Universal File Translator for First Principles Codes

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Abstract:

Currently, over twenty density functional (DFT) codes exist for calculating properties of crystal structures and molecules using first principle approaches. While each has its own strengths and weaknesses when describing a particular system, the ability to migrate from one approach to another easily is essential for comprehensive research.

In this work, we create a program that can convert between multiple formats of DFT codes. As a test case, we examine a magnetic nanowire system, converting between two popular DFT codes, LMTO and Abinit. LMTO uses a compact basis set derived from atomic-like orbitals to calculate system properties quickly. While LMTO is very efficient for closed pack systems, special care is required for structures with large amounts of open space. Abinit, by contrast, is based on a plane wave basis and can handle a wide range of systems at the expense of greater computation time. Since the plane wave basis set is not localized, Abinit treats empty space more effectively than LMTO. The system properties calculated using both techniques are compared and situations where format conversion would be ideal are also discussed.

Introduction:

While each of the DFT codes uses its own approach for determining the total energy of a system, they all rely on the underlying tenets of density functional theory. Density functional theory basically takes an *n*-body problem for all electrons and neutrons and reduces it to a function (the charge density, $r(x,y,z)$) of three variables. The assumption made (originally by the Hartree-Fock method) is that the electrons do not interact, which allows the problem to be viewed by using a Schrödinger equation that deals with only a single electron.

One of the major goals of density functional theory is to calculate the equilibrium crystal structure for a molecule. This can be done by adjusting the system volume for DFT calculations. If this data is plotted as energy versus volume (as seen in Figure 1) it will appear to be parabolic in shape. We say that the equilibrium structure for the given system occurs at the minimum of that curve. The reason this distribution appears parabolic is due to electron-electron repulsion that raises the energy as the system becomes too closely packed or too spread apart.

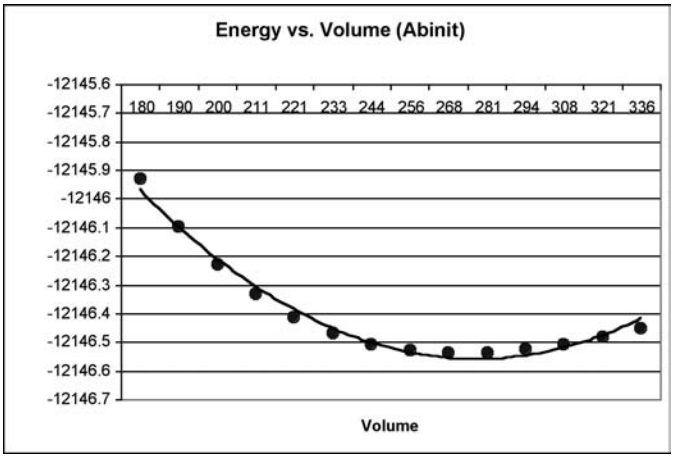

Figure 1: Abinit energy plot with a quadratic curve fit.

Procedure:

The majority of the project consisted of programming a file format translator. After work on the file translator program was completed, the next step was to test the quality of the program's ability to translate between file formats. To do this, we inserted a LMTO input file into the translation program to obtain a converted Abinit input file describing the same system. We would then analyze the results of parallel computations of the two codes to determine how well the computed equilibrium lattice constants and magnetic moment per atom agree.

While converting between Abinit and LMTO was the main concern of the project, another function intended for the translation utility was to make it able to convert to a simple file format for use in the program called "RasMol." RasMol takes Z-numbers and atomic positions and plots atoms in a three-dimensional graph. This is a feature that we felt would be important to a user of the translation utility as it allows a simple way to view the system with which the user is working.

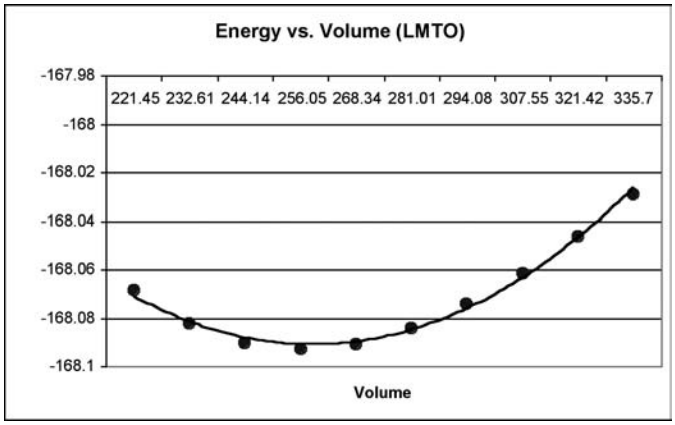

Figure 2: LMTO energy plot with a quadratic curve fit.

Results and Conclusions:

The results that we analyzed were those of calculations run by Abinit and LMTO using information about the same structure. To run tests, we ran calculations on a single atom Nickel-Face Centered Cubic (Ni-FCC) system; first with Abinit, and again with a converted input file for LMTO. The data obtained by the calculations was for a small range of lattice constants centered about the experimentally accepted value for nickel. The data that we wanted was the value that each of the calculations claimed to be the energy minimum for the system. For the Abinit calculation, the equilibrium lattice constant was calculated to be 6.35 Bohr (approximately 3.36Å). LMTO found the lattice constant to be 6.45 Bohr or 3.41Å (percent difference of 1.48%). The magnetic moment calculated by Abinit was 0.603 Bohr-Magnetons with a percent difference of 2.01% from the LMTO value of 0.591 Bohr-Magnetons.

Future Work:

The current status of the project is functional, but largely incomplete. The translation program presently converts between LMTO and Abinit input file formats as well as from Abinit and LMTO to RasMol. Since there are more than twenty density functional theory codes available, more coding can be done to add translation capabilities for additional codes. In the future a universal file format is planned that can be read by multiple DFT codes. The success of this future project will depend on its ease of use and readability as well as the potential acceptance and implementation by DFT code authors. Since the translator program is coded in Java, a web-based interface for use on the Cornell NanoScale Facility web site will be created for remote users who wish to convert between available file formats.

Acknowledgements:

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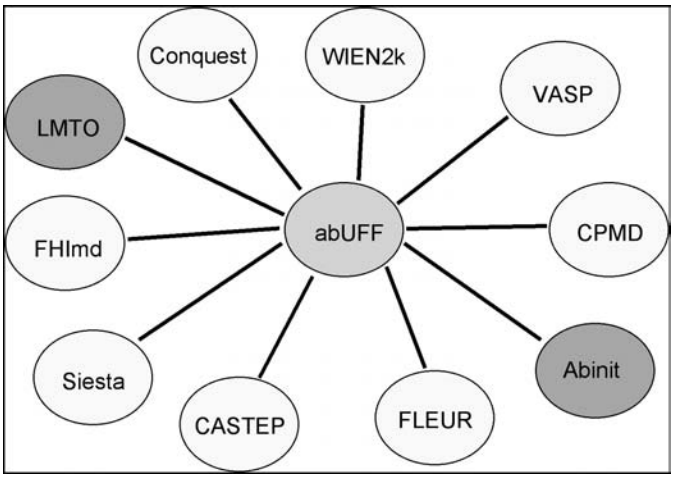

Figure 3: Some of the available DFT codes with the file translator in the center.