November 19, 2015

Tools and Techniques of Computational Science - Fall 2014

Assignment 3

Exercise 3.0

The following points are "real" data for the potential energy surface of the H_2 molecule. Fit these to a sixth-order polynomial in terms of r (the internuclear separation) and also fit them to a sixth-order polynomial in terms of $exp(-r)$. That is fit them to:

$$V(x) = \alpha_0 + \alpha_1 exp(-r) + \alpha_2 exp(-2r)... \tag{1}$$

Plot the fitted functions and the data points over the range of r between 0.2 and 5 Å.

r (Angstroms)	Energy (hartrees)
0.400000000000000	-0.976798125297645
0.500000000000000	-1.100869770567898
0.600000000000000	-1.153517976992553
0.700000000000000	-1.171014611491842
0.800000000000000	-1.170406254407191
0.900000000000000	-1.160412786280990
1.000000000000000	-1.145758813825982
1.100000000000000	-1.129119870077057
1.200000000000000	-1.112067541332630
1.300000000000000	-1.095549013746680

Again, use a compiled langue for this exercise.

Exercise 3.1

The error function is defined by the equation

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x exp(-u^2) du \tag{2}$$

Using various approaches to numerical integration, including trapezoid rule, Simpson's rule, gaussian quadrature and monte carlo integration, calculate erf(1) and compare with the most accurate tabulated values that you can find. For gaussian quadrature and monte carlo (mc) integration, I recommend that you use GSL. Demonstrate verification by providing asymptotic convergence analysis for all methods. Also, provide a Makefile to build your code on Stampede and a companion slurm job script to run your code in the development queue. All of these codes should be in a compiled language.