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CHM 548 PROGRAMMING HOMEWORK 1

(1) Write a program that solves the one-dimensional Schrödinger equation for an arbitrary bound potential using a finite-difference method.
(2) Solve the particle in a box problem numerically with this program and compare the results with the analytical solutions. Plot the wave functions if possible.
(3) Solve the particle in a finite depth well problem. Examine the degree of permeation of wave functions into the wall.
(4) Solve the particle in a box problem with a rectangular barrier in the middle. Observe the tunneling splitting of energies.
(5) Solve the harmonic and Morse oscillator problems. Compute Franck–Condon factors across two (displaced) potentials and simulate a vibrational progression in an electronic absorption spectrum.

PuTTY (download this program and use it to connect to a remote computer through secure shell)
LINUX tutorial (a common operating system for scientific computing)
Vi tutorial (a widely used text editor on Linux)
Fortran 90 tutorial
C/C++ tutorial
Numerical Recipes (theories and sample codes of numerical analysis)
Gnuplot (a graphics utility)
Software Carpentry (software engineering tutorials)

Fortran77/90/95

```
[sohirata@inferno ~]$ mkdir proj1
[sohirata@inferno ~]$ cd proj1
[sohirata@inferno ~/proj1]$ cp /mnt/people/sohirata/chem548/oned/tqli.f .
[sohirata@inferno ~/proj1]$ cp /mnt/people/sohirata/chem548/oned/sort.f .
[sohirata@inferno ~/proj1]$ cp /mnt/people/sohirata/chem548/oned/pythag.f .
[sohirata@inferno ~/proj1]$ vi oned.f
[sohirata@inferno ~/proj1]$ ls
oned.f  pythag.f  sort.f  tqli.f
[sohirata@inferno ~/proj1]$ ifort oned.f pythag.f sort.f tqli.f
[sohirata@inferno ~/proj1]$ ls
a.out  oned.f  pythag.f  sort.f  tqli.f
[sohirata@inferno ~/proj1]$ a.out
 mass =    100.000000000000
 analytical
           1  4.934825280000000E-002
           2  0.197393011200000
           3  0.444134275200000
           4  0.789572044800000
           5   1.23370632000000
 numerical
           1  4.740917256227306E-002
           2  0.189590824936438
           3  0.426407405556491
           4  0.757629809675279
           5   1.18293760100845
```

C/C++

```
[sohirata@inferno ~]$ mkdir proj1
[sohirata@inferno ~]$ cd proj1
[sohirata@inferno ~/proj1]$ cp /mnt/people/sohirata/chem548/oned/tqli.f .
[sohirata@inferno ~/proj1]$ cp /mnt/people/sohirata/chem548/oned/sort.f .
[sohirata@inferno ~/proj1]$ cp /mnt/people/sohirata/chem548/oned/pythag.f .
[sohirata@inferno ~/proj1]$ vi oned.c
[sohirata@inferno ~/proj1]$ icc -c oned.c
[sohirata@inferno ~/proj1]$ ifort -c pythag.f sort.f tqli.f
[sohirata@inferno ~/proj1]$ ls
oned.c  oned.f  oned.o  pythag.f  pythag.o  sort.f  sort.o  tqli.f  tqli.o
[sohirata@inferno ~/proj1]$ icc -L/opt/intel/Compiler/11.1/064/lib -lifcore oned.o sort.o tqli.o
pythag.o
```

```
/opt/intel/Compiler/11.1/064/lib/intel64/libimf.so: warning: warning: feupdateenv is not implemented
and will always fail
[sohirata@inferno ~/proj1]$ a.out
mass = 100.000000
analytical
1    0.0493482528
2    0.1973930112
3    0.4441342752
4    0.7895720448
5    1.2337063200
numerical
1    0.0474091726
2    0.1895908249
3    0.4264074056
4    0.7576298097
5    1.1829376010
```