Computational Physics - Project 3

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October 23, 2015

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We are looking at the six-dimensional integral, which is used to determine the ground state correlation energy between to electrons in a helium atom. This integral is given by:

$$I = \int_{\mathbb{R}^6} d\mathbf{r_1} d\mathbf{r_2} e^{-4(r_1+r_2)} \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} \tag{1}$$

Or in spherical coordinates:

$$\begin{aligned} I = \int_0^\infty \int_0^\infty \int_0^{2\pi} \int_0^{2\pi} \int_0^\pi \int_0^\pi & dr_1 dr_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2 r_1^2 r_2^2 sin(\theta_1) sin(\theta_2) \\ & \cdot \frac{e^{-4(r_1+r_2)}}{\sqrt{r_1^2 + r_2^2 - r_1 r_2 (cos(\theta_1)cos(\theta_2) + sin(\theta_1)sin(\theta_2)cos(\phi_1 - \phi_2))}} \end{aligned} \tag{2}$$

The analytical solution of this integral is $I = \frac{5\pi^2}{16^2}$.

To solve this integral numerical. We will first apply the Gauss-Legendre quadrature for every variable in Cartesian coordinates. After that we use the Gauss-Laguerre quadrature in Spherical coordinates. Next we will study the solution for the Monte Carlo method. Where we first apply a brute force algorithm in Cartesian coordinates and then improve the algorithm with importance sampling, by eliminating the exponential term of the integral.

2.1 Analytical derivation of the integral

We want to calculate the analytical solution to the integral:

$$I = \int d\vec{r}_1 \int d\vec{r}_2 \frac{1}{|\vec{r}_1 - \vec{r}_2|} \cdot e^{-4(r_1+r_2)}$$

Therefore, we first transform to spherical Coordinates for each variable. In addition to that, we choose while calculating the integral over r_2 the axis of r_1 as z-axis. With simple scalar product ($\vec{r}_1 \cdot \vec{r}_2 = r_1 \cdot r_2 \cdot cos(\theta)$) we get the following expression: (don't forget about Jacobi-determinant)

$$I = \int_0^{2\pi} d\phi_1 \int_0^\pi sin(\theta_1) d\theta_1 \int_0^\infty r_1^2 \cdot e^{-4\cdot r_1} dr_1 \cdot \int_0^{2\pi} d\phi_2 \int_0^\pi sin(\theta_2) d\theta_2 \int_0^\infty r_2^2 dr_2 \frac{1}{\sqrt{r_1^2 + r_2^2 - 2\cdot r_1 \cdot r_2 \cdot cos(\theta_2)}} \cdot e^{-4\cdot r_2} \tag{3}$$

$$= 4\pi^2 \cdot \int_0^\pi sin(\theta_1) d\theta_1 \int_0^\infty r_1^2 \cdot e^{-4\cdot r_1} dr_1 \cdot \quad \int_0^\infty dr_2 \int_0^\pi d\theta_2 \cdot \frac{r_2^2 \cdot sin(\theta_2)}{\sqrt{r_1^2 + r_2^2 - 2\cdot r_1 r_2 cos(\theta_2)}} \cdot e^{-4\cdot r_2} \tag{4}$$

$$= 4\pi^2 \cdot \int_0^\pi sin(\theta_1) d\theta_1 \int_0^\infty r_1^2 \cdot e^{-4\cdot r_1} dr_1 \cdot \quad I(\vec{r}_1)_2 \tag{5}$$

We now calculate the integral $I(\vec{r}_1)_2$:

$$\begin{aligned} I(\vec{r}_1)_2 &= \int_0^\infty dr_2 \int_0^\pi d\theta_2 \cdot \frac{r_2^2 \cdot sin(\theta_2) \cdot e^{-4\cdot r_2}}{\sqrt{r_1^2 + r_2^2 - 2\cdot r_1 r_2 cos(\theta_2)}} && (6) \\ &= \int_0^\infty dr_2 \cdot r_2^2 \cdot e^{-4\cdot r_2} \cdot \left[\frac{1}{r_1 r_2} \sqrt{r_1^2 + r_2^2 - 2 r_1 r_2 cos(\theta_2)} \right]_0^\pi && (7) \\ &= \int_0^\infty dr_2 \cdot r_2^2 \left(\sqrt{r_1^2 + r_2^2 + 2\cdot r_1 \cdot r_2} - \sqrt{r_1^2 + r_2^2 - 2\cdot r_1 \cdot r_2} \right) \cdot e^{-4 r_2} && (8) \\ &= \int_0^\infty dr_2 \frac{r_2}{r_1} (r_1 + r_2 - |r_1 - r_2|) \cdot e^{-4\cdot r_2} && (9) \end{aligned}$$

