arrays

Two-dimensional arrays in Fortran may be defined as follows:

```
integer a(2,3)                          !F77 convention
integer, dimension(2,3) :: a            !F90 convention
```

This defines a matrix in which the first indices will vary from 1 to 2, and the second from 1 to 3 (recall that the default starting array index is 1 in Fortran).

Here is a test program that illustrates how the numbers in a can be specified and how they are stored in memory:

```
program testmatrix
   implicit none
   integer, dimension(2,3) :: a
   a(1, 1:3) = (/ 1, 2, 3 /)
   a(2, 1:3) = (/ 4, 5, 6 /)
   print *, a
end program testmatrix
```

The output of this program is:

```
 1 4 2 5 3 6
```

First, note how the array values are specified. (/ 1, 2, 3 /) is an example of what is called an "array constructor" and is a sequence of scalar values along one array dimension only. We equate this to the desired part of the a matrix by writing, for example:

```
a(1, 1:3) = (/ 1, 2, 3 /)
```

thus setting a(1,1)=1, a(1,2)=2, and a(1,3)=3.

Finally note how the array is printed. The 'print *, a' statement will dump the values of a in the same order that they are stored in memory. In doing this, Fortran varies the first array element first, then the second, etc. In this case, the result is:

```
a(1,1), a(2,1), a(1,2), a(2,2), a(1,3), a(2,3)
```

Similarly a three-order array b(2,2,2) would be stored as:

```
b(1,1,1)
b(2,1,1)
b(1,2,1)
b(2,2,1)
b(1,1,2)
b(2,1,2)
b(1,2,2)
b(2,2,2)
```

This is important to remember when passing arrays to and from subroutines for cases when the array in the main program has more dimensions than the array in the subroutine. For example, suppose we wished to store 100 seismograms of 1000 points each in the main program. We have a filtering subroutine that will act on a single time series vector. If we dimension the array in the main program as b(1000,100) then we can call the subroutine using a statement like:

```
call FILTER(b(1,i),npts)
```

where i is the seismogram number. The filter can then act on b(1:npts, i) and would be of the form:

```
subroutine FILTER(c, n)
   real, dimension(n) :: c
   .
   .
```

This is a very common type of construction. Note that this would not work if the array was dimensioned as b(100,1000) because then each 1000-point time series would not be continuous in memory.

Here is an example program to multiply two matrices:

```
program matmult
   implicit none
   real, dimension(3,3) :: a, b, c
   integer :: i, j, k

   a(1,1:3) = (/ -5.1,  3.8,  4.2 /)
   a(2,1:3) = (/  9.7,  1.3, -1.3 /)
   a(3,1:3) = (/ -8.0, -7.3,  2.2 /)

   b(1,1:3) = (/  9.4, -6.2,  0.5 /)
   b(2,1:3) = (/ -5.1,  3.3, -2.2 /)
   b(3,1:3) = (/ -1.1, -1.8,  3.0 /)

   do i = 1, 3
      do j = 1, 3
         c(i,j) = 0.0
         do k = 1, 3
            c(i,j) = c(i,j) + a(i,k) * b(k,j)
         enddo
      enddo
   enddo

   print *, "Matrix a follows"
   call PRINTMAT(a)
   print *, "Matrix b follows"
   call PRINTMAT(b)
   print *, "Matrix c = a*b follows"
   call PRINTMAT(c)

contains

subroutine PRINTMAT(x)
   real, dimension(3,3) :: x
   do i = 1, 3
      print "(3f8.3)", (x(i,j), j=1,3)
   enddo
end subroutine PRINTMAT

end program matmult
```

Note the use of the internal subroutine PRINTMAT to display the results.

This example performs the matrix multiplication exactly as one would in F77; it does not take advantage of some of the new array capabilities of F90. In fact, there

is a built in function, MATMUL, in F90 that performs matrix multiplication. My plan is to have more to say about these special F90 capabilities later in the class.

ASSIGNMENT F14

Modify the matmult program so that the matrix multiplication is done in a subroutine. Add another subroutine that computes the transpose of a square matrix. Compute the transpose of c and add this to the output listing.

5.15.1 Arrays of strings

As we have discussed, a string is just an array of characters. Thus, a 1-D array of strings will be a 2-D character array. Here is an example of this:

```
program stringarray
   implicit none
   character (len = 80), dimension(10) :: name
   name(1) = "Bill Clinton"
   name(2) = "George Bush"
   print *, "Our last president was ", trim(name(1))
   print *, "Our current president is ", trim(name(2))
end program stringarray
```

The program can store up to 10 name of 80 characters each. Note the use of the 'trim' function when printing the names. This is very handle to cut off the trailing blanks and limit unnecessary extra spaces (and sometimes lines) in the output.

5.16 A more complex example of data processing

Suppose we have a data file (e.g., datafile1) that contains a series of measurements that has the following form:

```
980204 22:03:34.42
  10.8
  10.2
   9.8
  11.6
980205 08:45:22.20
   5.5
   7.2
   6.6
980205 20:13:42.88
  15.0
  13.8
  12.9
  14.2
```

```
etc.
```

The structure is that there are date/time identifiers and then a series of measurements made at that time. The problem in reading this file is that we don't know how many measurement lines will follow each date/time line so we can't simply perform a formatted read on each line from the file.

Let us assume that we want to compute the mean of these measurements and write a new file which stores this information on the same line as the date/time. In this case, our desired output file (e.g., datafile2) will look like:

```
980204 22:03:34.42   10.60     4
980205 08:45:22.20    6.43     3
980205 20:13:42.88   13.97     4
```

where the final column gives the number of measurements.

Here is how such a program could be written:

```
program procfile
   implicit none
   character (len=100) :: infile, outfile
   character (len=20) :: linebuf, event
   integer :: ios, nevent=0, ndata=0
   real :: x, sum=0.0, xavg

   print *, 'Enter input file name'
   read "(a)", infile
   open (11, file=infile, status='old')

   print *, 'Enter output file name'
   read "(a)", outfile
   open (12, file=outfile)

   do
      read (11,'(a)', iostat = ios) linebuf
      if (ios < 0) exit
      if (linebuf(1:1) /= ' ') then  ! no init blank, must be event
         nevent = nevent + 1
         if (nevent /= 1) then          !need to output previous event info
            call WRITE_EVENT
            ndata = 0
            sum = 0
         end if
         event = linebuf
      else                       ! has starting blank, must be measurement
         read (linebuf,*) x
         sum = sum + x
         ndata = ndata + 1
```

```
      end if
   enddo
   call WRITE_EVENT
   close (11)
   close (12)

contains

subroutine WRITE_EVENT
   if (ndata /= 0) then
      xavg = sum/real(ndata)
   else
      xavg = 0.
   end if
   write (12,"(a20, f7.2, i5)") event, xavg, ndata
end subroutine WRITE_EVENT

end program procfile
```

The beginning of the program where the files are opened is the same as in fileinout.f90 (our earlier example of file I/O).

Using an infinite do loop, we read lines from the input file using:

```
   read (11,'(a)', iostat = ios) linebuf
```

Because we don't know the format of each line before we read it, we read into a character string (linebuf) that will serve to temporary store the contents of the line (a line "buffer" as they say in the computer world).

We use iostat=ios to set ios to a flag that can be used to identify when the end of the file occurs so that we can exit the do loop. As discussed previously, we really should also check for an error condition (i.e., ios > 0), but we don't bother here because errors are unlikely when reading in a string (yes, we are being a bit sloppy!).

Next, we check the contents of the first character in linebuf. If is not a blank, then we know we have an event line. In this case we increment the nevent counter variable by one. If we have not just read the first event, then we have read a new event, thus terminating the data input from the previous event. In this case we need to write the processed event info to the output file (we can't do this until this point because we don't know how many data points there will be) and reset sum and ndata to zero. Finally we set event = linebuf to store the event line until we need to output it.

If, on the other hand, the first character in linebuf is blank, then we have a data line. We then read the value of x out of linebuf:

```
read (linebuf,*) x
```

This is called an "internal read" and is the first time that we have shown this. It allows the program to do a formatted read from a string, rather than from an external file. We do a free format read (*), but one could also use a format specifier. After reading the measurement value into x, we suitably increment a running sum of x and the number of measurements.

When we reach the end of the input file, we have to output the results of the final set of measurements. To avoid repeating a block of code for this operation, we use an F90 internal subroutine (WRITE_EVENT). This is used twice, inside the loop as we output information from the last event before going on to the next one, and outside the loop where we output the information from the last event. Note that we must check to see if there are no measurements for an event line, in which case we do not divide by zero but simply set xavg to zero. There should be no possibility of mistaking this for a real measurement in the output file because the number of measurements in this case will also be zero.

ASSIGNMENT F15

Obtain the data file, scsn.phase.dat, from the class web site. This is a list of earthquakes and arrival time data from the Southern California Seismic Network (SCSN) for the first two days of August 2000. (Files like this are readily obtainable from the SCEC Data Center at http://www.scecdc.scec.org if you ever want to obtain more of these data. The format is called the SCEC_DC phase format.)

