Bio

I am a first year PhD student in the Earth and Planetary Science Department at UC Berkeley. I graduated with a BS in Geology and Geophysics and minor in Math from the University of Hawai‘i at Manoa in August 2015. As an undergraduate I used experimental and measurement-based research to understand olivine nucleation and growth and the dynamics of volcanic eruptions. Currently, my research focuses on using first-principles molecular dynamics (MD) simulations, based on density functional theory (DFT), to determine the behavior of planetary materials at high temperatures and pressures. Codes implementing quantum mechanical MD simulations are massively parallel and are computationally expensive. Through this course I hope to learn about computer architectures, implementation and design of parallel codes, and optimization of parallel code efficiency.

Parallel Application: Molecular Dynamics

Introduction

Quantum mechanical first-principles molecular dynamics (MD) simulations provide a means of determining a material’s behavior under the high temperatures and pressures realized in planetary interiors. Results obtained from these simulations are combined with seismological data to determine the composition and mineralogy of Earth’s interior. For example, previous studies have found that the presence of post-perovskite phases (Figure 1) explain the seismic signatures of the D’’ layer [1]. By determining the mineralogy, composition, and thermal structure of Earth’s interior we provide more accurate inputs for geodynamical simulations of Earth’s evolution.

![Figure 1](image.png)
Method

Experiments replicating the high temperatures and pressures of Earth’s lower mantle and core face many challenges. As a result, first-principles MD simulations have become a common way to study earth materials. These simulations are most commonly based on density functional theory (DFT) and are implemented using a number of parallel codes. One parallel computer program used for these simulations is VASP (Vienna Ab Initio Simulation Package).

The DFT-based VASP program solves the Kohn-Sham equations to approximate a solution to the many body Schrödinger equation. Quantities such as one-electron orbitals, electronic charge density, and local potentials are expressed by plane wave basis sets. Pseudo potentials are used to describe interactions between electrons and ions. Iterative matrix diagonalization schemes and a Pulay mixer are used to calculate the electronic ground-state for the system in self-consistent cycles (2). These techniques may include blocked Davidson algorithms or such as the residual minimization method with direct inversion of the iterative subspace (2).

For VASP programs using plane wave basis sets, computational run-time scales as $N^3$ for certain portions of the code, $N$ is the number of valence electrons in the system (2). As the number of valence electrons increases, other portions of the code start to approach execution time scales of $N^3$, making VASP most useful for systems with up to 4000 valence electrons (2). VASP.4 was rewritten to take advantage of the flexibility of Fortran 90 and runs equally well on super-scalar processors, vector computers, and parallel computers. In the 1990s the code was updated with MPI (message passing) parallelization.

VASP has been able to replicate prior experimental measurements and proves a valuable tool for MD simulations in the Earth Sciences (3).

References

