Project 3

For the course FYS3150

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Week 40 - ??

HETER DET PARALLIZED ELLER PARALLILIZED ?????????

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 openMP eller MPI, kommenter resultatene (hovedsakelig i tiden brukt)

Det som mangler:

- må se gjennom abstract
- skrive mer på introduction
- lime inn theory
- skrive noe på method
- lime inn results
- skrive discussion
- skrive conclusion and perspective
- sjekke om vi skal ha noe i appendix
- sjekke references (den er skrevet dobbelt, er dette mulig å fjerne ?)

Abstract

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

In this scientific study we will compute an integral with different numerical methods of integration to approximate the ground state correlation energy between two electrons in a helium atom. Our integral is given by equation (1), which is not normalized. The integral has the analytical answer $\frac{5\pi^2}{16^2} \approx 0.192765710958777$. The main interest and the goal of this study is to look at how the methods compare with different amount of mesh points and integration limits. 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. The study was a success and proved Monte Carlo to be the fastest and most accurate method. Being based on big data, it required many more sampling points. However, as it did not manually calculate the integral, it was much more efficient.

SETT INN NOEN TALL SOM BEVIS HER

Contents

1 Introduction

The integral we are evaluating comes from the solution of Schrödinger's equation for a simplified case of determining the ground state correlation energy between two electrons in a helium atom.

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

The integral is not properly normalized. However, that is not important for the study. If you are interested in how the integral is found, see [1].
Our aim is, as written in the abstract, to approximate this integral using two types of Gaussian Quadrature, and some variations of Monte Carlo. We have created a code that evaluates the integral using each method and compares them. Alongside the actual value we get the absolute value, and time used. Using this we present our data showing that Monte Carlo massively outperforms the other methods.
The report will go through the theory and methods behind our study and following that we will present our results and discuss them.

2 Theory

HER SKAL ERIK SITT INN

3 Method

The methods used in this project are Gauss-Legendre quadrature, Gauss-Laguerre quadrature, brute force Monte Carlo, Monte Carlo with importance sampling, and Monte Carlo with parallization.

3.1 Gauss-Legendre

This method is excepted to give to worst approximation to the integral. This is because it uses approximations and other short cuts to more easily compute the integral. For instance the limits are originally given by $\pm\infty$ and in this method they have to be approximated to finite numbers.
integrand diverges.
THIS SHOULD ALSO BE ERIK SITT?

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?
- plottene for lambda, integrationspoints, montecarlo og timings
- tror ikke skal ha noen tabeller

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

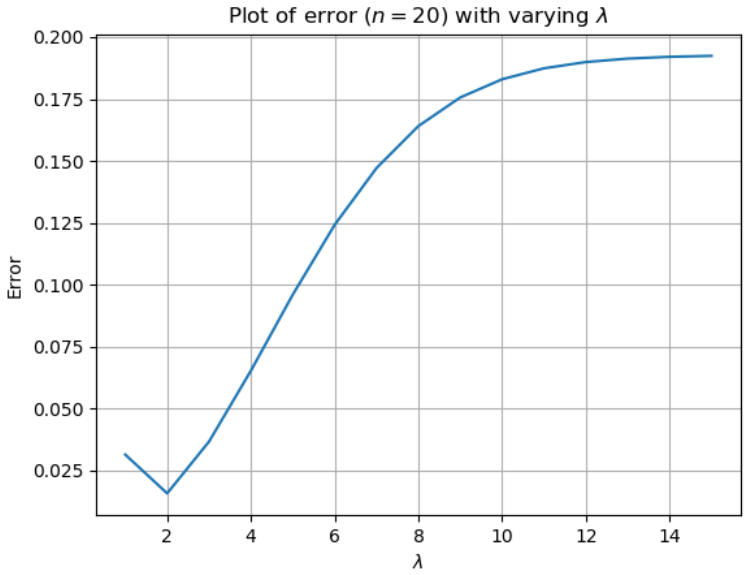

Figure 1: The plot of error as a function of lambda for Gauss-Legendre.

