Project for Computational Physics Course

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February 25, 2010

1 Proposal

The proposed problem for this project is given below in brief.

- **Specification of the problem**

  To determine the ground-state correlation energy between two electrons in Helium atom, the following six-dimensional integral is needed to be evaluated,

$$\int d\overrightarrow{r_1} d\overrightarrow{r_2} e^{-2(r_1+r_2)} \frac{1}{|\overrightarrow{r_1} - \overrightarrow{r_2}|}, where \overrightarrow{r_1}, \overrightarrow{r_2} \quad (1)$$

  are position vectors of two electrons of helium atom.

- **Numerical techniques to be used**

  To perform this integration the following methods ,

  1.Gauss-Legendre quadrature

  2.Monte Carlo integration

  will be used .

  To learn those Numerical techniques,necessarily the

  1.Numerical stability

  2.Error propagation during evaluation

  3.The CPU time taken
  etc. will be checked in both the methods.