Here is what part of the file looks like:

```
2000/08/01 14:44:12.6 L 1.1 c  35.962 -117.693   5.2 A 9159024   8  51  0  0
 WRC  VHZ   911      P IU1   4.41    1.26
 WCS  VHZ   885      P E 3   9.98    1.85
 WVP  VHZ   925      P IU1  11.54    2.25
 TOW  VHZ   813      P E 2  18.28    3.78
 CLC  VHZ   202      P E 2  18.49    3.37
 WMF  VHZ   906      P E 3  22.86    3.94
 WMF  VHZ   906      S E 2  22.86    7.08
 WNM  VHZ   908      P E 3  23.74    4.23
2000/08/01 14:45:36.8 L 1.3 h  34.806 -116.271   7.3 A 9159025   7  79  0  0
 CDY  VHZ   184      P IU0   6.66    1.73
 RAG  VHZ  1034      P IU1  17.58    3.19
```

```
 RAG  VHZ  1034      S E 2  17.58    5.77
 RMM  VHZ   647      P ID1  37.23    6.33
 TPM  VHZ  1033      P IU1  52.29    8.88
 GRP  VHZ   355      P IU1  61.21   10.14
0299    C 65535      P IU1 11395.79    7.39
2000/08/01 15:04:17.9 L 1.4 h  34.810 -116.268   7.1 A 9159030  19  83  0  0
 CDY  VHZ   184      P IU0   6.76    1.73
 RAG  VHZ  1034      P IU1  17.76    3.16
etc.
```

There is a line for each earthquake with the date and time (UT not local time). For the first line in the above example, the additional bits include:

```
L   = local event
1.1 = magnitude
c   = how magnitude was computed (coda in this case)
35.962   = lat
-117.693 = lon
5.2      = depth (km)
A        = SCSN assigned quality (A=best)
9159024  = cusp id number
8        = number of lines of phase arrival time info

The station info lines include:
WRC = station name
VHZ = station channel
911 = ?
P   = phase name (normally P or S)
IU1 = phase pick info
4.41 = station-event distance (km)              (=X for assignment)
1.26 = travel time (s from event origin time)   (=T for assignment)
```

Your task is to write a F90 program to read this file and write to an output file a series of (X,T) points with (one X-T pair per line) for all P arrivals for all events between 3 and 8 km depth. Then make an X-Y plot of the T-X points using whatever plotting method you are most familiar with. That is, plot time on the y-axis and distance on the x-axis and plot the coordinates of each point. E-mail me a copy of the F90 program source code and a PDF file of the X-Y plot.

The good news about this data format is that it does include a number in the event line that lists the number of phase lines that will follow. The bad news is that sometimes the last 1 or 2 phase lines are "garbage" in that they have numbers instead of station names and are some kind of calibration info. You will have to figure out how to recognize and discard these lines in your program. Also the phase lines begin with a tab character rather than a long series of blanks; this may complicate things somewhat.

Hint: Don't try to write your entire program all at once. First, get a version working that simply reads the input file and prints out the parts of each line that you will need (i.e., the depth and number of phase lines for the event line, the phase name and the X and P values for the phase lines). Once you have this working correctly, then go on to add the part to output the (X,T) points.

5.17 Example sorting routine from Numerical Recipes

The book Numerical Recipes contains a large number of useful subroutines (there are both Fortran and C versions) that are fully explained in the text. You can find F77 source code (1st edition of NR) for these routines in:

```
~shearer/PROG/SUBS/NUMRECIP
```

To illustrate the use of the Numerical Recipes routines, here is an example program that generates a list of random numbers, sorts them using the NR function piksrt, and then prints out the sorted list.

```
program sortrand
   implicit none
   integer, parameter :: NPTS=100
   integer :: i
   real, dimension(npts) :: xran

   do i = 1, NPTS
      call random_number(xran(i))
   enddo

   call PIKSRT(NPTS,xran)

   print "(10f7.4)", (xran(i), i=1,npts)
end program sortrand
```

The program sets the xran array to random numbers. It then calls the NR subroutine PIKSRT to sort the numbers before printing them out. We must either include the PIKSRT source code or link with a PIKSRT object code when we compile this program. Here is the PIKSRT source code:

```
      SUBROUTINE PIKSRT(N,ARR)
      DIMENSION ARR(N)
      DO 12 J=2,N
        A=ARR(J)
        DO 11 I=J-1,1,-1
```

```
          IF(ARR(I).LE.A)GO TO 10
          ARR(I+1)=ARR(I)
11      CONTINUE
        I=0
10      ARR(I+1)=A
12    CONTINUE
      RETURN
      END
```

This ugly code is typical of old Fortran programs. It has all capital letters and has line numbers, 'go to' statements, and uses 'continue' statements in the do loops. Actually, it's better than many examples, because the do loops are indented. The important thing for us is that the code works—we don't want to bother rewriting it and possibly breaking it.

In general, F77 and older code will not compile under F90 because of old-style comment lines ('C' in column 1) and old-style line continuation flags (non-& character in column 6). This example, however, does not have these problems and is fully F90 compatible. Thus, we could just append the source code onto the end of our program. Alternatively, we could compile the subroutine under F90 as follows:

```
f90 -c piksrt.f -o piksrt_f90.o
```

which will create a piksrt_f90.o file (replace f90 with gfortran if you are using gfortran). The _f90 is my own convention to label f77 source code that has been compiled under f90 so that I don't try to link piksrt_f90.o with a f77 program. Unfortunately, f77 and f90 object files are not always compatible (they are in this case, but it is dangerous to assume that they always will be, so it is safest to separately compile the source code in each case).

```
f90 sortrand.f90 piksrt_f90.o -o sortrand
```

or by using a Makefile as discussed earlier. This would be our best choice if the subroutine source code is lengthy and/or is non-F90 compatible.

ASSIGNMENT F16

Modify the sortrand program to return the median of a user-specified number of random numbers. Do the median computation in the form of a subroutine that returns the median value, but does NOT resort the input array in the process. The random number generation should be in your main program, not within the

MEDIAN subroutine which should be a general purpose routine that simply inputs an array of numbers and returns the median value. Then whenever you need to compute a median of some numbers within a program, you can simply call the same subroutine, e.g.,

```
call MEDIAN(x, n, xmed)     !x=array, n=# of points, xmed=median
```

Hint: Within your median-computing subroutine, copy the input array to another array before calling PIKSRT. Make sure that your program gives the correct result for both even and odd numbers of points.

5.18 Example of saving values in a subroutine

A common convention in geophysics is to name an instrument site with a short ascii string. In seismology, for example, station names are usually designated with 3 to 4 character names. Southern California GPS sites are usually identified with 4 character names.

Often data products are labeled by the station name, without including information about the station, such as its location. Data processing programs will often require this information. Thus, there is frequently a need for a computer routine that will retrieve information about a station, given the station name. One could hardwire this information into the program with a series of if statements, but this would become very cumbersome for large numbers of stations and would limit the flexibility and portability of the code. A better approach is to save the station information in a file and have the computer read from the file to access the information when necessary. However, file I/O is relatively slow so we won't want to open, read, and close the file every time we need to determine a station location. It would be much faster to read the station information file once and then save the information during the time that the program is running. For portability, ideally all of this overhead would be performed in a function that we could use in many programs without having to worry about the format of the station file or the size of the array that are required to store it.

In order to do this, we need to retain the values of certain variables within the function for subsequent calls.

Here is an example that will return station coordinates for some of the GSN (Global Seismic Network) stations.

```
program testgetstat
   implicit none
   character (len = 4) :: stname
   real :: slat, slon, selev
   do
      print *, 'Enter station name (stop to stop)'
      read (*,'(a)') stname
      if (stname == 'stop') exit
      call GET_STAT(stname,slat,slon,selev)
      print *, 'slat,slon,selev = ',slat,slon,selev
   enddo
end program testgetstat


! subroutine GET_STAT gets the lat/lon/elev of a station
! with a given name from the GSN station list
!
! Inputs:  snam  =  station name (a4)
! Returns: flat  =  station latitude
!          flon  =  station longitude
!          felev =  station elevation (m)
! NOTES: Station list must be alphabetized
!        If station name is not found, then returned
!          variables are set to -999.
!        Program reads and saves station info on first call
!
subroutine GET_STAT(snam,flat,flon,felev)
   implicit none
   integer, parameter :: NMAX=5000
   character (len = 4) :: snam
   character (len = 4), dimension(NMAX) :: stname
   real, dimension(NMAX) :: slat, slon, selev
   real :: flat, flon, felev
   integer :: i, i1, i2, nsta, it
   logical :: firstcall = .true.
   save firstcall, stname, slat, slon, selev, nsta

   if (firstcall) then
      firstcall = .false.
      open (11, file='stlist.gsn', status='old')
      print *, 'Reading station file: stlist.gsn'
      do i=1,NMAX
        read (11,7,end=12) stname(i), slat(i), slon(i), selev(i)
7       format (a4, f10.5, f11.5, f5.0)
      enddo
      print *,'***Warning: number of stations in file may exceed ',NMAX
      i = NMAX + 1
12    nsta = i-1
      close (11)
      print *,'Number of stations read = ',nsta
   end if
```

```
   i1 = 1
   i2 = nsta
   do it = 1, 15
      i = (i1+i2)/2
      if (snam == stname(i)) then
         flat = slat(i)
         flon = slon(i)
         felev = selev(i)
         return
      else if (snam < stname(i)) then
         i2 = i-1
      else
         i1 = i+1
      end if
   enddo
   print *, '***station not found ', snam
   flat  = -999.
   flon  = -999.
   felev = -999.
end subroutine GET_STAT
```

The main program is a short driver program that enables us to test that the GET_STAT subroutine is working properly. It is always a good idea to use little programs like this to test functions that are being developed, BEFORE using the functions in larger programs.

For efficiency, the subroutine reads the station file only the first time the subroutine is called. It then saves the information in memory to use for subsequent calls. Normally, the values of variables in a subroutine are not retained between calls. The "save" command is used to specify those variables that are to be saved between calls.

This is our first example of a logical variable:

```
   logical :: firstcall = .true.
```

firstcall can have two possible values: .true. or .false. Here we set it to .true. the first time (and only the first time) that the subroutine is called.

The save statement specifies which variable values are to be saved between subroutine calls:

```
   save firstcall, stname, slat, slon, selev, nsta
```

To read the station file upon the first call to the subroutine, we write

```
if (firstcall) then
```

Notice that a logical variable can be the sole argument for an if test. We then set firstcall = .false. so that this block of code will not be excuting upon subsequent calls to the subroutine.

The station file has the form:

```
AAE    9.02920   38.76560 2442
AAK   42.63900   74.49400 1645
ABKT  37.93040   58.11890  678
ADK   51.88370 -176.68440  116
AFI  -13.90930 -171.77730  706
ALE   82.50330  -62.35000   60
ALQ   34.94620 -106.45670 1840
ANMO  34.94620 -106.45670 1840
ANTO  39.86890   32.79359  883
AQU   42.35389   13.40500  720
.
.
```

In routines like this, I like to print out information about the file that is being read during the first call. This reminds the user of the program about what is being done and it helpful in case there is a problem or error later in the program. For example, perhaps we have a faulty station file that has only 1 station. Or perhaps the firstcall flag is not working properly, in which case these output lines will result each time we call the routine, not just the first time.

