

Introduction

When studying systems with large numbers of electrons, current methods often face issues with:

- Accurately treating electron interactions
- Incorporating temperature effects

The research being performed is out of a desire to simulate large electron clusters.

Path Integrals are a way to effectively analyze these systems at the cost of the inaccuracies associated with a “sign problem”, an issue related to fermion statistics.

It is this sign problem that we set out to solve through our research.



Materials and Methods

Materials for Research:

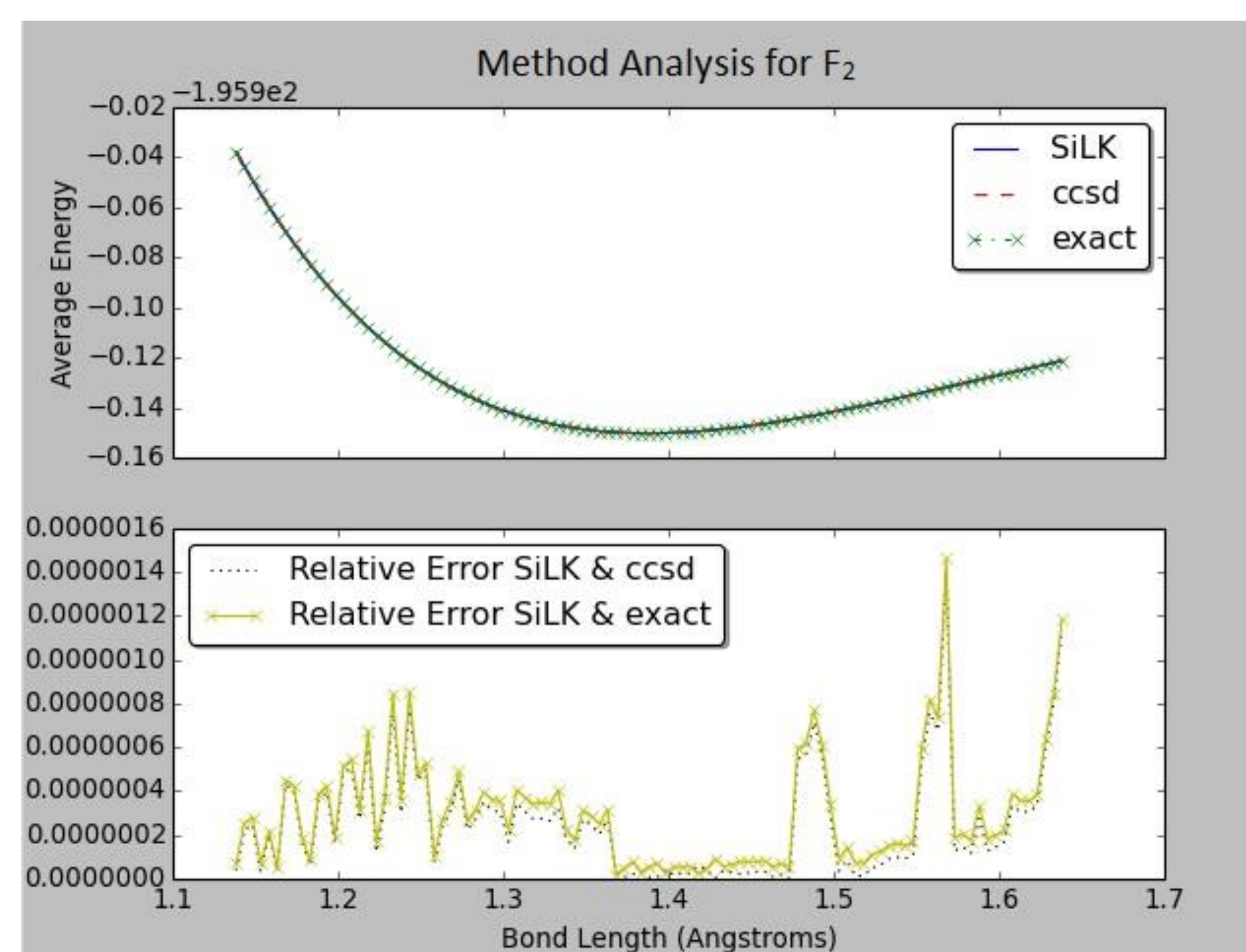
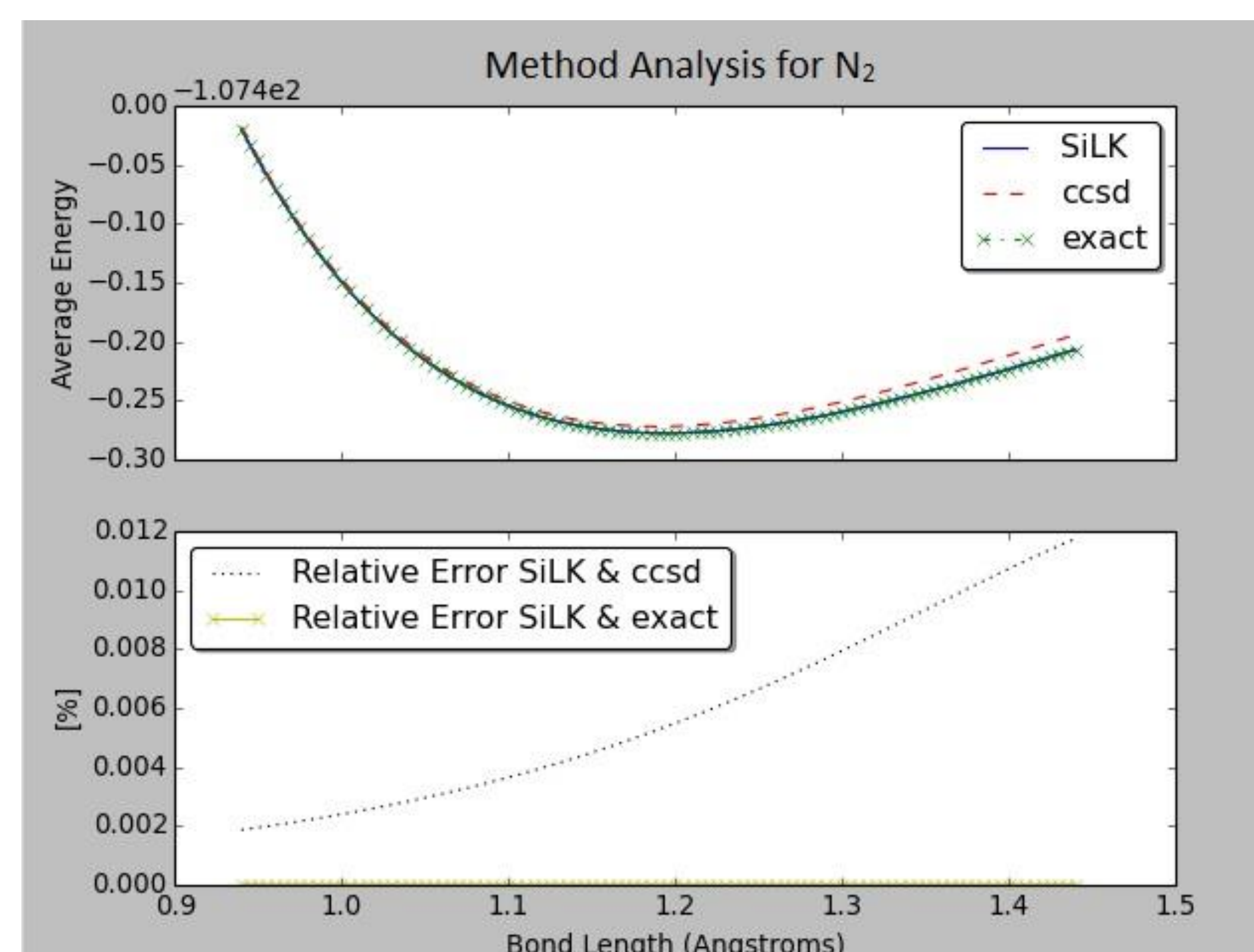
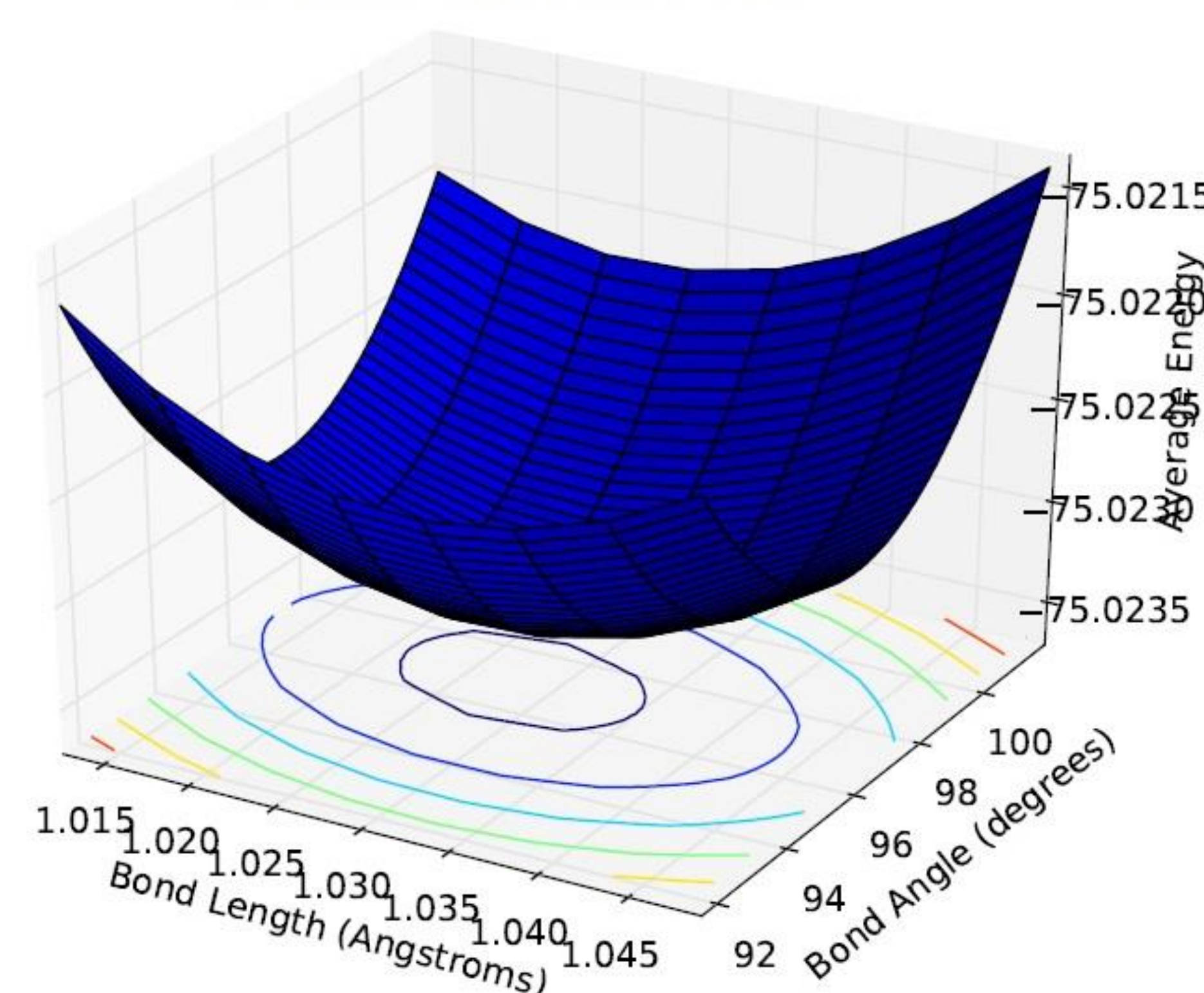
- Supercomputing clusters at Super Mike II
- NWChem ab initio computational chemistry software