5 Discussion

diskutere resultatetene: altså hvilke metoder som brukte lengst tid, hvilke som var mest nøyaktig osv
koble dette til teori for hvorfor resultatene ble slik som de er

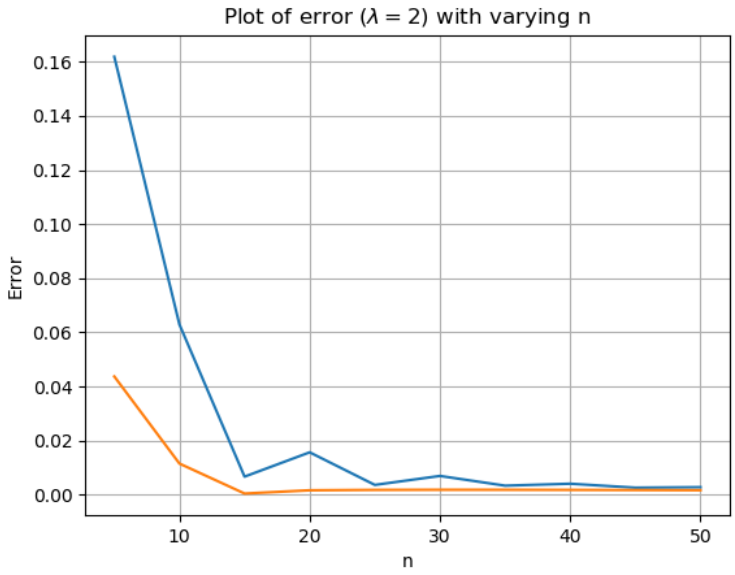

Figure 2: The plot of error as a function of integrations points n for Gauss-Legendre and Gauss-Laguerre.

The results show that the parallized code actually isn't better than the non-parallized code. This is strang. However, it can be from the fact that the computer running the code only has two cores so there is less of an effect.

6 Conclusion and perspective

To conclude the Monte Carlo integration methods exceeded the Gauss quadrature methods for both computation time and accuracy of the answer to the integral. As expected the parallized spherical Monte Carlo with importance sampling is the fastest method with the highest degree of accuracy. This is mainly because ...

legge inn mer her som knytter det opp til teorien.

7 Appendix

Figure (5) does not include all larger data points from our `.txt`-files. These can be found in table (???????)

8 References

[1] Morten H. Jensen (2019), Project 3, Departement of Physics, University of Oslo, Norway

[2] Erik B. Grammeltvedt, Alexandra Jahr Kolstad, Erlend T. North (2019), GitHub, Students of Departement of Physics, University of Oslo, Norway