For speed, the subroutine does not simply loop through the station list until it finds a match. Instead, it exploits that fact that the stations are in alphabetical order. i1 and i2 are indices that are designed to bracket the target station in the list. Initially, they are set to 1 and nsta, the first and last station indices. Next, i is set to a point halfway between i1 and i2. The station in the station list at i is compared to the target station. If they are the same, then we can set the return variables. If the stlist station is greater than the target station (later in the alphabet), then i2 is set to i-1. If the stlist station is less than the target station, then i1 is set to i+1. We iterate using this procedure 15 times to narrow in on the station name. (2e15 must be greater than NMAX to make sure we do enough iterations)

Note that

```
else if (snam < stname(i)) then
```

is a valid check to see if string variables are in alphabetical order.

If we don't find the target stname in the station list, then we print out a warning message. We also set the station coordinates to numbers that are unlikely to be confused with real station locations in case the user of the function does not notice the warning message (or chooses to ignore it!).

ASSIGNMENT F17

Modify GET_STAT to find the nearest station to a given (lat, lon) point and return the station name and its coordinates. You can get the stlist.gsn file from http://igppweb.ucsd.edu/ shearer/SIO233/. Name your new function NEAR_STAT and also include a testnearstat driver program to test the operation of the function. To find the nearest station, you will need to be able to compute the distance between two points on a sphere. Use the SPH_AZI from the notes or the SPH_DIST subroutine from ~shearer/SUBS/sphere_subs.o

Don't bother to do the separate calculation for small values of del.

The NEAR_STAT suboutine should be of the form:

```
subroutine NEAR_STAT(plat, plon, stname, slat, slon, sdep)
```

where plat and plon are the coordinates going into the subroutine and stname, slat, slon and sdep are passed back from the function to the main program.

5.19 Complex numbers

A nice aspect of Fortran is that complex numbers are a standard feature. Here is a program to show how they can be declared and used:

```
program testcomplex
   implicit none
   complex :: a, b, c
   print *, 'Enter first complex number'
   read *, a
   print *, 'Enter second complex number'
   read *, b
   c = a*b
   print *, 'Product = ', c
   print *, 'abs of product = ', abs(c)
   print *, 'sqrt of product = ', sqrt(c)
end program testcomplex
```

Here is an example of running the program:

```
rock% testcomplex
 Enter first complex number
(1, 1)
 Enter second complex number
(-.5, .1)
 Product =  (-0.6,-0.4)
 abs of product =  0.7211103
 sqrt of product =  (0.2460795,-0.81274545)
```

Complex numbers are represented as a pair of numbers in parenthesis separated by a comma (first number is the real part, second number is the imaginary part). This is the only format that will work for the free format read. If you try to enter

```
          1, 1
or        1 1
or even   (1 1)
```

you will get an error.

Notice that in F90 you don't need to use special forms for the functions abs and sqrt (e.g., cabs and csqrt as you will see sometimes in older code).

There are conversion functions to build complex numbers from two real numbers and vice versa, as shown in this example code:

```
program testcomplex2
   implicit none
   complex :: a
   real :: ar, ai
   print *, 'Enter real part'
   read *, ar
   print *, 'Enter imaginary part'
   read *, ai
   a = cmplx(ar, ai)
   print *, 'a = ',a
   a = exp(a)
   print *, 'Exp(a) = ', a
   ar = real(a)
   ai = aimag(a)
   print *, 'Real part = ', ar
   print *, 'Imag part = ', ai
end program testcomplex2
```

and its output

```
rock% testcomplex2
 Enter real part
1
 Enter imaginary part
```

```
 2
  a =  (1.0,2.0)
  Exp(a) =  (-1.1312044,2.4717266)
  Real part =  -1.1312044
  Imag part =  2.4717266
```

ASSIGNMENT F18

Write a program to test the built in complex exponential function against the formula

```
e^z = e^(x+iy) = e^x e^(iy) = (e^x cos y) + i (e^x sin y)
```

which you will have to adapt for your program. Include a driver program to test your function for selected input values. Make sure that your code gets the correct answer for these examples:

```
exp( 1.1 + 2.3i) = -2.002 + 2.240i
exp( 0.0 + 1.2i) =  0.362 + 0.932i
exp(-0.5 + 0.0i) =  0.607 + 0.000i
```

Can you find any differences between the built in exp function are the results obtained with the formula?

5.20 Array operations in F90

F90 allows many operations on vectors and matrices to be performed in single statements without the necessity of writing do loops over the array indices (as was necessary in F77). Here is an example program that demonstrates some of these operations on vectors.

```
program vectormath
   implicit none
   real, dimension(5) :: a = (/ 1.0, 2.0, 3.0, 4.0, 5.0 /), b = 2.0, c
   real :: x

   print *, 'a = ', a
   c = a + 1
   print *, 'a + 1 = ', c
   c = 2 * a
   print *, '2 * a = ', c
   c = a * a
   print *, 'a * a = ', c
   c = sqrt(a)
```

```
   print *, 'sqrt(a) = ', c
   c = sin(a)
   print *, 'sin(a) = ', c
   c = exp(a)
   print *, 'exp(a) = ', c
   print *, 'b = ', b
   c = a + b
   print *, 'a + b = ', c
   c = a * b
   print *, 'a * b = ', c
   x = sum(a)
   print *, 'sum(a) = ', x
   c = a
   c(4:5) = 0.0
   print *, 'a with two zeros on end = ', c
   x = dot_product(a, b)
   print *, 'a dot b = ', x
   x = sum( (a - sum(a)/5. )**2)
   print *, 'sum of squares of difference from mean = ', x

end program vectormath
```

Note that even fairly complicated expressions are possible provided the programmer keeps track of what is a vector and what is a scalar.

Operations are also possible on matrices. Here are some examples:

```
program matrixmath
   implicit none
   real, dimension(2, 3) :: a23, b23, c23
   real, dimension(3, 2) :: a32, b32, c32
   real, dimension(2,2) :: a22, b22, c22
   integer, dimension(2) :: loc2
   integer :: i, j, k

   a23(1,1:3) = (/ -5.1,  3.8,  4.2 /)
   a23(2,1:3) = (/  9.7,  1.3, -1.3 /)
   print *, 'Matrix a23 follows'
   call PRINTMAT(a23, 2, 3)

   b32(1:3, 1) = (/  9.4, -6.2,  0.5 /)
   b32(1:3, 2) = (/ -5.1,  3.3, -2.2 /)
   print *, 'Matrix b32 follows'
   call PRINTMAT(b32, 3, 2)

   c22 = matmul(a23, b32)        !this works but matmul(b32, a23) does not

   print *, "Matrix c22 = matmul(a,b) follows"
   call PRINTMAT(c22, 2, 2)

   print *, 'maxval(a23) = ', maxval(a23)
```

```
   print *, 'maxloc(a23) = ', maxloc(a23)
   loc2 = maxloc(a23)
   print *, 'loc2 = ', loc2
   print *, 'a23(loc2(1), loc2(2)) = ', a23(loc2(1), loc2(2))

   b23 = a23 + transpose(b32)
   print *, 'Matrix b23 = a32 + transpose(b32) follows'
   call PRINTMAT(b23, 2, 3)

   print *, 'size(a23) = ', size(a23)
   print *, 'size(a23(1,:)) = ', size(a23(1,:))

contains

subroutine PRINTMAT(x, m, n)
   real, dimension(m, n) :: x
   integer :: m, n
   do i = 1, m
      print "(10f8.3)", (x(i,j), j=1,n)
   enddo
end subroutine PRINTMAT

end program matrixmath
```

This demonstrates the intrinsic functions matmul, maxval, maxloc, transpose, and size. Note that matmul(a,b) is true matrix multiplication, not the multiplication of the individual array elements as occurs from writing simply a*b.

The maxloc function returns the location of the maximum value in the array. Note that the statement

```
   loc2 = maxloc(a23)
```

works only if loc2 is defined as an integer array with dimension(2).

NOTE: If maxloc is applied to a one-dimensional array, for example to find the index of the maximum value of a vector bvec:

```
   loc = maxloc(a)
```

Note that loc must be defined as an integer array with dimension(1). You will get an error message during compilation if loc is defined simply as an integer.

There are corresponding functions, minval and minloc, that determine the minimum value and location within an array.

It would be interesting to test whether programs using the intrinsic array functions in F90 run any faster than those written using do loops.

5.20.1 ANY and ALL

Sometimes you may want to check whether something is true for any or all elements of an array. This could be done using a few lines of code in which the appropriate if statement is contained inside a do loop over all of the array indices. However, the test can often be done more compactly using ANY or ALL. For example,

```
program anyall
   implicit none
   integer :: i
   integer, dimension(3) :: x, y, z

   x = (/ 1, 2, 3 /)
   y = 1
   z = x

   if (ANY(x == y)) print *, 'x(i) = y(i) for some i'
   if (ALL(x == z)) print *, 'x(i) = z(i) for all i'

   print *, ANY(x == y), ALL(x == y)
   print *, ANY(x == z), ALL(x == z)

end program anyall
```

will result in

```
./anyall
 x(i) = y(i) for some i
 x(i) = z(i) for all i
 T F
 T T
```

Notice that .true. and .false. are output as T and F, respectively. Interestingly, you can use this form to print out the true/false part of if statements without the ANY and ALL, i.e.,

```
   print *, (1 == 2)
```

results in

```
 F
```

Although the anyall.f90 code above uses 1D arrays (vectors), ANY and ALL can also be applied to check corresponding values of matrices and other multidimensional arrays.

