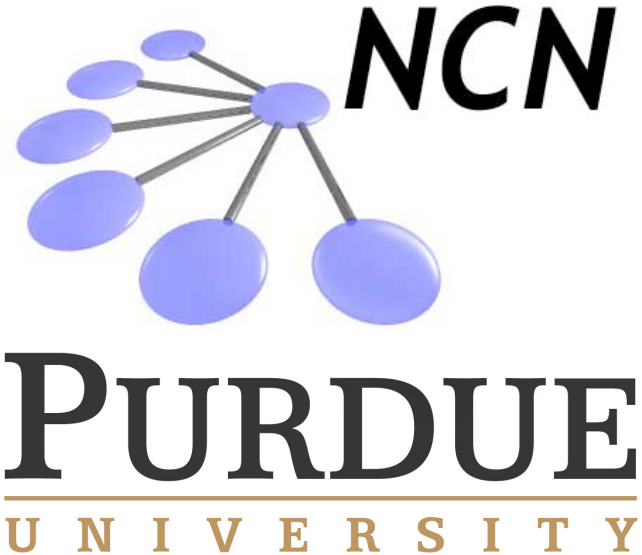
ABINIT: First Time User Guide



Benjamin P. Haley
Network for Computational Nanotechnology (NCN)
Purdue University

bhaley@purdue.edu

A very brief introduction

- Many problems in atomic scale physics and chemistry require a solution to the many-electron Schrödinger equation.

$$\hat{H}\Psi = \left[\hat{T} + \hat{V} + \hat{U}\right]\Psi = \left[\sum_{i}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i}^{N} V(\vec{r}_i) + \sum_{i<j}^{N} U(\vec{r}_i, \vec{r}_j)\right]\Psi = E\Psi$$

- This equation can not be solved exactly; the U term, denoting electron-electron interactions is particularly intractable. One of the most popular approximation methods for this equation is called Density Functional Theory (DFT), which uses the electron density n to re-write the many-electron problem into a single electron problem in which the electron moves in an effective potential

$$V_s(\vec{r}) = V(\vec{r}) + \int \frac{e^2 n_s(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|}\mathrm{d}^3 r' + V_{\mathrm{XC}}[n_s(\vec{r})]$$

Equation images from http://en.wikipedia.org/wiki/Density_functional_theory)

A very brief introduction II

- The effective potential V_s is a function of the electron density

$$n(\vec{r}) \stackrel{\text{def}}{=} n_s(\vec{r}) = \sum_i^N |\phi_i(\vec{r})|^2$$

- The exchange-correlation energy V_{xc}, which describes the many -electron interactions, is a functional of n.
- The electron density n is itself a function of the solutions ϕ_i of the Kohn-Sham [see References] equations

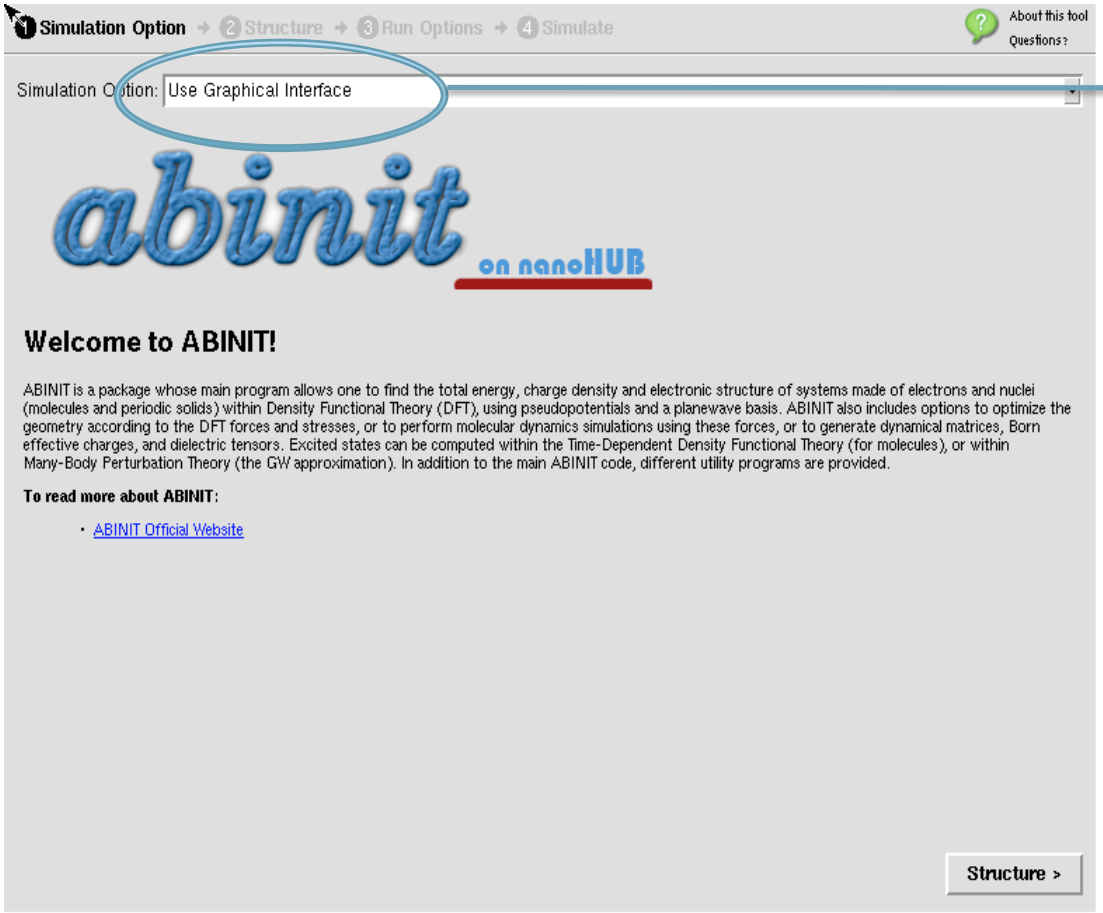
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_s(\vec{r})\right]\phi_i(\vec{r}) = \epsilon_i\phi_i(\vec{r})$$

