Project 3

For the course FYS3150

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Week 40 - ??

Kommentarer fra project 1 på devilry:

- Abstract: short motivation and presentation of the results and the findings
- Introduction: you want to motive the reader about the problem and why you want solve it
- Theory: explaining the theory behind the solution method and the problem
- Method/implementation: how you implement the solution in order to fix/solve the problem
- Results/graphs/tables: presenting the results
- Discussion: Discussing the result from previous section
- Conclusion: concluding the findings, your neutral opinion, etc... and future work
- Appendix: How you derived your method, theory, etc... , altså utledning av ting i teori som ikke spesifikt er et bevis

Ting å gjøre for de ulike oppgavene:

- 3a: beregne integralet, how many mesh points, lage et plott for å sjekke om grensene er passende å bruke
- 3b: finne grensene, erstatte Gauss-Legendre metoden med Laguerre polynomer, sammenligne med resultater fra a
- 3c: nå bruke brute force Monte Carlo, sammenligne resultatene med tidligere
- 3d: forbedre Monte Carlo med bruk av importance sampling, kommentere resultatene, lage en liste over tidene, sammenligne resultatene
- 3e: parallellisere koden fra 3d med openMPI eller MPI, kommenter resultatene (hovedsakelig i tiden brukt)

Abstract

hensikt: tilnærme løsningen til integralet så best som mulig 5 pi**2 / 16**2 .

In this project we will compute an integral with different numerical methods of integration, while comparing these values to the exact answer. Our integral is

$$\left\langle \frac{1}{|\vec{r_1}-\vec{r_2}|} \right\rangle = \int_{-\infty}^{\infty} d\vec{r_1} d\vec{r_2}\; e^{-2\alpha(r_1+r_2)}\; \frac{1}{|\vec{r_1}-\vec{r_2}|} \tag{1}$$

which is not normalized. The answer to the integral is $\frac{5\pi^2}{16^2} \approx 0.192765710958777$. The numerical integration methods we will use in this project are Gauss-Legendre quadrature, Gauss-Laguerre quadrature, brute force Monte Carlo, Monte Carlo with importance sampling, and Monte Carlo with parallization.

In this numerical study we are going to use different numerical integration methods to approximate the ground state correlation energy between two electrons in a helium atom. The main interest and the goal of this study is to look at how the different methods compare and

```
  1x-193-157-253-38:project3 Alexandra$ ./ni.o 1000000000 3

Gauss-Legendre quad =     0.00000000000000
Exact answer =          0.192765710958777
Error =                 0.192765710958777
Time used by Gauss-Legendre = 1.73000000000000E-07s

Gauss-Laguerre quad =     0.00000000000000
Exact answer =           0.192765710958777
Error =                   0.192765710958777
Time used by Gauss-Laguerre = 1.17000000000000E-07s

Brute Force Monte Carlo =    0.193462755727606
Exact answer =           0.192765710958777
Error =                0.000697044768829452
Time used by Brute Force Monte Carlo = 653.636127568000s

Spherical Monte Carlo w/ Imp.Sampling =    0.192692246996587
Exact answer =           0.192765710958777
Error =                7.34639621890743E-05
Time used by Spherical Monte Carlo w/ Imp.Sampling = 772.072297750000s

Standard deviation BMC = 0.00111909179849692
Standard deviation SMC = 3.31038411626575E-05
```

Contents

1 Introduction

All programs are found at our GitHub-repository.

2 Theory

$$\begin{bmatrix} d & a & 0 & \dots & 0 & 0 \\ a & d & a & \dots & 0 & 0 \\ 0 & a & d & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & a & d & a \\ 0 & 0 & 0 & 0 & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{bmatrix}$$

3 Method

4 Results

Our results are as shown in the Appendix. We also have `.txt`-files for all the raw data generated by the projects up on GitHub.

- How many mesh points do you need before the results converges at the level of the third leading digit?

Burde ha at lambda er 2 siden det gir best resultater, se plottet fra plot_data.txt.

Table 1: Execution time for the two methods.

n	Tridiagonal	LU-Decomposition
10	kcmdkcmdkmcdkmdkcmk kdmckdcm	
eokfodfk	$3.17 \cdot 10^{-4}$	
100	$1,40 \cdot 10^{-6}$	$1.40 \cdot 10^{-3}$
1000	$1.44 \cdot 10^{-5}$	$3.36 \cdot 10^{-2}$

5 Discussion

6 Conclusion and perspective

7 Appendix

8 References

Link to the PDF for Project 2.

Our GitHub-repository.

Link to lecture slides in FYS3150 - Computational Physics.

Offical Armadillo website for documentation of all contents in the library.

Analytical results for specific oscillator frequencies.