5.21 Allocatable arrays

An awkward aspect of older Fortran programs is the need to declare arrays to the maximum possible size that could ever be needed when running the program. This memory must be set aside even when it is not needed—a wasteful practice. F90 avoids this by allowing memory to be allocated and deallocated on the fly. Here is an example program:

```
program setarray
   implicit none
   real, dimension(:), allocatable :: x
   real, dimension(:, :), allocatable :: y, yy
   real :: xsum
   integer :: n, i, j, m

   print *, 'Enter number of points'
   read *, n

   allocate (x(n))
   do i = 1, n
      call random_number(x(i))
   enddo
   xsum = sum(x)
   print *, 'sum = ', xsum
   deallocate(x)        !this frees up memory

   print *, 'Enter m, n (# rows, # columns)'
   read *, m, n
   allocate (y(m,n))
   allocate (yy(n,n))
   do i = 1, m
      print *, 'Enter row # ', i
      read *, (y(i, j), j = 1, n)
   enddo
   yy = matmul(y, transpose(y))
   print *, 'y * yt = '
   call PRINTMAT(yy, m, m)
   deallocate(y)
   deallocate(yy)

contains

subroutine PRINTMAT(x, m, n)
   real, dimension(m, n) :: x
   integer :: m, n
   do i = 1, m
      print "(10f8.3)", (x(i,j), j=1,n)
   enddo
end subroutine PRINTMAT
```

```
end program setarray
```

5.22 Structures in F90

It is often convenient to have a user-defined array of data elements that may, or may not, be of the same data type. This is called a "Structure" in C and a "Derived Data Type" in F90. This is a new feature that was not included in F77. Suppose, for example, we wanted to set up a data base containing information (name, age, height, weight) about 3 different people. Here is a program that uses a structure to read in this information and print the name of the lightest person:

```
program namebase
   implicit none
   integer, parameter :: nmax=3
   type person
      character (len=20) :: name
      integer :: age
      real :: height, weight
   end type person
   type(person), dimension(nmax) :: student
   integer :: i
   real :: weightmin

   do i = 1, nmax
      print *, 'Enter first name, age, height, weight (e.g., Bob 27 69 183)'
      read *, student(i)%name,    &
              student(i)%age,       &
              student(i)%height,   &
              student(i)%weight
   enddo

   print *, 'Lightest student = ', student(minloc(student%weight))%name
   print *, 'Oldest student = ', student(maxloc(student%age))%name

end program namebase
```

The statements:

```
type person
   character (len=20) :: name
   integer :: age
   real :: height, weight
end type person
```

create a defined type that can be used to name a variable later in the program. The contents are a character string (of length 20), an integer for the age, and real number for the height and weight. These contents are termed the "members" or "components" of the structure.

In this example, the defined type is given the name "person" which is NOT a variable name. Rather it is a name that can later to used to define the actual variable name(s) that will have this structure. The next line creates the array student that has this structure:

```
type(person), dimension(nmax) :: student
```

In this line, type(person) acts just like the integer and real statements that we are used to. It can be used to define more than one variable name and these variables do not need to be arrays. Here is another example of this:

```
type(person), dimension(nmax) :: grads, undergrads
type(person) :: teacher
```

which sets up structure arrays for grads and undergrads and a single structure for teacher.

The members of the structure are referenced by appending %member to the name, where member refers to the specific member defined in the structure. So, for example, student(1)%age is the age of student(1). Note that the array index goes BEFORE the %member, not after. The % operator is also sometimes called the "component selector."

Note the nifty use of the minloc and maxloc functions, avoiding the need to write do loops.

This example does not really make obvious the advantages of a structure because we could easily have maintained separate arrays for name, age, height and weight. A clearer advantage of the structure approach is that we can reassign all of the members with a single statement, i.e., we can say:

```
student(3) = student(2)
```

rather than having to say:

```
student(3)%name = student(2)%name
student(3)%age = student(2)%age
etc.
```

However, we cannot compare structures as in the statement:

```
if (student(3) == student(2) ) then    !   ILLEGAL!!
```

ANY or ALL also do not work for structures, i.e.,

```
if (ALL(student(3) == student(2)) ) then    !   ILLEGAL!!
```

5.23 Writing fast programs

Modern computers are amazingly fast compared to those from 10 to 20 years ago and thus even inefficient code will often run fast enough. But any code that takes more than a few seconds to run is potentially more useful if it could run faster. So it's always good to think about ways to make code more efficient.

In most cases, there is one key part of the program that takes most of the time. The first step is to identify that part. If it's not obvious by inspection, then one can add print statements that keep track of how long the different parts take to run. In F90, this can be done using the builtin function system_clock, as illustrated in this example program that tests how long different types of math take:

```
program testspeed
   implicit none
   integer :: n, i, count1, count2, count_rate, k=2, k2
   real :: dt, x=1.2, x2

   print *, 'Enter number of operations'
   read *, n

! test integer math
   call system_clock(count1, count_rate)
   k2 = 5
   do i = 1, n
      k = k + k2
      k = k - k2
   enddo
   call system_clock(count2, count_rate)
   dt = real(count2-count1)/real(count_rate)
   print *, ' integer +-, dt = ', dt
   call system_clock(count1, count_rate)
   k2 = 5
   do i = 1, n
      k = k*k2
      k = k/k2
```

```
   enddo
   call system_clock(count2, count_rate)
   dt = real(count2-count1)/real(count_rate)
   print *, ' integer */, dt = ', dt

! test real math
   call system_clock(count1, count_rate)
   x2 = 3.14159
   do i = 1, n
      x = x + x2
      x = x - x2
   enddo
   call system_clock(count2, count_rate)
   dt = real(count2-count1)/real(count_rate)
   print *, ' real +-, dt = ', dt
   call system_clock(count1, count_rate)
   x2 = 3.14159
   do i = 1, n
      x = x*x2
      x = x/x2
   enddo
   call system_clock(count2, count_rate)
   dt = real(count2-count1)/real(count_rate)
   print *, ' real */, dt = ', dt

! test trig functions
   call system_clock(count1, count_rate)
   x2 = 5.14159
   do i = 1, n
      x = sin(x2)
      x = cos(x2)
   enddo
   call system_clock(count2, count_rate)
   dt = real(count2-count1)/real(count_rate)
   print *, ' sin/cos, dt = ', dt

! test if statement
   call system_clock(count1, count_rate)
   k2 = 5
   do i = 1, n
      k = k + k2
      k = k - k2
      if (k > 2) k = k - k2
   enddo
   call system_clock(count2, count_rate)
   dt = real(count2-count1)/real(count_rate)
   print *, ' integer +- with if statement, dt = ', dt

end program testspeed
```

On my Macbook Air (2 GHz Intel Core i7), this produces:

```
shearer@khan 84> ./testspeed
 Enter number of operations
99999999
  integer +-, dt =   0.44499999
  integer */, dt =    1.1700000
  real +-, dt =   0.57099998
  real */, dt =   0.95999998
  sin/cos, dt =    1.7980000
  integer +- with if statement, dt =   0.44499999
```

Before we continue, we should stop for a minute to be amazed. My little laptop is doing 200 million operations in about a second or less!

Somewhat surprisingly, real arithmetic is comparable to integer arithmetic and sometimes even faster. Even more surprisingly, the trig functions only take about a factor of two longer. And it appears that if statements take hardly any time at all! Thus much of the advice that I was prepared to give you (try to use integers instead of reals, avoid computing trig functions and using if statements inside do loops) is not accurate. Some really smart people must be optimizing computer chips and the F90 compiler. But it's still worth knowing how to identify the slow part of your code, so that you can devise ways to make it run faster.

5.23.1 The -O option

But there is another way to make your code run faster and it's always surprising to me how many students don't know about it. Most modern computer compilers have an option to "optimize" code to make it run faster. In gfortran, this is done using the "-O" option, i.e.,

```
gfortran -O testspeed.f90 -o testspeed
```

Here is what I get for this program after optimization:

```
shearer@khan 86> ./testspeed
 Enter number of operations
99999999
  integer +-, dt =   3.50000001E-02
  integer */, dt =   0.22499999
  real +-, dt =   0.19100000
  real */, dt =   0.63099998
  sin/cos, dt =   3.20000015E-02
  integer +- with if statement, dt =   0.12400000
```

The integer add/subtract is 13 times faster, the integer mult/divide is 5 times faster, the real add/subtract is 3 times faster, the real mult/divide is 1.5 times faster, and the sin/cos is an astonishing 560 times faster[1].

Since -O makes code run faster, why not use it all the time? It takes longer to compile programs using -O and the executables are not as stable, i.e., your program is more likely to crash or give the wrong answer (!). Thus, I recommend that you debug your programs without using -O, but then once they are stable and working, use -O to improve their speed (if necessary).

ASSIGNMENT F19

Compile and run the program testspeed.f90, compiled both with and without the -O option. Send me the output results for 99,999,999 operations, along with the details of your computer (i.e., name, type, chip, clock speed). For example, on Macs go to 'About This Mac' under the Apple menu and send me the processor details.

5.24 Fast I/O in Fortran

Unless you are a serious "number cruncher" you are likely to find that input/output operations (reading and writing to file) take more time than any arithmetic operations. FORTRAN has generally not been considered to be as flexible as C in the way that it handles i/o operations. However, with a little deviousness, it is possible to write FORTRAN programs that are capable of extremely fast i/o. The key to making FORTRAN do fast i/o is to use unformatted binary read/write operations.

Suppose we have a 100000 × 10 real array that we wish to store on disk. We could output this simply as an ascii file:

```
program testio1
   implicit none
   real, dimension(100000,10) :: a = 1.1
   integer :: i, j, count1, count2, count_rate
   real :: dt

   open (12, file='out.testio1')

   call system_clock(count1, count_rate)

   do i = 1, 100000
      write (12, '(10e12.4)') (a(i,j), j=1,10)
   enddo
```

[1]Does it recognize that we are computing the same thing? I suspect so!

```
   call system_clock(count2, count_rate)
   dt = real(count2-count1)/real(count_rate)
   print *, 'dt = ',dt

   close (12)
end program testio1
```

Notice the use of the intrinsic function, system_clock, to monitor how long the output takes. On my laptop (Macbook Air, 2 GHz Intel Core i7), this takes about 0.7 s and creates a 12.1 Mb file.

Next, we could output this as a binary file using similar loops over the indices:

```
open (12, file='out.testio2', form='unformatted')
do i = 1, 100000
   write (12) (a(i,j), j=1,10)
enddo
close (12)
```

On my laptop, this takes about 0.067 s (10 times faster) and generates a 4.8 Mb file. A further improvement occurs when we store the entire array directly:

```
   open (12,file='out.testio3',form='unformatted')
   write (12) a
   close (12)
```

On my laptop, this generates a 4.1 Mb file in about 0.006 s. The total speed improvement compared to ASCII is about a factor of 120.

