AMath 483/583 — Lecture 7

This lecture:

- Python debugging demo
- Compiled langauges
- Introduction to Fortran 90 syntax
- Declaring variables, loops, booleans

Reading:

- class notes: Python debugging
- class notes: Python plotting
- class notes: Fortran
- class notes: Fortran Arrays

Notes:

Changes in uwhpsc repository

A new branch has been added to the uwhpsc repository on bitbucket.

The coursera branch will be used for modifications needed for the Coursera version.

Ignore this branch and stay on master.

Note that git fetch will also fetch history into origin/coursera

You want to:

```
$ git fetch origin
$ git branch   # make sure you are on master
$ git checkout master  # if you weren't
$ git merge origin/master
```


Notes:

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- class notes: Fortran
- class notes: Fortran Arrays

Notes:

Compiled vs. interpreted language

Not so much a feature of language syntax as of how language is converted into machine instructions.

Many languages use elements of both.

Interpreter:

- Takes commands one at a time, converts into machine code, and executes.
- Allows interactive programming at a shell prompt, as in Python or Matlab.
- Can't take advantage of optimizing over a entire program — does not know what instructions are coming next.
- Must translate each command while running the code, possibly many times over in a loop.

Notes:

Compiled language

The program must be written in 1 or more files (source code).

These files are input data for the compiler, which is a computer program that analyzes the source code and converts it into object code.

The object code is then passed to a linker or loader that turns one or more objects into an executable.

Why two steps?

Object code contains symbols such as variables that may be defined in other objects. Linker resolves the symbols and converts them into addresses in memory.

Often large programs consist of many separate files and/or library routines — don't want to re-compile them all when only one is changed. (Later we'll use Makefiles.)

Notes:

Fortran history

Prior to Fortran, programs were often written in machine code or assembly language.

FORTRAN = FORmula TRANslator

Fortran I: 1954–57, followed by Fortran II, III, IV, Fortran 66.

Major changes in Fortran 77, which is still widely used.

> *"I don't know what the language of the year 2000 will look like, but I know it will be called Fortran."*
> *– Tony Hoare, 1982*

Notes:

Fortran history

Major changes again from Fortran 77 to Fortran 90.

Fortran 95: minor changes.

Fortran 2003, 2008: not fully implemented by most compilers.

We will use Fortran 90/95.

gfortran — GNU open source compiler

Several commercial compilers also available.

Notes:

Fortran syntax

Big differences between Fortran 77 and Fortran 90/95.

Fortran 77 still widely used:

- Legacy codes (written long ago, millions of lines...)
- Faster for some things.

Note: In general adding more high-level programming features to a language makes it harder for compiler to optimize into fast-running code.

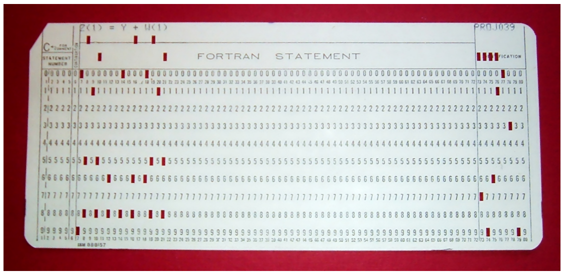
Notes:

Fortran syntax

One big difference: Fortran 77 (and prior versions) required fixed format of lines:

Executable statements must start in column 7 or greater,

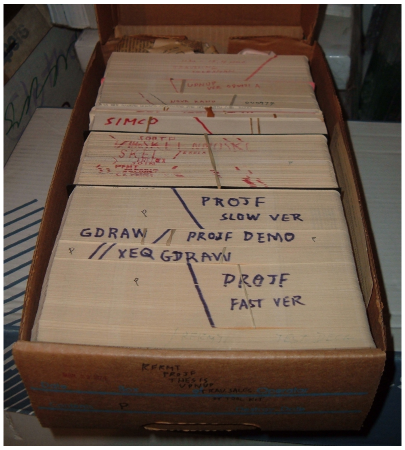
Only the first 72 columns are used, the rest ignored!



http://en.wikipedia.org/wiki/File:FortranCardPROJ039.agr.jpg

Notes:

Punch cards and decks



http://en.wikipedia.org/wiki/File:PunchCardDecks.agr.jpg

Notes:

Paper tape

http://en.wikipedia.org/wiki/Punched_tape

Notes:

Fortran syntax

Fortran 90: free format.

Indentation is optional (but highly recommended).

gfortran will compile Fortran 77 or 90/95.

Use file extension `.f` for fixed format (column 7 ...)

Use file extension `.f90` for free format.

Notes:

Simple Fortran program

```
! $UWHPSC/codes/fortran/example1.f90
program example1
    implicit none
    real (kind=8) :: x,y,z

    x = 3.d0
    y = 1.d-1
    z = x + y
    print *, "z = ", z
end program example1
```

Notes:

- Indentation optional (but make it readable!)
- First declaration of variables then executable statements
- implicit none means all variables must be declared

Notes:

Simple Fortran program

```
! $UWHPSC/codes/fortran/example1.f90
program example1
    implicit none
    real (kind=8) :: x,y,z

    x = 3.d0
    y = 1.d-1
    z = x + y
    print *, "z = ", z
end program example1
```

More notes:

- `(kind = 8)` means 8-bytes used for storage,
- `3.d0` means 3×10^0 in double precision (8 bytes)
- `2.d-1` means $2 \times 10^{-1} = 0.2$

Notes:

Simple Fortran program

```
! $UWHPSC/codes/fortran/example1.f90
program example1
    implicit none
    real (kind=8) :: x,y,z

    x = 3.d0
    y = 1.d-1
    z = x + y
    print *, "z = ", z
end program example1
```

More notes:

- `print *, ...`: The * means no special format specified
  As a result all available digits of z will be printed.
- Later will see how to specify print format.

