

12.010 Computational Methods of Scientific Programming

Lecturers
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Review of last lecture

- Start examining the FORTRAN language
- Development of the language
- “Philosophy” of language: Why is FORTRAN still used (other than you can’t teach an old dog new tricks)
- Basic structure of its commands
- Communications inside a program and with users
- This lecture will go into commands in more detail
- There are many books on Fortran and an on-line reference manual at:
http://www.fortran.com/fortran/F77_std/rjcnf0001.html

Today's Class

- Fortran Details
 - Subroutines and functions
 - Intrinsic routine (e.g., sin, cosine)
 - Constants and variables (plus example)
 - Input/Output
 - Open and close statements
 - Read and write statements
 - Formats
 - Character strings

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Subroutines (declaration)

- Subroutine name(list of variables)
- Invoked with
 - Call name(same list of variable types)

- Example:
 - Subroutine sub1(i,value)
 - Integer*4 I
 - Real*8 value

In main program or another subroutine/function:

```
integer*4 j
Real*8 sum
Call sub1(j, sum)
```

Note: Names of variable do not need to match, just the type needs to match, although it is good practice to do so if possible

Variables used in subroutines (and functions) are in general are lost after the subroutine completes execution. Use the "Save" command if variables values are to be remembered.

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Functions

Real*8 function func(list of variables)

- **Invoked with**

Result = func(same list of variable types)

- **Example**

Real*8 function eval(i,value)

Integer*4 i

Real*8 value

eval = i*value

In main program or subroutine or function

Real*8 result, eval

Integer*4 j

Real*8 sum

Result = eval(j,sum)

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Functions 02

- Functions can be of any of the variable types
- The last action of the function is to set its name to the final result
- The function type must be declared in the main program (looks like any other variable)
- There are other forms of the declaration. Often simply function is used and the type declared in the function.
- The function must always appear with the same name and type.
- Fortran has special functions called intrinsic which do not need to be declared.

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Intrinsic functions

- These functions are embedded in the language and often go by “generic names”
- Examples include sin, cos, tan, atan2. Precisely which functions are available depend on machine.
- Generic names means that the actual loaded code depends on the variable types used in the call (i.e., if real*8 argument is used in sin, then the real*8 version of the sin function is loaded).
- Link to standard intrinsic functions is provided on the lecture notes section
- Not all of the intrinsic listed on this page are available always. If not available: Get an undefined external message or undeclared variable when program compiled and linked.

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Variables and constants

- In Fortran variable names point to an address in memory and so most of the time when variables are passed only the address is passed. There is usually no check that information about the variable type between the modules.
- Character strings are treated differently since the string is defined not only by an address but also a length. Unlike Fortran arrays, inside a module you can tell the length of string passed (LEN intrinsic function). (Fortran90 does have features that allow the sizes of arrays to be determined: size, shape, lbound,ubound)
- Constants may be passed by address or by value. Passing by value is the more common technique now.
- Variable type Fortran Program

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IO: Read, write, open, close

- These are the main routines used to get data into and out of a program.

- Format of the read and write commands are:

Read(unit,format,<options>) list of variables

Write(unit,format,<options>) list of variables

Where unit is either:

A numeric number associated with a device or file. Set with an open statement

* which is generic for screen or keyboard

A character string (call internal reads and writes).

Format is a format statement defining how variables are read/written or a * for free-format.

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IO Open

- To open a unit number for IO you use the open command. Its basic format is

Open(unit=nnn,file=<string>, status=<status>,iostat=<ierr>,...)

Where nnn is a numeric value, e.g., 80

<string> is a string containing the file name. This can be a character variable or the name of the file contained in single quotes e.g., 'prog.dat'

<status> is a string with type options

'unknown' status unknown

'old' file should already exist

'new' file should not exist.

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IO Open continued 02

`<ierr>` is an integer*4 variable for the IO Status (IOSTAT) return. Most important here is that 0 return means the open was successful. Any non-zero return means an error occurred and the file is not open.