Similar speed improvements can be noted upon reading these files. The message is that for speedy i/o of large data sets in FORTRAN, we should read/write large arrays in blocks. This is how Guy's GFS programs work and my routines to store travel time data.

Of course, it is not always convenient to refer to data within a big array. To make it easier to keep track of things, it is often a good idea to define a data type (structure). For example, suppose our array actually consists of 10000 "lines" of data with 10 values for each line, consisting, for example, of a 4 character station name, coordinates for the station, and date/time information. In this case, we can define a suitable data type and then create an array of these data types.

```
type station_info
   character (len=4) :: stname
   real :: slat, slon, selev, sec
```

```
      integer :: iyr, imon,iday, ihr, imn
   end type station_info
   type(station_info), dimension(10000) :: stlist
```

We can now perform i/o very simply using the stlist array, while preserving the ability to access its individual parts. For example, stlist(5633)%stname is the station name of the 5633th line of data, stlist(232)%slat is the latitude of the 232th line, etc.

F77 does not allow for structures, but a kludge is possible using the equivalence statement. For example, we could we define a small array aa with 10 elements and set these elements to be equal to the individual variable names that we want:

```
      real aa(10)
      common/com1/stname,slat,slon,selev,iyr,
     &            imon,iday,ihr,imn,sec
      equivalence (aa(1),stname)
```

The equivalence statement sets the values of aa to the same place in memory as the 10 variable names defined in the common block. The beauty of this is that these variables can be of mixed data types. In order to examine the record 523, we just set aa to the appropriate part of a:

```
      i=523
      do 50 j=1,10
         aa(j)=a(i,j)
50    continue
```

The stname, slat, etc., are now set. This trick is used in Guy's GFS routines and in many of my older I/O routines.

5.24.1 Ascii versus binary files

There is a tradeoff between speed and convenience for ascii versus binary files. ascii is easier to work with and to understand and is often the preferred format when file size or speed is not a problem. However, for large data sets and data processing, binary is often better because it permits much faster I/O and the files will generally be smaller than their ascii counterparts. You are also assured of retaining the full machine precision for numerical values (you don't risk deciding later that you really should have stored 4 places to the right of the decimal, not 3). However, binary formats are somewhat less portable then ascii and require more user knowledge about their format.

ASSIGNMENT F20

Compile and run the program testio.f90 on your computer and send me the timing results for the three different ways to perform the I/O, along with the details of your computer (name, type, chip, clock speed). Then try it again after compiling with the -O option. Does -O help with I/O speed?

Chapter 6

Fun programs

Let's be honest—the examples in most programming books are pretty boring. Devising efficient sorting algorithms may be of academic interest, but these programs are pretty far from the science that most of us do. But the only way to get good at programming is to write lots of programs. It doesn't really matter what they do, as long as they do *something*. So to help us stay motivated, this chapter contains examples of programs that are fun to write and fun to run.

6.1 Tic-tac-toe

> *...nearly all the people I take down there have precisely the same response to the prospect of playing ticktacktoe with a chicken. After looking the situation over, they say, 'The chicken gets to go first!'*
>
> *'But she's a chicken,' I say. 'You're a human being. Surely there should be some advantage in that.'*
>
> *Some of my guests, I always report with some embarrassment, don't stop there. Some of them say, 'The chicken plays every day. I haven't played in years.'*
>
> Calvin Trillin, The New Yorker, Feb. 8, 1999

As a goal for some of our F90 programming exercises, we are going to write a program to play tic-tac-toe. Although tic-tac-toe is a fully solved game in the sense that it is well known that a draw always results if both players play optimally (indeed even chickens have been trained to play the game), it is of sufficient complexity that writing a working program may seem a daunting task to the beginning programmer.

As is usually the case, however, the problem can be made more tractable by splitting the task up into smaller pieces.

Let us consider how we are going to approach this problem. Clearly we will need a way to store the current state of the board (who has moved where), some kind of flag for who is x and who is oh, some kind of flag for who goes first, etc. We will also need a way to display the board and to input moves from the human player.

There are obviously many, many different ways to write this program. However, to make sure that our programs will readily be able to play each other, it will be good to agree on some standardization of the different components.

First, let us assume that the spaces on the board are defined by the numbers 1-9, e.g.,

```
 1 | 2 | 3
---+---+---
 4 | 5 | 6
---+---+---
 7 | 8 | 9
```

Thus, when the program asks the human for a move, the human will enter a number from 1 to 9. For convenience, let's use the same convention for storing the moves within the program. Define an array called board that will store the moves that have been made:

```
integer, dimension(9) :: board
```

Now, let us specify that board will have the value 0 if the space is still open, 1 if the human has moved in the space, and 2 if the computer has moved in the space. Obviously there are other choices that we could have made for this (1 for x, 2 for oh; 1 for 1st player, 2 for 2nd player), but this makes the most sense to me because the human vs. computer difference is fundamental to the program. x vs. oh is simply a naming convention; 1st vs. 2nd will simply determine where the program starts.

Let us begin by writing an external subroutine that will print to the screen the current state of the board. We will need to input to the subroutine the board variable and a variable to define which player is x in the game. In other words, this subroutine might have the form:

```
subroutine printboard(board, playerx)
```

We assume that playerx = 1 if the human is x, playerx = 2 if the computer is x.

ASSIGNMENT TTT1

Write the external subroutine printboard, together with a test main program to check if it is working properly. Here are some examples:

```
board = (/ 1, 2, 1,   &
           0, 2, 0,   &
           0, 0, 0 /)
playerx = 1
```

printboard should produce something like:

```
 x | o | x
---+---+---
   | o |
---+---+---
   |   |
```

```
board = (/ 0, 0, 0,   &
           0, 2, 1,   &
           0, 0, 2 /)
playerx = 2
```

printboard should produce something like:

```
   |   |
---+---+---
   | x | o
---+---+---
   |   | x
```

Note that in these examples *board* is a 1-D array with nine elements. The '&' line continuation characters are used only to make the mapping to the 3x3 board more obvious. Make sure that you do not change any of the values in the *board* array or that of *playerx*. You only want to print out the current state of the board.

Note: Print out the state of the board within the printboard subroutine, not the main program. You only need to pass the board array and the integer variable playerx to the subroutine. Do not pass any values back to the main program.

Hint: Define a character array cboard(9) within your subroutine, the elements of which you set to ' ', 'x', or 'o', depending upon the contents of board and playerx. Then write a series of print statments to do the actual output.

Next, our program will need some way to determine if a proposed move is a valid move, i.e., if there is currently a blank space in the move location. To implement this, let us write a function of the form:

```
integer function checkmove(board, move)
```

which will return 1 if the move is valid, 0 otherwise. Note that board is the array defined above and move is the proposed move.

ASSIGNMENT TTT2

Write the function checkmove, together with a test main program to check if it is working properly. To make the function robust, return zero if move is outside of the range 1 to 9. Make sure you do not change any of the values in the *board* array or of the *move* variable. Also, do NOT print out anything within this function to warn of an invalid move. We may want to use this function for multiple purposes in the program and we don't necssarily want it to print anything out. If a warning is necessary, the calling program can print out the message.

Next, we need a function that will prompt the human for a move. It should check to see if the move is valid and prompt the human again in the cases of invalid moves. Let's call this function readmove:

```
integer function readmove(board)
```

which will return a valid move as entered by the keyboard.

ASSIGNMENT TTT3

Write the external function readmove, together with a test main program to check if it is working properly. The function should ask the user to enter a move, then use the checkmove function to check whether it is valid. If it is valid, return the move to the main program. If it is invalid, then alert the user and prompt again for a valid move. Repeat until a valid move is entered. IMPORTANT: Do not change the *board* array within the readmove function. That should be done later in the main program.

Next, we need a function to determine if there is a current winner (3 in a row)

or if the game is drawn (all spaces filled, no winner). This function will have the form:

```
integer function checkwinner(board)
```

and will return 1 if player 1 has won, 2 if player 2 has won, 3 if the game is drawn, and 0 otherwise.

ASSIGNMENT TTT4

Write the external function checkwinner, together with a test program to check if it is working properly. Make sure you do not change the *board* array.

Hint: Define an 2-D integer array that stores the locations of the eight possible ways to win, e.g.,

```
integer, dimension(8,3) :: win
win(1,1:3) = (/ 1, 2, 3 /)
win(2,1:3) = (/ 4, 5, 6 /)
win(3,1:3) = (/ 7, 8, 9 /)
win(4,1:3) = (/ 1, 4, 7 /)
.
.
etc.
```

Then loop over these 8 possibilities and check to see if the 3 board values are all ones or all twos. If there is no winner, then check to see if all board locations are full (the draw criteria).

The most challenging part of your TTT program will be determining the best move for the computer to make. We will implement this as a function:

```
integer function findmove(board)
```

which will return the "best" move for the computer (player 2) to make. Testing this function will be easiest once the complete program is finished. To complete the program, however, one needs a working version of findmove. To get around this problem, let's write findmove in two stages. First, let's write a very stupid version that will simply return a valid move. Then, after we have the complete program working, we can make improvements to findmove.

ASSIGNMENT TTT5

Write a working version of findmove, together with a test main program to check if it is working properly. Important: Do NOT change the *board* array within the function; that should be done only within the main program. Your function should not use any arguments other than *board*, that is *playerx* is not needed and should not be used, nor should your findmove function need to know who is going first. Of course, you can figure out if you are making the first move within find move simply by checking to see if the board is empty. Hint: Just loop through the moves 1 to 9 until you find an empty space (board(i) = 0). For a slightly more interesting "stupid" program, pick a random valid move.

Now we are ready to put these pieces together into a main program that will actually play the game. This program should ask the user if he/she wants to go first and if he/she wants x or oh (the latter is the playerx flag in the printboard function). The board array should be initialized to zero. For each move, the program will have to determine whose move it is (a function of the move number and who went first) and then either prompt the user or use the findmove function to pick a move. Following the move, the program should check for a win or draw. If there is a win or draw, a suitable message should be printed and the program stopped. If there is not a winner/draw, then the program should continue with the next move.

ASSIGNMENT TTT6

Construct a working version of the complete tic-tac-toe program.