Now, we split up the integral in two parts:

$$\begin{aligned} I(\vec{r}_1)_2 &= \int_0^{r_1} dr_2 2 \cdot \frac{r_2^2}{r_1} e^{-4 r_2} + 2 \cdot \int_{r_1}^\infty dr_2 e^{-4 r_2} && (10) \\ &= \frac{2}{r_1} \cdot \hat{I}_1 + \hat{I}_2 && (11) \end{aligned}$$

Through partial integration, we can calculate the following integral:

$$\hat{I}_1 = \int_0^{r_1} dr_2 \cdot r_2^2 e^{-4r_2} \tag{12}$$
$$= -\frac{1}{4} r_1^2 e^{-4r_2}|_0^{r_1} + \int_0^{r_1} \frac{1}{2} r_2 e^{-4r_2} dr_2 \tag{13}$$
$$= -\frac{1}{4} r_1^2 e^{-4r_1} - \frac{1}{8} r_2 e^{-4r_2}|_0^{r_1} + \int_0^{r_1} \frac{1}{8} e^{-4r_2} dr_2 \tag{14}$$
$$= -\frac{1}{4} r_1^2 e^{-4r_1} - \frac{1}{8} r_1 e^{-4r_1} + \frac{1}{32} - \frac{1}{32} \cdot e^{-4r_1} \tag{15}$$
$$\tag{16}$$

Similarly, we determine the second integral:

$$\hat{I}_2 = 2 \cdot \int_{r_1}^{\infty} dr_2 e^{-4r_2} \tag{17}$$
$$= -\frac{1}{2} r_2 e^{-4r_2}|_{r_1}^{\infty} + \int_{r_1}^{\infty} \frac{1}{2} e^{-4r_2} dr_2 \tag{18}$$
$$= \frac{1}{2} r_1 e^{-4r_1} + \frac{1}{8} e^{-4r_1} \tag{19}$$

In total, we can now determine the integral I_2:

$$I_2 = \frac{2}{r_1}\left(-\frac{1}{4} r_1^2 e^{-4r_1} - \frac{1}{8} r_1 e^{-4r_1} + \frac{1}{32} - \frac{1}{32} \cdot e^{-4r_1}\right) + \frac{1}{2} r_1 e^{-4r_1} + \frac{1}{8} e^{-4r_1} \tag{20}$$
$$= -\frac{1}{16} \frac{\left(2\,\mathrm{e}^{-4\,r_1} r_1 + \mathrm{e}^{-4\,r_1} - 1\right)}{r_1} \tag{21}$$

Finally, we can calculate the integral:

$$I = 4\pi^2 \cdot \int_0^{\pi} sin(\theta_1) d\theta_1 \int_0^{\infty} r_1^2 \cdot e^{-4\cdot r_1} dr_1 \left(-\frac{1}{16} \frac{\left(2\,\mathrm{e}^{-4\,r_1} r_1 + \mathrm{e}^{-4\,r_1} - 1\right)}{r_1}\right) \tag{22}$$
$$= 8\pi^2 \cdot \int_0^{\infty} r_1^2 \cdot e^{-4\cdot r_1} dr_1 \left(-\frac{1}{16} \frac{\left(2\,\mathrm{e}^{-4\,r_1} r_1 + \mathrm{e}^{-4\,r_1} - 1\right)}{r_1}\right) \tag{23}$$
$$= -\frac{1}{2}\pi^2 \cdot \int_0^{\infty} e^{-4\cdot r_1} dr_1 \left(2e^{-4r_1} \cdot r_1^2 + e^{-4r_1} \cdot r_1 - r_1\right) \tag{24}$$
$$= -\frac{1}{2}\pi^2 \cdot \int_0^{\infty} dr_1 \left(2e^{-8r_1} \cdot r_1^2 + e^{-8r_1} \cdot r_1 - r_1 \cdot e^{-4\cdot r_1}\right) \tag{25}$$
$$\tag{26}$$

We can derive with partial integration the expression:

$$\int_0^{\infty} dx \cdot x^n \cdot e^{-\beta x} = \frac{n!}{\beta^{n+1}} \tag{27}$$

Then, we can calculate the integral as follows:

$$I = -\frac{1}{2}\pi^2 \cdot \left[\frac{2\cdot 2!}{8^{2+1}} + \frac{1!}{8^{1+1}} - \frac{1!}{4^{1+1}}\right] \tag{28}$$
$$= -\frac{1}{2}\pi^2 \cdot \left[\frac{4}{8\cdot 8\cdot 8} + \frac{8}{8\cdot 8\cdot 8} - \frac{1}{8\cdot 2}\right] \tag{29}$$
$$= -\frac{1}{2}\pi^2 \cdot \left[\frac{12}{8\cdot 8\cdot 8} - \frac{32}{8\cdot 8\cdot 8}\right] \tag{30}$$
$$= \pi^2 \cdot \left[\frac{16}{8\cdot 8\cdot 8} - \frac{6}{8\cdot 8\cdot 8}\right] = \pi^2 \frac{10}{8\cdot 8\cdot 8} = \pi^2 \frac{5}{16^2} \approx 0.19277 \tag{31}$$

