PC5215, Numerical Recipes with Applications, Lab 2 (Due Thursday, 4 Oct 2018)

1. Copy the polynomial interpolation code polint() of "Numerical Recipes in C" in a machine readable form. Use it to compute and then plot a curve for x in the interval [-1, 4], passing through exactly the points (x,y) = (-1, 1.25), (1, 2), (2,3), (4,0) with a cubic polynomial. For plotting, you can use gnuplot, or Origin, or the plotting function in MATLAB. Label the axis, mark the points with circles and the interpolated curve with solid line.

2. Implement the Romberg integration routine [following the "Numerical Recipes" code qromb(), and polint()], and compute the integral:

$$\int_0^2 x^4 \ln\left(x+\sqrt{x^2+1}\right) dx.$$

The ln means natural logarithm (base e). Use different precisions (float and double, or even long double) and change parameters, compare the results. What is your most accurate estimation of the integral? Give an error estimate of the answers. Compare with the exact answer. Also try with the symbolic integration system, such *Mathematica* to get exact, or highly accurate (say 16 digits) results.

3. (This is a more challenging problem) The Hamiltonian of a hydrogen molecule with two fixed protons and two electrons is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{e^2}{4\pi\varepsilon_0 r_{A1}} - \frac{e^2}{4\pi\varepsilon_0 r_{B1}} - \frac{e^2}{4\pi\varepsilon_0 r_{A2}} - \frac{e^2}{4\pi\varepsilon_0 r_{B2}} + \frac{e^2}{4\pi\varepsilon_0 r_{12}} + \frac{e^2}{4\pi\varepsilon_0 r_{AB}},$$

where m is the mass of the electron, ε_0 is the dielectric constant in vacuum, e is the magnitude of the electron charge, $\hbar$ is the reduced Planck constant. We assume that the two protons are located at (3D) fixed vector positions $\mathbf{r}_A$ and $\mathbf{r}_B$, and the two electrons are at $\mathbf{r}_1$ and $\mathbf{r}_2$. The distance is defined by $r_{\alpha\beta} = |\, \mathbf{r}_\alpha - \mathbf{r}_\beta \,|$, where α or β can be A, B, 1 or 2. In a simplest possible approximation for the electron wave function, we use atomic orbital of the ground state hydrogen atom in the symmetrized form,

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \varphi(r_{A1})\varphi(r_{B2}) + \varphi(r_{A2})\varphi(r_{B1}), \quad \varphi(r) = e^{-r/a_0}$$

where a_0 is Bohr radius. Note that the wave function is not normalized.

Estimate numerically lower bounds to the hydrogen molecule bonding energy by evaluating the integrals through a Monte Carlo method with Metropolis algorithm,

$$E(r_{AB}) = \frac{\left\langle \Psi \mid \hat{H} \mid \Psi \right\rangle}{\left\langle \Psi \mid \Psi \right\rangle} \ .$$

For internal computer calculation, it is best to use atomic units ($\hbar$=1,e=1,m=1,$4\pi\varepsilon_0$=1). Outline your method, and report the results in units of ångström (for distance r_{AB} between two protons) and eV (for energy). Make a plot of energy (with error bars) vs. r_{AB}.

[For background, read any quantum mechanics textbooks, or Chapter 2 of "Molecular Modelling, principles and applications", by Andrew R. Leach.]