# Progress report FYS4411 project

Filip Sund
filipsu@fys.uio.no

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I have done tasks 1a through 1c, and parts of 2a. I have not made a method for computing the onebody density and the charge density in task 1d, mostly because I don't know how to do it, and I haven't looked into it yet. I made a method that found the optimal variational parameters using Newton's method, but I have since rewritten my whole program, and have yet to re-implement this method.

After writing a lot of bad not-really-class-oriented code I decided to rewrite my whole program, and I'm now using a proper Jastrow and Slater class, a Wavefunction class and a Hydrogen-like orbitals-class. I have not yet implemented the 2p wavefunction, so the program can't do Neon yet, but this should be easy to implement. I am still using the numerical derivatives to find the local energy, because I haven't implemented the closed form gradient or laplacian functions in the Jastrow and Slater classes. The Slater class is also currently using the slow/stupid method for calculating the Slater-wavefunction and the Slater-ratio:

```
1  double Slater::wavefunction(const mat &r)
2  {
3      /* For use in the numerical derivative, in the numerical local energy,
4       * and in the temporary ratio function */
5
6      mat slaterUP(N, N);
7      mat slaterDOWN(N, N);
8
9      for (int i = 0; i < N; i++)
10     {
11         for (int j = 0; j < N; j++)
12         {
13             slaterUP(i,j) = orbitals->wavefunction(i, r.row(j));
14             slaterDOWN(i,j) = orbitals->wavefunction(i, r.row(j+N));
15         }
16     }
17
18     return det(slaterUP)*det(slaterDOWN);
19 }
20
```

```
21 double Slater::getRatio()
22 {
23     return wavefunction(rNew)*wavefunction(rNew) /
24             (wavefunction(rOld)*wavefunction(rOld));
25 }
```

The program is running correctly in parallel using MPI, but I haven't implemented blocking yet.

My plan is to have a proper Slater class working before the end of easter, including proper "smart" updating of the inverse of the Slater determinant matrix, and closed for expressions for the gradient and laplacian ratios for both the Jastrow and the Slater classes. I'm a bit behind because I have been working a lot on FYS4460, and I have also had some trouble with the quantum mechanics.