Finally, we will want to improve on our initial findmove function to make the program smarter. An obvious strategy for this is to first check to see if any winning moves are possible. If not, then next check to see if there is a winning move for the human that should be blocked. Beyond this, you're on your own!

Hint: Use your checkwinner function to implement these strategies. Make a copy of the board array within findmove (e.g., board2 = board, where board2 is also a 9 vector). Loop over i values from 1 to 9 and for each blank square (i.e., board(i) = 0), try setting board2(i) = 2 and then use your checkwinner function to see if the computer has won (or in the later test, to see if the human can win by setting board2(i) = 1). Be sure to always reset board2 back to board before trying each new move.

ASSIGNMENT TTT7

Refine your program to incorporate a smart findmove function. Send me the complete program, including all functions in an e-mail. I will check the operation of your program and also attempt to have the programs play each other. To facilitate the latter goal, please give your findmove function the name:

```
function findmove_lastname(board)
```

where lastname is your last name. This will make it easier for me to test your routines all at once. Please only include 'board' in the argument list to findmove—this function should not need to know who is 'X' or who went first. Please also make sure that you do not modify the board array within findmove. If you use the checkwinner function (recommended), make sure that it is the standard version discussed in the notes. Also, please be aware that I will use your findmove functions for more than one game within the same main program run, so make sure that there are not move counters or other parameters that are not reset appropriately for new games.

6.2 Fractals

Generating beautiful images of fractals, such as the Mandelbrot set, is surprisingly easy on the computer and provides good practice in using complex numbers. The basic idea behind most fractal calculations is that there are certain complex functions that, when computed over and over again, will either diverge or remain bounded. Whether or not they diverge turns out to be extremely sensitive to small changes in the initial complex value that starts the calculation, at least in certain regions of the complex plane.

The most famous of all fractal images is the Mandelbrot set. To generate the Mandelbrot set, we begin by considering a complex number, c. We then apply the following algorithm:

```
set z = 0 to start

then repeatedly compute z = z*z + c

until |z| > 2 OR the number of iterations exceeds some threshold

then output the number of iterations
```

For example, if c = 0.3 + 0.3i then

```
1st iteration:  z =  0.30 + 0.30i    |z| = 0.42
2nd iteration:  z =  0.30 + 0.48i    |z| = 0.57
3rd iteration:  z =  0.16 + 0.59i    |z| = 0.61
4th iteration:  z = -0.02 + 0.49i    |z| = 0.49
```

In this case, z will remain bounded even after an infinite number of iterations. However, if c = 0.5 + 1.0i then

```
1st iteration:  z =  0.50 + 1.00i    |z| =  1.1
2nd iteration:  z = -0.25 + 2.00i    |z| =  2.0
3rd iteration:  z = -3.44 + 0.00i    |z| =  3.4
4th iteration:  z = 12.32 + 1.00i    |z| = 12.4
5th iteration:  z = 151.19 + 25.63i  |z| = 153.4
```

and the size of z explodes toward infinite values. By the 10th iteration it will exceed the floating point range of most computers. However, we can stop computing z once its absolute value (the complex absolute value or modulus is defined as the distance of a point in the complex plane from the origin, i.e. $|z| = \text{abs}(a+bi) = \text{sqrt}(a^2+b^2)$ exceeds 2 because it can be shown that divergence is guaranteed at this point.

We repeat this calulation for a series of different values of c and plot the resulting output as a function of the location of c on the complex plane. The Mandelbrot set is the set of all complex numbers c for which the size of $z^2 + c$ is finite even after an infinite number of iterations. We may obtain a good approximation, however, by checking after some large number of iterations (1000 is a common choice). We also may take advantage of the fact that it is known that $z^2 + c$ will diverge whenever $|z| > 2$.

Here is an example F90 program that performs this calculation for user-specified parts of the complex plane and outputs a binary file that can be read and plotted using MatLab or Python:

```
program mandel
   implicit none
   real, dimension(:), allocatable :: dat
   real :: x1, x2, y1, y2, dx, dy, cr, ci
   integer :: nx, ny, ix, iy, it, idat, ndat, nbytes, status
   integer, dimension(2) :: nxny
   complex :: c, z, z2
   real, dimension(4) :: wind

   print *, 'Enter x1, x2, y1, y2, nx, ny'
   read *, x1, x2, y1, y2, nx, ny
```

```
   dx = (x2 - x1) / real(nx)
   dy = (y2 - y1) / real(ny)

   allocate(dat(nx*ny))

   idat=0
   do ix = 1, nx
      do iy = 1, ny
         cr = x1 + dx/2. + dx*real(ix-1)
         ci = y1 + dy/2. + dy*real(iy-1)
         c = cmplx(cr, ci)
         z = cmplx(0.0, 0.0)
         do it = 1, 1000
            z = c + z*z
            if (cabs(z) > 2) exit
         enddo
         idat = idat + 1
         dat(idat) = it
      enddo
   enddo
   print *, 'Finished calculation'
   ndat = idat
   print *, 'ndat = ',ndat

   open (12, file='fractal.bin', form='unformatted')
   nxny(1) = nx
   nxny(2) = ny
   write (12) nxny
   wind(1) = x1
   wind(2) = x2
   wind(3) = y1
   wind(4) = y2
   write (12) wind
   write (12) dat
   close (12)

end program mandel
```

The program computes the result for a grid of points in the complex plane, defined by the user-defined limits x1 and x2 for the real part and y1 and y2 for the complex part. The number of points computed in x and y are input as nx and ny. This will determine the resolution of the plot. For example, nx=50 and ny=50 will result in an image 50 pixels wide by 50 pixels tall. Although the image is really two-dimensional, I store the results in the 1-D array, dat, because this simplies the output of the results. Notice how allocate is used to set dat to dimension(nx*ny) on the fly.

The spacing in x and y are defined by:

```
dx = (x2 - x1) / real(nx)
dy = (y2 - y1) / real(ny)
```

Note the conversion of the integer variables nx and ny to floats prior to performing the division.

Here are the main loops that actually do the calculation:

```
idat=0
do ix = 1, nx
   do iy = 1, ny
      cr = x1 + dx/2. + dx*real(ix-1)
      ci = y1 + dy/2. + dy*real(iy-1)
      c = cmplx(cr, ci)
      z = cmplx(0.0, 0.0)
      do it = 1, 1000
         z = c + z*z
         if (cabs(z) > 2) exit
      enddo
      idat = idat + 1
      dat(idat) = it
   enddo
enddo
```

The real and imaginary parts of c are set to the center of the "pixel" with sides dx and dy. The calculation is done for a maximum of 1000 iterations. The calculation is halted if $|z| > 2$ by exiting the for loop. The iteration number is saved in the dat array, using idat as a counter.

The next step is to save this information to a file. For speed in the case of a large dat array, we use a binary file. We create and open the file with

```
open (12, file='fractal.bin', form='unformatted')
```

We use form='unformatted' to specify that this is a binary file, not an ascii file.

Before writing the dat array to the file, we write some header information that will help MatLab or Python to know the size of the array and the values of x1, x2, y1, and y2. Writing to a binary file in Fortran is done using the write statement without a format. We set up the 2-element int array, nxny, to handle the output of nx and ny:

```
nxny(1) = nx
nxny(2) = ny
write (12) nxny
```

and we set up a 4-element float array, wind, to handle the output of x1, etc.

```
wind(1) = x1
wind(2) = x2
wind(3) = y1
wind(4) = y2
write (12) wind
```

Finally, we write the output array to the file

```
write (2) dat
```

For this program, it is a good idea to compile with the -O compiler option to make it run faster:

```
gfortran -O mandel.f90 -o mandel
```

The Mandelbrot set is approximated in our program by places on the complex plane where the output value (contained in the dat array) is 1000, i.e., the z function has not diverged even after 1000 iterations. Output values less than 1000 provide a message of how quickly the function diverges (small values indicate rapid divergence, larger values indicate slower divergence). Plots of the output usually use colors to indicate the different output values.

6.2.1 Plotting using MatLab

Here is how to plot our output using Matlab:

```
clf reset
clear
[fid, message] = fopen('fractal.bin')

% Fortran I/O has extra four bytes at beginning and end of writes
[dum, count] = fread(fid, [1], 'int');
[size, count] = fread(fid, [2], 'int');
[dum, count] = fread(fid, [1], 'int');

nx = size(1)
ny = size(2)

[dum, count] = fread(fid, [1], 'int');
[wind, count] = fread(fid, [4], 'float')
[dum, count] = fread(fid, [1], 'int');

x1 = wind(1)
```

```
x2 = wind(2)
y1 = wind(3)
y2 = wind(4)

[dum, count] = fread(fid, [1], 'int');
[z, count] = fread(fid, [nx,ny], 'float');
fclose(fid);

z2 = log10(z);
axis( [x1, x2, y1, y2] ); axis('square'); hold on;
imagesc( [x1, x2], [y1, y2], z2 );
colorbar;
```

One important detail is that Fortran (unlike C) writes an extra 4 bytes before and after each of the binary writes. So we need to read these extra btyes with our Matlab script into a dummy variable or we will not be properly aligned with the data fields.

We set the output array to z and use imagesc to plot the result using the default color scheme. We plot log(z) rather than z because it shows some of the details a little better.

6.2.2 Plotting using Python

Here is one way to plot our output using Python, a script called plotfractal.py

```
#! /usr/bin/env python
import numpy as np
from scipy.io import FortranFile
import matplotlib
matplotlib.use("TkAgg")
import pylab

# Open the Fortran unformatted binary
f = FortranFile('fractal.bin', 'r')

# Read the contents from fractal.bin in the order that they were written
# Read nx, ny
[nx, ny] = f.read_ints(np.int32)
print 'nx, ny = ', nx, ny
# Read wind
wind = f.read_record('float32')
x1 = wind[0]
x2 = wind[1]
y1 = wind[2]
y2 = wind[3]
print 'x1,x2,y1,y2 =', x1, x2, y1, y2
# Read dat, then reshape into a 2D array Z for plotting (need to do transpose)
```

```
dat = f.read_record('float32')
Z = np.transpose(dat.reshape(nx,ny))

# Construct the x and y vectors for plotting
dx = (x2 - x1)/nx
dy = (y2 - y1)/ny
x = np.arange(x1 + dx/2., x2, dx)
y = np.arange(y1 + dy/2., y2, dy)

# plot
pylab.pcolormesh(x,y,np.log10(Z),cmap='jet')
pylab.xlabel('x', fontsize=16)
pylab.ylabel('y', fontsize=16)
pylab.colorbar()
pylab.show()
```

I got this script from Robin Matoza at UCSB and it works more cleanly than an older Python script I had kludged together. It takes advantage of the scipy.io.FortranFile method for reading Fortran unformatted binary files (see https://docs.scipy.org/doc/scipy-0.16.0/reference/generated/scipy.io.FortranFile.html) This has the advantage that it knows about the extra 4 bytes that Fortran puts before and after every binary-write, so we do not need to explicitly read these, as we did in the Matlab script above.

