

Unix/Linux commands

Fortran sample code

Homework 1

Due 1 February 2023

A. Read Sections 1.1 to 1.4 of Chapter 1 in *Introduction to Computational Physics for Undergraduates*.

B. Use vim, MacVim, Emacs, gedit or another text editor of your choice to create a text file named `UnixCommands.txt` on your computer. In this file, describe briefly (not more than a sentence per command) the meaning of the following Unix/Linux commands:

cd	ls -a	mkdir	rmdir	pwd	cp	touch
cd ..	mv -iv	rm -iv	rm -rf	more	head	tail
cd .	chmod	date	df	./Einstein.o	cpp Newton.cpp	wc
cd ~/	gfortran Einstein.f90	gunzip	gzip	chmod	sftp	ssh
tar -tvf	tar -tzvf	tar -xvf	tar -xzvf	tar -cvf	tar -czvf	cd ../../

C. The Fortran code shown below reads x (real number) from standard input (i.e., keyboard), computes $\psi(x)$ given by

$$\psi(x) = \sin^3(x^2) \cos^2(\sqrt{|x|}) \left(1 - e^{-x^2/4}\right) + \frac{1}{7} e^{\sqrt{|x|} \cos(|x|)},$$

and writes the value of $\psi(x)$ to standard output (i.e., terminal).

```
PROGRAM evalMathExpression
```

```
! This program reads x (real number) from keyboard and computes and writes the
! value of psi(x) to standard output (terminal).
```

```
! History:
```

```
!   Version      Programmer      Date      Description/Comments
!   -----      -
!       1         Your Name      xx/xx/xxxx  Code created from scratch
!
```

```
! INPUT:
```

```
!   Quantity      Units      Description
!   -----      -
!         x         none      Keyboard input
!
```

```
! OUTPUT:
```

```
!   Quantity      Units      Description
!   -----      -
!         psi         none      wave function of a QM object
!
```

```
! SPECIAL REQUIREMENTS: none
```

```
IMPLICIT none
```

```
REAL :: x, psi_x, term1, term2, term3, term4
```

```
! Input x value from standard input (keyboard)
```

```
WRITE(*,*) "Input value for x:"
```

```

READ(*,*) x

term1 = SIN(x*x)**3
term2 = COS(SQRT(ABS(x)))**2
term3 = 1.0 - EXP(-x*x/4)
term4 = EXP(SQRT(ABS(x)) * COS(ABS(x))) / 7.0

! Compute function f(x)
psi_x = term1 * term2 * term3 + term4

! Write results to standard output (screen)
WRITE(*,*) x, psi_x

STOP 'Regular stop encountered'
END PROGRAM evalMathExpression

```

Tasks

1. Open `evalMathExpression.f90` with a text editor of your choice (e.g. `vim`, `MacVim`, `Emacs`, `gedit`) and enter the Fortran program line by line into this file.

2. Compile the program:

```
gfortran -o evalMathExpression.o evalMathExpression.f90
```

Check whether or not the binary (executable) file `evalMathExpression.o` has been created. If errors have occurred, correct them and recompile the code until the Fortran compiler generates the binary version of the code.

4. To run the program, type

```
./evalMathExpression.o
```

at the shell prompt and hit the return button. You will be prompted to input a value for x . Run the code for $x = 0.5$ and 1.5 . The results will be

```

0.500000000    0.266236067
1.500000000    0.179099947

```

HOMEWORK SUBMISSION INSTRUCTIONS

1. Create a sub-directory named `LastFirst_HW1`.
2. Copy `UnixCommands.txt` and `evalMathExpression.f90` to `LastFirst_HW1`.
3. Create a gzipped archive file of your homework: `tar -czvf LastFirst_HW1.tgz LastFirst_HW1/`.
4. Email the archive file `LastFirst_HW1.tgz` to `ewhart317@gmail.com`. Put `PHYS 317 HW 1` in the subject line.