The specific numerical values for given types of errors depends on the machine.

The meaning of the numerical values can be found in the “runtime error” or “IOSTAT error” section of the manual for the fortran on your machine. (HP: 908 means file not found, g77 Linux: 2 means the same, Solaris: 1018).

- There are more options for direct access files (fixed length records), read-only, to append, binary files (unformatted)

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IO Close

- The close statement closes a unit number.

`Close(unit=<nnn>,iostat=<ierr>)`

Where `<nnn>` is the unit number, and `ierr` is IOSTAT error for the close.

- For both open and close, the `unit=` is not needed and the numeric value of the unit number of all that is needed.
- The unit number can be an integer*4 variable containing the unit number.
- In some cases, the default compilers require the unit number be less than 99.

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Open/close

- Some unit number are automatically opened when a program is executed.
- Unit 5 is for reading from keyboard
- Unit 6 is write to screen
- Unit 0 is often (but not always) the error output device.
- You should not close units 5 or 6
- Generically, * can be used in read and write for reading from keyboard and writing to screen. This is the preferred option.
- For reads and write to * or 5 or 6, the Unix IO redirect can be used (< file, > file, or | for piping.)

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Read/Write

- For read and write the most common <option> is IOSTAT=ierr which allows the IO error during read/write to be checked.
- If the IOSTAT= option is not included, and an error during reading or writing then your program will “core dump” or “abort”
- When the IOSTAT= option is included, it is your responsibility to check that the return is zero.
- The most common return is -1 mean End-of-file has been reached.
- Other options exist for reading specific records from direct access files

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FORMAT

- Allows the format of input or output to be specified.
- There are two ways to specify a format:
 - A numeric label can be given which refers to a labeled format statement
 - A character string containing the format can be given.
- The following two cases generate the same result.
Write(*,100) I
100 format(' The integer value is ',i4)
Form = (' The integer value is ',i4)
Write(*,form) I
- Note the use of single and double quotes

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FORMAT arguments

- The options in the format statements are:
 - Strings inside single or double quotes are written as is.
 - For numbers the generic type is <T><n>.<m>Where T is for type; I integer, F floating point notation, E exponential, L logical
<n> is total width of field
<m> is decimal places or leading zeros.
Examples: if 22.7 is written with:
F8.3 ^^ 22.700 (with spaces (^) 8 characters wide, 3 DP)
E11.3 ^^ 0.227E+02
For integer 10 I4.3 -> ^ 010 (The symbol ^ means space)

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FORMAT 02

- Character strings are output with the a format
A10 would write 10 characters, left justified (if the string to printed is longer than this it is truncated).
A without any numeric value following it will print the full declared length of the string.
- Other control characters are:
/ — carriage return, start a new line
Nx — print N spaces where N is integer
Enclosing part of the format in parentheses with with a numeric argument in front, repeated that parts of format N times, e.g., 20(I4,2x)

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Character strings

- Character strings are treated differently in Fortran than other variable types because an address and length is passed with the name.
- In side modules: Strings that are passed in can be declared as
Character*(*) <string name>
Where the second * says use the “passed length” of the string.
(Homework number 2 which will be due Oct 6 will use these concepts).

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Summary of Today's class

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 - Intrinsic routine (e.g., sin, cosine)
 - Constants and variables (plus example)
 - Input/Output
 - Open and close statements
 - Read and write statements
 - Formats
 - Character strings
- For the remainder of the class; examine, compile and run the poly_area.f and vars.f programs. Try modifications of these programs and see what happens.

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Exercises using FORTRAN

- In this exercise session we will write some simple FORTRAN programs:
 - Write a simple program that writes your name to the screen
 - Compile and load the poly_area.f program from the web page. Test the program to see how it works
 - Compile and load the vars.f routine from the web page. Test the following modifications to the program:
 - In the first call to var_sub_01, replace j with an integer constant and see what happens

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