Most of the script should be self-explanatory. Note how we read in the wind array and then assign the plot limits:

```
wind = f.read_record('float32')
x1 = wind[0]
x2 = wind[1]
y1 = wind[2]
y2 = wind[3]
```

We read in the big vector containing the data for the image and then reshape it into the correct matrix form for plotting:

```
dat = f.read_record('float32')
Z = np.transpose(dat.reshape(nx,ny))
```

Next, we compute dx and dy and set up the x and y vectors for plotting:

```
dx = (x2 - x1)/nx
dy = (y2 - y1)/ny
x = np.arange(x1 + dx/2., x2, dx)
y = np.arange(y1 + dy/2., y2, dy)
```

Note that the last value of x will be x2 - dx/2.

The plot looks nicer if we take the log before plotting. The 'jet' color scheme is a good choice.

```
pylab.pcolormesh(x,y,np.log10(Z),cmap='jet')
```

It's fun to explore the effect of different color maps in Python. Here is a site that shows lots of them: http://www.scipy.org/Cookbook/Matplotlib/Show_colormaps

6.2.3 Good targets and more about fractals

The entire Mandelbrot set may be imaged in the window

```
real -2 to 0.5, imag -1.25 to 1.25  (i.e., -2, 0.5, -1.25, 1.25)
```

It is also fun to zoom in on details of the image. Here are some suggestions for places to look:

```
-0.95 -0.90 0.25 0.30
-0.75 -0.65 0.25 0.35
-0.73 -0.72 0.282 0.292
-0.703 -0.693 0.26 0.27
```

Further details about generating fractals may be found in a series of articles by A.K. Dewdney in the Computer Recreations section that used to appear in Scientific American. The August 1985 article describes the Mandelbrot set, the November 1987 article talks about the related Julia sets, and the July 1989 article is about fractals called "biomorphs" that look like little creatures. There are also lots of books on fractals that have many beautiful images.

The study of fractals is related to chaos theory and the fact that in physical systems (weather is one example) are inherently unpredictable on large time scales because small perturbations to the starting conditions will cause large changes over time.

ASSIGNMENT FRAC1

Rewrite the mandel.c and plotfractal.m (or plotfractal.py) programs to plot examples of the Julia sets and the biomorphs. You will want to first read the appropriate Scientific American articles.

1. Produce PDF files of 3 especially nice images of Julia sets.

2. Reproduce and make images of as many of the biomorphs as you can that are shown on p. 110 of the biomorph article.

Part (2) is harder because you will have to generate more complicated complex functions than those that are used for the Mandelbrot and Julia sets. You may have to consult a book on complex numbers to find suitable formulae to compute $\sin(z)$, z^z, etc.

Please e-mail me the PDF files and copies of your F90 and Matlab or Python source code.

Have fun!

6.3 Fun with spectra

Computing Fourier transforms using the Fast Fourier Transform (FFT) algorithm is a standard tool in geophysical analysis. There are many books and articles on Fourier theory and how the FFT works. I am distributing the part of Numerical Recipes that discusses this, which seems as good a treatment as any. You will certainly learn much more about this if you take our Data Analysis class.

For brevity in this class I am simply going to focus on what you need to know to use an FFT program and leave the theory for you to pick up elsewhere.

We start with a "time series," which is a series of measurements that are made at some regular interval. These measurements are normally stored on the computer in an array. We also need to know the sample interval (the time between sample points, the reciprocal of the digitization rate) and the number of points in the time series. In most cases the time series consists of real (i.e., not complex) numbers and we will assume this is true for the examples shown.

The purpose of the FFT is to examine the different frequency waves that may be present in the data. The FFT is a linear transformation that allows us to look at the data in the "frequency domain" rather than the "time domain" of the original data. In fact, the original time series can be expressed exactly as a sum of harmonic waves of different frequency content and phase. The FFT allows us to readily compute what the frequencies and phases of these waves are.

The simplest FFT algorithms require that the number of points in the original time series be a power of two. We will assume that this is true here, but you should be aware that alternative FFT methods exist for non-powers of two.

Thus, the input to a typical FFT algorithm will consist of an array of data values, the number of time points (n), and the sample interval (dt). For a real time series, the FFT algorithm will then return a complex spectra that will give the amplitude

and phase at a series of equally spaced frequency points. There will be $n/2 + 1$ frequency points and the frequency spacing will be $df = 1/(n * dt)$.

The first frequency point is at $f = 0.0$

The last frequency point is at $f = 1/(2 * dt)$ and is called the Nyquist frequency.

The Nyquist frequency is the highest frequency that one can resolve in the time series. At the Nyquist frequency, there are two data points in the time series per wavelength. If higher frequencies are present in the data, they will be "aliased" so that they are seen at lower frequencies. From the time series alone, there is no way to discriminate between correctly resolved frequencies and aliased data from higher frequencies. Thus, sometimes filters (anti-aliasing filters) are applied to the data prior to digitization to remove the frequencies above the Nyquist so that this will not be a problem.

The FFT algorithm provides the spectra at $n/2+1$ frequency points which may be represented as $n/2 + 1$ complex numbers. (complex numbers are necessary to represent both the amplitude and phase of each harmonic component).

"Wait a minute," the alert reader might cry. We started with n real points in the time domain and now we have $n + 2$ real points in the frequency domain, if we count each complex number as two reals. Have we gained information compared to the original time series? The resolution to this apparent problem comes from the fact that the first and last frequency points always have zero imaginary parts. Thus the total number of independent data points is the same in both the time and frequency domains. In fact, most FFT algorithms return only $n/2$ frequency points by packing the real part of the Nyquist point into the imaginary part of the zero frequency point.

Once we have the frequency domain points we can make an amplitude spectra plot by plotting the absolute values (Cabs function) of the points versus frequency. If we want a power spectrum, then we square the amplitudes. Getting the correct units on the y-axis can be a tricky business (let's save that discussion until your time series analysis class); in many cases, however, we are only interested in the position of the peaks or the shape of the spectrum so we don't need to worry about this.

We can also transform back to the time domain by computing an inverse FFT. If your code is working correctly, you should get back exactly the same time series as you started with.