Notes:

Compiling and running Fortran

Suppose example1.f90 contains this program.

Then:

```
$ gfortran example1.f90
```

compiles and links and creates an executable named `a.out`

To run the code after compiling it:

```
$ ./a.out
 z =    3.20000000000000
```

The command `./a.out` executes this file (in the current directory).

Notes:

Compiling and running Fortran

Can give executable a different name with -o flag:

```
$ gfortran example1.f90 -o example1.exe
$ ./example1.exe
  z =    3.20000000000000
```

Can separate compile and link steps:

```
$ gfortran -c example1.f90 # creates example1.o

$ gfortran example1.o -o example1.exe
$ ./example1.exe
  z =    3.20000000000000
```

This creates and then uses the object code example1.o.

Notes:

Compile-time errors

Introduce an error in the code: (`zz` instead of `z`)

```
program example1
    implicit none
    real (kind=8) :: x,y,z
    x = 3.d0
    y = 2.d-1
    zz = x + y
    print *, "z = ", z
end program example1
```

This gives an error when compiling:

```
 $ gfortran example1.f90
   example1.f90:11.6:
    zz = x + y
     1
Error: Symbol 'zz' at (1) has no IMPLICIT type
```


Notes:

Without the "implicit none"

Introduce an error in the code: (`zz` instead of `z`)

```
program example1
    real (kind=8) :: x,y,z
    x = 3.d0
    y = 2.d-1
    zz = x + y
    print *, "z = ", z
end program example1
```

This compiles fine and gives the result:

```
 $ gfortran example1.f90
 $ ./a.out
    z =   -3.626667641771191E-038
```

Or some other random nonsense since `z` was never set.

Notes:

Fortran types

Variables refer to particular storage location(s), must declare variable to be of a particular type and this won't change.

The statement

```
    implicit none
```

means all variables must be explicitly declared.

Otherwise you can use a variable without prior declaration and the type will depend on what letter the name starts with.
Default:

- integer if starts with i, j, k, l, m, n
- real (kind=4) otherwise (single precision)

Many older Fortran codes use this convention!

Much safer to use `implicit none` for clarity, and to help avoid typos.

Notes:

Fortran arrays and loops

```
! $UWHPSC/codes/fortran/loop1.f90
program loop1
   implicit none
   integer, parameter :: n = 10000
   real (kind=8), dimension(n) :: x, y
   integer :: i

   do i=1,n
      x(i) = 3.d0 * i
      enddo

   do i=1,n
      y(i) = 2.d0 * x(i)
      enddo

   print *, "Last y computed: ", y(n)
end program loop1
```


Notes:

Fortran arrays and loops

```
program loop1
   implicit none
   integer, parameter :: n = 10000
   real (kind=8), dimension(n) :: x, y
   integer :: i
```

Comments:

- `integer, parameter` means this value will not be changed.
- `dimension(n) :: x, y` means these are arrays of length `n`.

Notes:

Fortran arrays and loops

```
   do i=1,n
      x(i) = 3.d0 * i
      enddo
```

Comments:

- `x(i)` means i'th element of array.
- Instead of `enddo`, can also use labels...

```
      do 100 i=1,n
         x(i) = 3.d0 * i
 100     continue
```

The number 100 is arbitrary. Useful for long loops.
Often seen in older codes.

Notes:

Fortran if-then-else

```
! $UWHPSC/codes/fortran/ifelse1.f90

program ifelse1
    implicit none
    real(kind=8) :: x
    integer :: i

    i = 3

    if (i<=2) then
        print *, "i is less or equal to 2"
    else if (i/=5) then
        print *, "i is greater than 2, not equal to 5"
    else
        print *, "i is equal to 5"
    endif
end program ifelse1
```


Notes:

Fortran if-then-else

Booleans: `.true.` `.false.`

Comparisons:

`<` or `.lt.` `<=` or `.le.`

`>` or `.gt.` `>=` or `.ge.`

`==` or `.eq.` `/=` or `.ne.`

Examples:

```
if ((i >= 5) .and. (i < 12)) then
```

```
if (((i .lt. 5) .or. (i .ge. 12)) .and. &
 (i .ne. 20)) then
```

Note: `&` is the Fortran continuation character.
Statement continues on next line.

Notes:

Fortran if-then-else

```
! $UWHPSC/codes/fortran/boolean1.f90
program boolean1
    implicit none
    integer :: i,k
    logical :: ever_zero

    ever_zero = .false.
    do i=1,10
        k = 3*i - 1
        ever_zero = (ever_zero .or. (k == 0))
        enddo

    if (ever_zero) then
        print *, "3*i - 1 takes the value 0 for some i"
    else
        print *, "3*i - 1 is never 0 for i tested"
    endif
end program boolean1
```


Notes: