CY40014 Introduction to Computational Chemistry
Autumn 2010-2011

Module 1: Introduction to FORTRAN programming

Worksheet 1

Essentials

- Log into your account
- Change directory to access your working sub-directory
- For each of the problems listed below, create a separate FORTRAN file. You may name it as you wish. But remember to have an extension .f

Useful linux commands	**Meaning**
• ls	list of files in current directory
• pwd	print working directory
• mkdir *dir_name*	make subdirectory *dir_name*
• cd *dir_name*	change current directory to subdirectory *dir_name*
• cp *file1 file2*	copy *file1* to *file2*
• mv *file1 file2*	rename *file1* to *file2*
• cd ..	change current directory to the one before

Useful vi-editor commands (Esc +)	**Meaning**
• :wq	write to disk and quit
• :q	quit
• :q!	forced quit
• i	insert text
• 0	go to beginning of current line
• $	go to end of current line
• a	append at end of current line
• dd	delete current line
• dw	delete current word
• x	delete current character
• w	move to the beginning of next word
• b	move to the beginning of last word

Reference: *Linux in a Nutshell by Ellen Siever, Stephen Figgins, Aaron Weber, and Robert Love* ***(2005)***

Background

- A program is a set of instructions being given to the computer written in a certain language. We are going to use FORTRAN77,FORTRAN90/95.
- After writing a program, we make the computer **compile** the program to convert the program file to an executable file.
- When prompted, the computer **runs** the executable file, i.e. executes the commands given in the program file.
- Useful commands:
  vi *filename*.f (to open and edit your FORTRAN program file)
  f95 *filename*.f (to compile)
  ./a.out (to execute/run the program)
- **Data Type**: The data you are dealing with may be of different types: number/character, real/complex, rational number/integers. You need to specify the data type in your program.

Aim of worksheet 1

To make the computer compute for you the value of a function $y=f(x)$ for a given value of x. The function to be evaluated may be quite complicated

Important note

Although we generally use $f(x)$ to represent an algebraic function of x in paper, you should not use the same notation in your program. Instead, write fx to represent the dependent variable if you wish to have a similar notation.

Useful instructions that you may follow

1. Log into your account with the following
   Username: chem*mn*
   Password: icc2010

   Where *mn* is a two digit number from your roll number.If your Roll No is 10CY40001, your user name is chem01. If it is 10CY40023, your user name would be chem23.

2. After you log into your account, **create a subdirectory called worksheet1** and go to this directory. **Write programs given in worksheet 1 in this subdirectory.**

3. You will find two types of tasks in the worksheet – **problems** and **assignments**. You are supposed to finish the **problems** within the class hours. You may start the assignments in class if time permits. Otherwise, you have to complete them before you come for the next class.

4. The first problem in your worksheet 1 is numbered as W1_1. So the corresponding program may be named as w1_1.f in the subdirectory worksheet1.

5. The first problem in your assignment 1 may thus be programmed in the file named a1_1.f in the same subdirectory.

Problems: Worksheet 1

W1_1. (a) Create a file named w1_1.f and type the program given on the right.

(b) Compile the program using the following command: f95 w1_1.f
(c) Run the program with an input x=5.0
(d) Run the program with other input values of x of your choice.

```
implicit real*4 (a-h, o-z)
read(*,*)x
y=x+1.0
write(*,*)y
stop
end
```

W1_2. (a) In a new file (named w1_2.f) type the following program.

(b) Compile the program using the following command: f95 w1_2.f
(c) Run the program with an input x=5.0, y=2.0
(d) Repeat the run with x=5.0 and y= - 5.0
(e) Run the program with input values of x and y of your choice.

```
implicit real*4 (a-h, o-z)
read(*,*)x,y
z=x+y
write(*,*)z
stop
end
```

W1_3. (a) In a new file (named w1_3.f) type the following program.

(b) Compile the program using the following command: f95 w1_3.f
(c) Run the program with an input i=3, y=8
(d) Repeat the run with i=3 and y= - 8
(e) Run the program with input values of i and j of your choice.

```
implicit real*4 (a-h, o-z)
read(*,*)i,j
k=i*j
write(*,*)k
stop
end
```

W1_4. (a) In a new file (named w1_4.f) type the following program.