Here is a set of routines, adopted from those in Numerical Recipes to do both forward and inverse FFTs.

```
! GETSPEC_NR computes the spectrum of a real time series using
! Numerical Recipes FFT routines
!
! Requires:  TAPER, REALFT, FOUR1
!
! Inputs:  ts  =  input time series with values from ts(1) to ts(ntime)
!         ntime = number of time points (int)
!         dt = sample interval (s) (float)
!         itap = 1 to apply Hann taper before computing sprectrum
!              = 0 otherwise
! Returns: spec = complex spectrum
!         nfreq = number of complex frequency points (int, = 1+ntime/2)
!         df = frequency spacing
!
!  spec(1)  =  value at zero frequency
!  spec(nfreq)  =  value at freq. of (nfreq-1)*df (Nyquist frequency)
!
!  (November, 2002, Peter Shearer)
!
subroutine GETSPEC_NR(ts, ntime, dt, itap, spec, nfreq, df)
   implicit none
   real, dimension(*) :: ts
   real, dimension(ntime) :: a
   complex, dimension(*) :: spec
   real :: dt, df
   integer :: ntime, itap, nfreq, i

   if (itap == 1) then
      call TAPER(ts, ntime, a)
   else
      do i = 1, ntime
         a(i) = ts(i)
      enddo
   end if

  call REALFT(a, ntime/2, 1)

   nfreq = 1 + ntime/2
   df = 1./(dt*float(ntime))

   spec(1) = cmplx(a(1), 0.)
   spec(nfreq) = cmplx(a(2), 0.)
   do i = 2, nfreq-1
      spec(i) = cmplx(a(2*i-1), a(2*i))
   enddo

end subroutine GETSPEC_NR
```

```
! GETTS_NR computes a real time series from a complex spectrum
! (stored as in GETSPEC_NR) using Numerical Recipes FFT routines
!
! Requires:  REALFT, FOUR1
!
! Inputs:  spec = complex spectrum stored as floats
!         nfreq = number of complex frequency points (int, = 1+ntime/2)
!         df = frequency spacing
!
! Returns: ts  =  input time series with values from ts(1) to ts(ntime)
!         ntime = number of time points (int)
!         dt = sample interval (s) (float)
!
!  spec(1)  =  value at zero frequency
!  spec(nfreq)  =  value at freq. of (nfreq-1)*df (Nyquist frequency)
!
!  (November, 2002, Peter Shearer)
!
subroutine GETTS_NR(spec, nfreq, df, ts, ntime, dt)
   real, dimension(*) :: ts
   real, dimension(ntime+2) :: a
   complex, dimension(*) :: spec
   real :: df, dt, scale
   integer :: nfreq, ntime, n, isign, i

   ntime = (nfreq-1)*2
   dt = 1./(df*float(ntime))
   scale = 2.0/float(ntime)

   a(1) = real(spec(1))*scale
   a(2) = real(spec(nfreq))*scale

   do i = 2, nfreq-1
      a(2*i-1) = real(spec(i))*scale
      a(2*i) = aimag(spec(i))*scale
   enddo

   call REALFT(a, ntime/2, -1)

   do i = 1, ntime
      ts(i) = a(i)
   enddo

end subroutine GETTS_NR


! TAPER multiplies ts1 for Hann taper and puts result in ts2
!
subroutine TAPER(ts1, n, ts2)
```

```
   implicit none
   real, dimension(n) :: ts1, ts2
   real :: pihalf, tsmid, frac, angle, tap
   integer :: n, i, i2
   pihalf = 3.1415927/2.
   i2 = n/2 +1
   tsmid = float(n)/2. + 0.5
   do i = 1, i2
      frac = float(i)/tsmid
      angle = pihalf*frac
      tap = sin(angle)**2
      ts2(i) = ts1(i)*tap
      ts2(n+1-i) = ts1(n+1-i)*tap
   enddo
end subroutine TAPER


      SUBROUTINE REALFT(DATA,N,ISIGN)
      REAL*8 WR,WI,WPR,WPI,WTEMP,THETA
      DIMENSION DATA(*)
      THETA=6.28318530717959D0/2.0D0/DBLE(N)
      C1=0.5
      IF (ISIGN.EQ.1) THEN
        C2=-0.5
        CALL FOUR1(DATA,N,+1)
      ELSE
        C2=0.5
        THETA=-THETA
      ENDIF
      WPR=-2.0D0*DSIN(0.5D0*THETA)**2
      WPI=DSIN(THETA)
      WR=1.0D0+WPR
      WI=WPI
      N2P3=2*N+3
      DO 11 I=2,N/2+1
        I1=2*I-1
        I2=I1+1
        I3=N2P3-I2
        I4=I3+1
        WRS=SNGL(WR)
        WIS=SNGL(WI)
        H1R=C1*(DATA(I1)+DATA(I3))
        H1I=C1*(DATA(I2)-DATA(I4))
        H2R=-C2*(DATA(I2)+DATA(I4))
        H2I=C2*(DATA(I1)-DATA(I3))
        DATA(I1)=H1R+WRS*H2R-WIS*H2I
        DATA(I2)=H1I+WRS*H2I+WIS*H2R
        DATA(I3)=H1R-WRS*H2R+WIS*H2I
        DATA(I4)=-H1I+WRS*H2I+WIS*H2R
        WTEMP=WR
        WR=WR*WPR-WI*WPI+WR
```

```
        WI=WI*WPR+WTEMP*WPI+WI
11    CONTINUE
      IF (ISIGN.EQ.1) THEN
        H1R=DATA(1)
        DATA(1)=H1R+DATA(2)
        DATA(2)=H1R-DATA(2)
      ELSE
        H1R=DATA(1)
        DATA(1)=C1*(H1R+DATA(2))
        DATA(2)=C1*(H1R-DATA(2))
        CALL FOUR1(DATA,N,-1)
      ENDIF
      RETURN
      END


      SUBROUTINE FOUR1(DATA,NN,ISIGN)
      REAL*8 WR,WI,WPR,WPI,WTEMP,THETA
      DIMENSION DATA(*)
      N=2*NN
      J=1
      DO 11 I=1,N,2
        IF(J.GT.I)THEN
          TEMPR=DATA(J)
          TEMPI=DATA(J+1)
          DATA(J)=DATA(I)
          DATA(J+1)=DATA(I+1)
          DATA(I)=TEMPR
          DATA(I+1)=TEMPI
        ENDIF
        M=N/2
1       IF ((M.GE.2).AND.(J.GT.M)) THEN
          J=J-M
          M=M/2
        GO TO 1
        ENDIF
        J=J+M
11    CONTINUE
      MMAX=2
2     IF (N.GT.MMAX) THEN
        ISTEP=2*MMAX
        THETA=6.28318530717959D0/(ISIGN*MMAX)
        WPR=-2.D0*DSIN(0.5D0*THETA)**2
        WPI=DSIN(THETA)
        WR=1.D0
        WI=0.D0
        DO 13 M=1,MMAX,2
          DO 12 I=M,N,ISTEP
            J=I+MMAX
            TEMPR=SNGL(WR)*DATA(J)-SNGL(WI)*DATA(J+1)
            TEMPI=SNGL(WR)*DATA(J+1)+SNGL(WI)*DATA(J)
```

```
            DATA(J)=DATA(I)-TEMPR
            DATA(J+1)=DATA(I+1)-TEMPI
            DATA(I)=DATA(I)+TEMPR
            DATA(I+1)=DATA(I+1)+TEMPI
12        CONTINUE
          WTEMP=WR
          WR=WR*WPR-WI*WPI+WR
          WI=WI*WPR+WTEMP*WPI+WI
13      CONTINUE
        MMAX=ISTEP
      GO TO 2
      ENDIF
      RETURN
      END
```

GETSPEC_NR, GETTS_NR and TAPER are my own inventions; REALFT and FOUR1 are from Numerical Recipes. Hopefully the documentation for GETSPEC_NR and GETTS_NR is self-explanatory.

The GETSPEC_NR function includes an option to multiply the time series by a cos**2 function (i.e., Hanning taper) before computing the FFT. This generally improves the appearence of the spectrum and avoids artifacts that may result from the abrupt truncation of the time series at the end of the data window.

A typical call to GETSPECNR would have the form:

```
call GETSPEC_NR(a, n, dt, itap, b, nfreq, df)
```

where a is the data array. You should define the sizes of a and b in the calling program as, for example:

```
integer, parameter :: maxpts = 8192
real, dimension(maxpts) :: a
complex, dimension(maxpts/2+1) :: b
```

WARNING: The routines do not check if n is a power of two. This would be a useful improvement to make the routines more robust with respect to user errors in the calling program.

6.3.1 Guitar string example

A properly tuned guitar will have strings with fundamental mode frequencies as follows: E = 82 Hz, A = 110 Hz, D = 147 Hz, G = 196 Hz, B = 247 Hz, E = 330 Hz.

There will be overtones (harmonics) at frequencies of $n*f0$ where $f0$ is the fundamental (lowest) frequency. Thus, for the A string, we should expect to see peaks at 110 Hz, 220 Hz, 330 Hz, 440 Hz, etc. The relative power between the different harmonics is what determines the tone of the guitar.

Unfortunately, the MacCRO program mentioned in the next paragraph does not seem to work/exist for modern Macs. Until I find a suitable replacement program, I will just have to use some files that I previously digitized.

The shareware program MacCRO (http://pderrin.cjb.net/ maccro.html) uses the audio input on the Mac to simulate an oscilloscope. For our purposes, its most useful feature is the ability to download digitized sounds to a file. For a class demo, my plan is to use the program to digitize the sound of the A string, save the result to a file, and then bring the file over to the Sun where it can be FFTed and the resulting spectrum plotted.

If we have time, it will be interesting to compare:

(1) string plucked near center vs. near one end

(2) sound sampled just after pluck vs. a few seconds later

(3) cheap vs. expensive guitar ————————————————————————-

Assuming we have a digitized ascii time series file (one point per line) with a header line for the sample rate, here is a program to read the data, compute the FFT, and output the spectrum:

```
! program to compute spectrum of MacCRO output file
program macfft
   implicit none
   integer, parameter :: maxpts = 8192
   real, dimension(maxpts) :: a, a2
   complex, dimension(maxpts/2+1) :: b
   real :: x, y, dt, df, samrat, samcount, freq, amp
   integer :: ios, i, j, idir, itap=0, n, nfreq, nn, menu
   character (len=100) :: infile, linebuf, outfile
   character (len=20) :: word1, word2

   print *, 'Enter input file name from MacCRO program'
   read *, infile
   open (11, file=infile, status='old')

   read (11, '(a)') linebuf
   print *, 'First line of file = ', linebuf
   read (11, *) word1, word2, samrat
   dt = 1.0/samrat
   print *, 'samrat, dt = ', samrat, dt
   read (11, *) word1, word2, samcount
```

```
   print *, 'samcount = ', samcount
   read (11, '(a)') linebuf

  do i = 1, 10000
      read (11, *, iostat=ios) x
      if (ios < 0) exit
      a(i) = x
   enddo
   n = i - 1
   print *, ' n= ',n
   do i = 1, 5
     print *, i, a(i)
   enddo

   print *, 'Enter desired power of two'
   read *, nn
   n = nn

   print *, 'Apply Hann taper?  (0) no,  (1) yes'
   read *, itap

   call GETSPEC_NR(a, n, dt, itap, b, nfreq, df)
   print *, 'nfreq, df = ', nfreq, df

   print *, 'Output spectrum to:  (1) screen  or  (2) file'
   read *, menu
   if (menu.eq.2) then
      print *, 'Enter file name'
      read *, outfile
      open (12, file=outfile)
   end if

   do i = 1, nfreq
      freq = float(i-1)*df
      amp = cabs(b(i))
      if (menu == 1) then
         print '(4f10.4)', freq, amp, real(b(i)), aimag(b(i))
      else
         write (12, '(4f10.4)') freq, amp, real(b(i)), aimag(b(i))
      end if
   enddo

end program macfft
```

We can then plot the spectrum using plotxy or another plotting program. In the case of the guitar string, the fundamental frequency will be the lowest frequency peak in the spectrum and the harmonics will be evenly spaced peaks in frequency going to higher frequencies. By plucking the string in different places, it is possible to excite the harmonics more than the fundamental mode.

6.3.2 ASSIGNMENT FFT1

Get the file bfo1 from the class website. This is a time series of the 1994 deep Bolivian earthquake as recorded at Black Forest Observatory, Germany (48.3319N,8.3311E). The sample interval is 40 s and there are 24225 points in the file, representing over 11 days of data. The sensor is vertical in orientation so primarily spheroidal modes are recorded.

(a) Plot the time series using whatever plotting program you want. Label the x-axis in units of hours.

(b) Write a F90 program to read the data and compute the spectrum, both with and without first applying a Hann taper.

(c) Make nice plots of the spectra that compare the results with and without the Hann taper. Label the x-axis in units of mHz. Make plots that go from zero to the Nyquist frequency and also some closeups from zero to 2 mHz.

(d) Using Table V from the PREM paper (Dziewonski and Anderson, PEPI 25, 297-356, 1981, see me if you want to make a copy), identify and label as many of the peaks below 2 mHz as you can.

NOTE: 24225 is not a power of two. You have two choices. You can either truncate the time series at 2**14=16384 or pad the time series with zeros to 2**15=32768. In the latter case, make sure you apply the taper to the 24225-point series and THEN pad with zeros (i.e., you can't just use the taper option in getspec).