Methods of Research:

- Submission of scripts as jobs within Mike clusters
- Monte Carlo sampling of data
- Sign Learning Kink-Algorithm (SiLK)
 - Simplest Metropolis-Monte Carlo method
- Pseudo-random numbers representing probabilities which are used to calculate the properties of the atoms and/or molecules evaluated within the system.

Results

Ground State Energy Variation in H₂O



Discussion

The graph for water shows how the Ground State Energy changes as the bond angle and lengths change. The ripples at the bottom of the graph correspond to the increase in the average (ground state) energy, with each ripple being a 0.0005 increase. The graphs for N₂ and F₂ compare the evaluation methods of exact diagonalization, ccSD, and SiLK. The top graph shows the relationship between the results of the different methods, while the lower graph emphasizes the error SiLK has when compared to the other two methods. The increasing error found within the N₂ graph is to be expected, as an increase in the bond distance of a triple bonded N₂ molecule creates a lot of inaccuracies at longer bond lengths, with more accuracy in the shorter bonds. The error within the F₂ graph is quite minimal, with the most accurate values near the textbook bond lengths, as expected for the molecule.

Conclusion

1. The water molecule ground state energies can be successfully mapped out as the molecule is manipulated to fit our desired specifications.
2. The energy variants based upon bond lengths are quite similar to those of the established methods for both N₂ and F₂.
3. With the error between the methods being so small, SiLK can be said to overcome the sign problem within smaller molecules.
4. Future steps could include adaptation and testing for larger, more complex molecules and systems as well as adding calculations for smaller and larger systems.

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