We have now derived an analytical expression for the integral. The integral has the value:

$$I = \frac{5\pi^2}{16^2} \tag{32}$$

3 Theoretical background for numerical integration

3.1 Gaussian quadrature

3.2 Montecarlo integration

4 Execution

4.1 Gaussian quadrature

4.2 Montecarlo integration

We calculated the same integral with montecarlo method. First, we calculated the integral in a brute force way. This means that we calculate the integral using (pseudo) random numbers, which obey uniform distribution functions. The random numbers for each of the six dimensional integral are uniform distributed in a chosen interval (-a to a). Furthermore, we don't transform the integral, but we calculate it in Cartesian coordinates. We got the values in table 1. (We used the interval for a=2) In one dimension, the montecarlo method can be described by formula 33.

$$I = \int_a^b f(x)dx \approx < f(x) > \cdot (b-a) = \frac{1}{n}\sum_{i=1}^{n} f(x_i)\cdot(b-a) = \hat{I} \tag{33}$$

In addition to that, we tried to improve our calculations. First, we transformed the integral into spherical coordinates. In spherical coordinates, we use the variables θ (from 0 to π), ϕ (from 0 to 2π) and r (from 0 to infinity) instead of using Cartesian coordinates $x_{i,k}$ [$-\infty$ t ∞) (i=1,2,3; k=1,2). We also used a distribution function in order to get appropriate values of the random numbers. Formula 34 to 36 describe the general one dimensional reformulation if you want to use a other particle distribution function.

$$P(x) = \int_0^x p(x)dx \tag{34}$$

$$I = \int_a^b \frac{f(x)}{p(x)}\cdot p(x)dx = \cdot \int_a^b \hat{f}(x)\cdot p(x)dx \approx \frac{1}{n}\sum_{i=1}^{n}\hat{f}(y_i)\cdot(b-a) = \hat{I} \tag{35}$$

$$y_i(x_i) = P^{-1}\left(p(y(x_i))\right) = P^{-1}(x_i) \tag{36}$$

In order to improve the precision of the integral, we used a not uniform distribution function, which can be found in formula 37ff.

$$P(x) = \int_0^x 4\cdot e^{-4x} = 1-e^{-4x} \tag{37}$$

$$y_i(x_i) = -\frac{1}{4}ln(1-x_i) \tag{38}$$

We transformate the integral to spherical Coordinates and use the distribution function for r_1 and r_2. Finally, the integral can be calculated through formula 40. The results are in table 2.

$$f(r_{1,i},r_{2,i},\theta_{1,i},\theta_{2,i},\phi_{1,i},\phi_{2,i}) = \frac{r_{1,i}^2\cdot r_{2,i}^2\cdot sin(\theta_{1,i})sin(\theta_{2,i})}{\sqrt{r_{1,i}^2+r_{2,i}^2-2\cdot r_{1,i}r_{2,i}cos(\theta_{1,i})cos(\theta_{2,i})+sin(\theta_{1,i})sin(\theta_{2,i})\cdot cos(\phi_{1,i}-\phi_{2,i})}\cdot 4^2} \tag{39}$$

$$\hat{I} = \frac{1}{n}\sum_{i=1}^{n} f(r_{1,i},r_{2,i},\theta_{1,i},\theta_{2,i},\phi_{1,i},\phi_{2,i})\cdot(2\pi-0)^2\cdot(\pi-0)^2 \tag{40}$$

5 Comparison and discussion of the results

6 Source-code

Table 1: Data from the brute force montecarlo algorithm (part c))

n	Integral	standart deviation	time in s
100	0.0563094	0.0362644	0
1000	0.226437	0.159513	0.001
10000	0.0986332	0.0263534	0.006
100000	0.155652	0.01757	0.062
1000000	0.178452	0.00754909	0.667
10000000	0.188683	0.00290854	6.645
100000000	0.19169	0.000942637	70.881

Table 2: Data from the montecarlo algorithm with distribution function (in spherical coordinates) (part d))

n	Integral	standart deviation	time in s
100	0.216734	0.0769193	0
1000	0.173694	0.0241284	0.002
10000	0.186069	0.00885492	0.021
100000	0.19571	0.00343622	0.21
1000000	0.193259	0.00101078	2.07