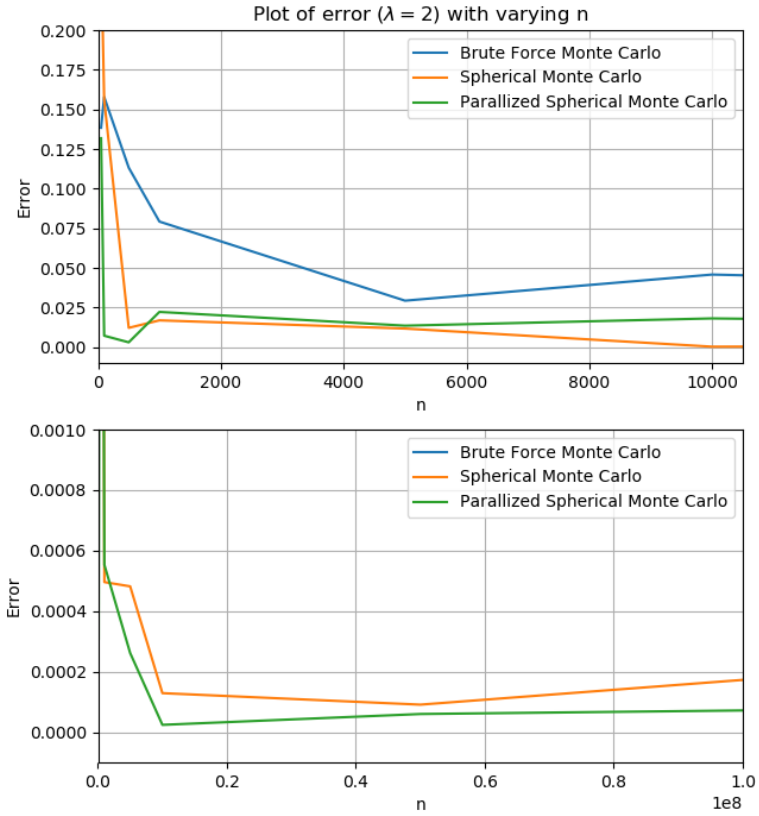

Figure 3: The plot of error as a function of integration points n for brute force Monte Carlo, spherical Monte Carlo with importance sampling, and parallized spherical Monte Carlo with importance sampling.

[3] Morten H. Jensen (2015), Lecture slides for FYS3150, Department of Physics, University of Oslo, Norway

Table 1: Error and execution time for Gauss-Legendre and Gauss-Laguerre.

Legendre error	Laguerre error	Legendre time	Laguerre time
0.161836	0.0437248	0.00082727	0.0022169
0.0629315	0.0115411	0.0520311	0.150486
0.00670907	0.000476827	0.609131	1.69456
0.0157005	0.00167232	3.35013	9.3416
0.00365618	0.00181852	12.8663	35.5266
0.00697009	0.00186703	38.0615	105.708
0.00337855	0.00186074	95.5971	264.104
0.00409558	0.00181934	214.105	608.182
0.00263748	0.00176034	433.725	1191.8
0.00281127	0.00169433	831.449	2314.1

Table 2: Error and execution time for brute force Monte Carlo, spherical Monte Carlo with importance sampling, and parallized spherical Monte Carlo with importance sampling.

BMC error	SMC error	PSMC error	BMC time	SMC time	PSMC time
0.138417	0.251552	0.131809	0.00011814	8.7853e-05	0.00038
0.157825	0.156198	0.0071997	0.00014777	0.0001193	0.00037
0.113224	0.012164	0.00302251	0.0003764	0.0003822	0.00051
0.079204	0.0168798	0.022215	0.00066215	0.0007048	0.00098
0.029304	0.011712	0.013536	0.0029481	0.00338986	0.002612
0.0457817	0.00027297	0.018113	0.005808	0.006558	0.005258
0.0096648	0.0038374	0.0012646	0.029013	0.032508	0.025366
0.024003	0.0043587	0.00030587	0.056982	0.067961	0.047938
0.0137398	0.0046188	0.00356363	0.287352	0.328019	0.18964
0.0161491	0.00049579	0.0005530	0.57400	0.654257	0.354581
0.00311977	0.00048176	0.00026134	2.85616	3.27695	1.82245
0.00481115	0.00012881	2.40583e-05	5.70269	6.54182	3.3623
0.00265522	9.08138e-05	5.988e-05	29.7091	33.0613	16.5097
0.00117823	0.0001726	7.16594e-05	58.8054	67.2903	33.4236
6.0793e-05	2.5923e-05	1.6625e-05	415.953	448.229	208.211

