Spring 5-2019

Hartree-Fock Implementation for Pedagogical & Research Purposes

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Computational Chemistry is the use of computers and quantum mechanics to simulate chemical experiments, saving time and money for scientists and researchers. Despite the benefits of computational chemistry, few undergraduate students are exposed to computational chemistry methods. Because of this, there is a need for an easily understandable computational-chemistry code with a focus on pedagogical use, leading to the implementation of the Hartree-Fock method in Python, with a focus on legibility and conceptual understanding for undergraduate students. The overall logic flow of the program is depicted below.

Specify Molecular System

- Atomic Numbers
- Nuclear Coordinates
- Number of Electrons
- Basis Set
- Object-Oriented Structure (Atoms build Molecules)

Evaluate Integrals

- Gaussian Basis Set allows for simplification of integral evaluation
- Evaluate integrals for overlap, electron kinetic energy, electron repulsion, and nuclear-electron attraction values

Prepare for SCF

- Construct Hamiltonian
- Construct Guess Fock Matrix, Assume no Electron-Electron Interactions for Guess
- Create Transformation Matrix

SCF Procedure

Diagonalize Fock Matrix

- Compute molecular orbitals and energies from transformed Fock matrix

Convergence Not Reached
Perform Another SCF Iteration

Build Density Matrix

- Use molecular orbitals to compute density of electrons

Build Two Electron Term

- Use density matrix to build two electron term

Rebuild Fock Matrix

- Sum two electron term and Hamiltonian to create a new Fock matrix

Compute Expectation Energy

- Determine energy of the molecule from the Fock matrix

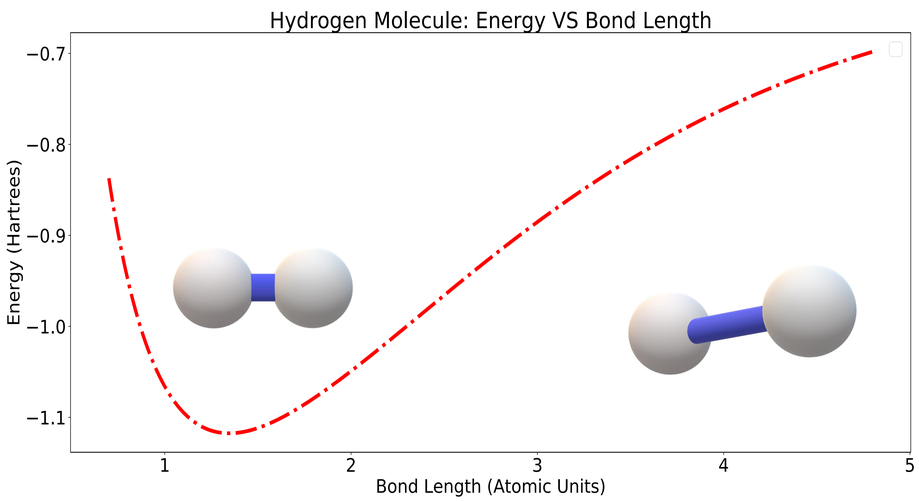
Check For Convergence

- Check if difference between expectation energies is less than a certain threshold

Convergence Reached
Output Computed Energy & Bond Distance

Simulated Results

Graph of hydrogen atom ground state energies at varying bond lengths. Data was generated from pedagogical Hartree-Fock code.



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