(b) Compile the program using the following command: f95 w1_4.f
(c) Run the program with an input x=20.0 and y=4.0
(d) Repeat the run with x=20.0 and y=3.0
(e) Run the program with input values of x and y of your choice.

```
implicit real*4 (a-h, o-z)
read(*,*)x,y
z=x/y
write(*,*)z
stop
end
```

W5. (a) In a new file (named w1_5.f, for example) type the following program.

(b) Compile the program using the following command: f95 w1_5.f
(c) Run the program with an input i=32, y=8
(d) Repeat the run with i=32 and y= 7
(e) Run the program with input values of i and j of your choice.

```
implicit real*4 (a-h, o-z)
read(*,*)i,j
k=i/j
write(*,*)k
stop
end
```

Assignment 1

While writing the program, assume that names of all integer variables start with i,j,k,l,m or n. Variable names starting with any other alphabet indicate real variables. Note that this is not necessarily so when we write down a formula on paper.

A1_1. In each case, write a program that (i) reads a value of x, (ii) evaluates the value of a function, y of x using this value and (iii) writes the calculated value of the function as output.

1. $y = x^2$
2. $y = 1 + x^2$
3. $y = 1 + x + x^2 + x^3$
4. $y = c + px; \quad c = \text{intercept}, \; p = \text{slope of a straight line (to be given as additional input)}$
5. $y = (x/4) * 4$

A1_2. In the following, write small FORTRAN programs to evaluate the following FORTRAN formulae:

$(a)\; w = \dfrac{(a+b)b^n}{2.7(c-d+1)}$

$(b)\; f = \dfrac{(x_1 + x_2)^m (y_1 + y_2)^n}{(x_1 / y_1)^{m+n} (x_2 / y_2)^{m-n}}$

$(c)\; a = \sqrt{5x^2 + 8y^2}$

$(d)\; y = a + b(c + d(e + f))^2$

$(e)\; y = \dfrac{1}{2}\exp\left(-\dfrac{(x-m)^2}{2}\right)$

A1_3. (i) Evaluate π using a suitable trigonometric formula and write a program to do this.
(ii) Write simple FORTRAN programs to estimate the following expressions:

1. $y = a\sin\left(\dfrac{m\pi x}{L}\right) + b\cos\left(\dfrac{m\pi x}{L}\right)$
2. $y = \log(a + bx); \; a, b, x > 0$
3. $y = \dfrac{1}{\sqrt{2\pi\sigma}}\exp\left(-\dfrac{(x-\mu)^2}{2\sigma^2}\right)$
4. $f = 5\cos(A) + 9\sin(B)$

A list of mathematical functions in FORTRAN
Arithmetic expressions

Operation	Symbol	Example of application in Fortran program
Addition	+	x+y
Subtraction	-	x-y
Multiplication	*	x*y
Division	/	x/y
Exponentiation (power)	**	x**2

Intrinsic library functions

These are built-in functions used by the compiler to evaluate the corresponding values. If you are trying to calculate fx=sqrt(x), x is called the argument.

Function	Meaning	Argument	Value	Example of application
sqrt(x)	$\sqrt{x}$	real	real	fx=sqrt(x)
exp(x)	e^x	real	real	fx=exp(x)
log(x)	$\log_e(x)$	Real, x>0	real	fx=log(x)
log10(x)	$\log_{10}(x)$	Real, x>0	real	fx=log10(x)
abs(x)	|x|	-	-	fx=abs(x)
sin(x)	sin(x)	real, x is in radians	real	fx=sin(x)
cos (x)	cos (x)	real, x is in radians	real	fx=cos (x)
tan (x)	tan (x)	real, x is in radians	real	fx=tan (x)
asin(x)	$\sin^{-1}(x)$	real, $-1 \le x \le 1$	real, resultant angle given in radian	fx=asin(x)
acos (x)	$\cos^{-1}(x)$	real, $-1 \le x \le 1$	real, resultant angle given in radian	fx=acos (x)
atan (x)	$\tan^{-1}(x)$	real	real, resultant angle given in radian	fx=atan (x)
atan2(x,y)	$\tan^{-1}\left(\frac{x}{y}\right)$	real	real, resultant angle given in radian	fx=atan2 (x,y)
sinh(x)	$\sin h(x)$	real	real	fx=sinh(x)
cosh(x)	$\cos h(x)$	real	real	fx=cosh(x)
tanh(x)	$\tan h(x)$	real	real	fx=tanh(x)

---------- **End of Worksheet 1**----------