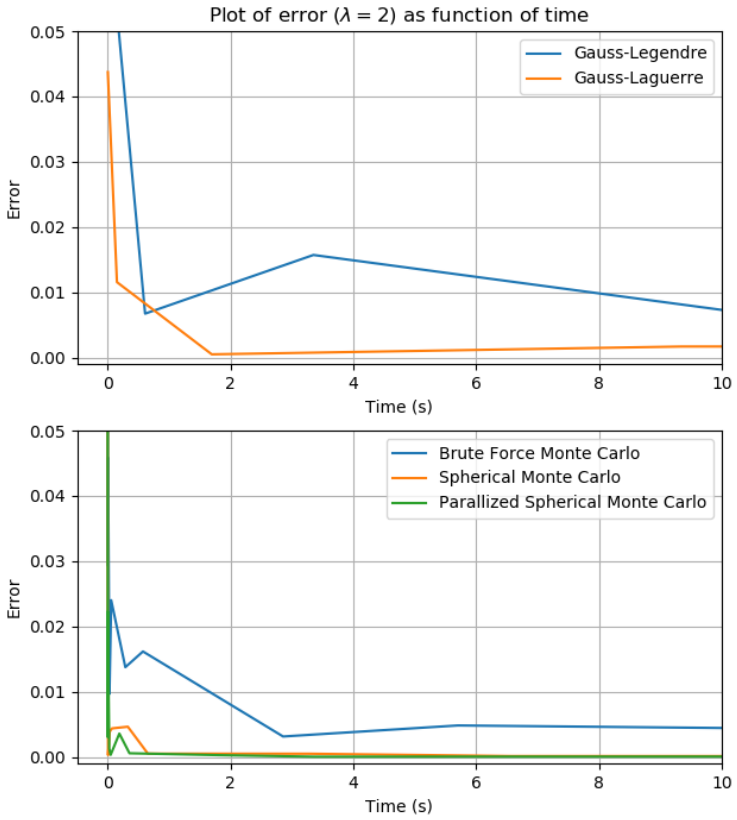

Figure 4: The plot of error as a function of time for all the numerical integration methods used in this scientific study.

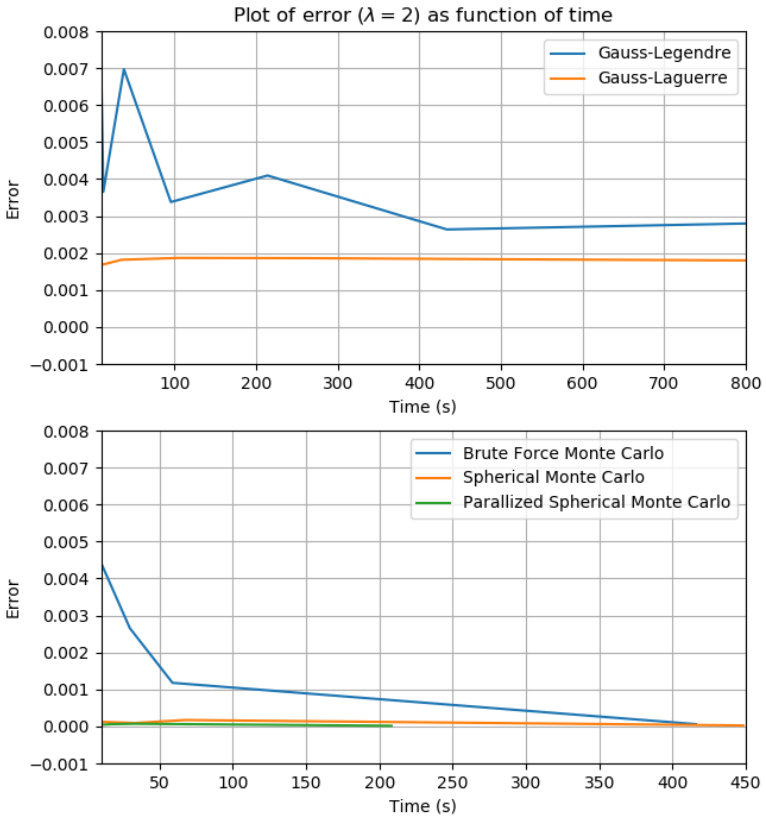

Figure 5: This figure is a continuation of the previous figure, (4).