

I. Program layout-- execution part

PROGRAM program-name

IMPLICIT NONE
[specification part]

[execution part]

Stop
end

[subprogram part]

The execution part is control statements, subroutine calls, functions, and intrinsic functions

II. Details... radioactive decay program

- Multiplication.... Use the * symbol
- Division... Use the / symbol

`nuclei=nuclei*(1.0d0-dt/tau)`

- Boolean logic... not like an ordinary equation!
- Comparison to exact result... intrinsic function dexp

`nexact=n0*dexp(-time/tau)`

III. Details... chemical reaction program

$$\frac{dn_A}{dt} = -k_{AB}n_A n_B + k_C n_C$$

$$\frac{dn_B}{dt} = -k_{AB}n_A n_B + k_C n_C$$

$$\frac{dn_C}{dt} = k_{AB}n_A n_B - k_C n_C$$

- Must save prior concentrations to use on right-hand side!

nao=na

nbo=nb

nco=nc

- Euler integration... you figure it out, but use nao,nbo,nco!

na=nao+dt*(???)

nb=nbo+dt*(???)

nc=nco+dt*(???)

IV. More details... output to screen, unit=6

`write(6,100) time,na,nb,nc,ntota,ntotb`

`100 format(f8.4,5f12.6)`

Line number

Float with 8
columns, 4
after decimal

5 float number with
12 columns each, 6
after decimal

V. More on editing

- In command mode, several commands to manipulate text

- x Delete character
 - dd Delete entire line
 - yy “Yank” a single line
 - y5 “Yank” 5 lines
 - p “Place” yanked line(s)

- Recall from before the following commands, preceded by colon

- :w Write file to disk
 - :wq Write file to disk, then quit
 - :q Quit
 - :q! Quit without saving changes (forces quit)

VI. Compiling and running your code

- After the code is written, compile it

```
ifort -o prog1 prog1.f
```

- Then run it, directing the data to a file “output.dat”

```
./prog1 > output.dat
```

- Now you can view the results, and then plot them

```
vi output.dat
```

VI. Plotting results with gnuplot

- Type gnuplot at command line to enter gnuplot
- At the gnuplot cursor, set the terminal to “dumb”

```
gnuplot> set terminal dumb
```

- Then plot your results, will come up on screen

```
gnuplot> plot 'output.dat'
```

- Now make a .jpg file

```
gnuplot> set terminal jpeg  
gnuplot> set output 'decay.jpg'  
gnuplot> plot 'output.dat'  
gnuplot> quit
```

VII. Getting the results to your machine

- For Mac OSX, linux operating systems, scp utility

```
scp patrick@odin.engr.ucf.edu:decay.jpg decay.jpg
```

- For windows, need windows scp utility (much like putty)

<http://winscp.net/eng/index.php>

- Once installed and run, winscp will open a window to click and drag files between the odin machine and the windows machine

VIII. Decay results