- The DFT method, then, is an iterative process, in which an initial n is used to calculate V_s, which is used to solve for ϕ_i, which updates n, and so on.

What is ABINIT?

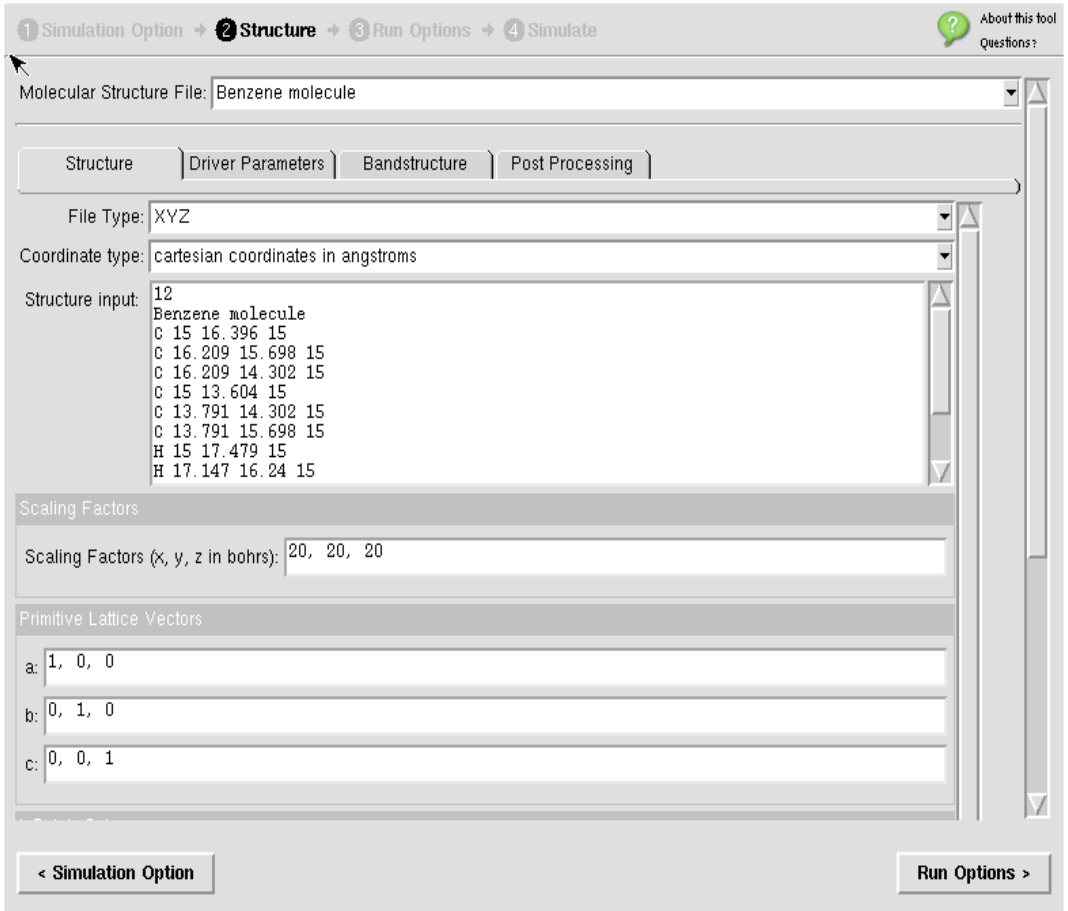
- A program which calculates the total energy, electronic structure, and charge density of atomic systems (nuclei and electrons) using DFT, plane waves, and pseudopotentials.
- ABINIT can also do geometry optimization and molecular dynamics (MD).
- Many body perturbation theory (GW approximation) is also possible.
- The rest of this guide will focus on the nanoHUB interface for ABINIT.
- For more information, see http://www.abinit.org/about/

First input phase: Simulation Option



- ABINIT supports two interfaces
- **Use Graphical Interface** allows the user to select simulation options. This is the default option and the focus of this user guide.
- **Upload Abinit Inputdeck** allows an expert user to upload his own input file.

Second input phase: Structure I



- Choose one of the preloaded molecular structures (benzene, carbon nanotube, crystalline silicon) or upload your own.
- PDB and XYZ coordinate formats are supported.
- All calculations must be done in a periodic supercell; this is a consequence of using a planewave basis.
- Define primitive vectors and scaling factors (lattice constants) for the supercell holding the system.
- Determine the distribution of *k*-points in the supercell.

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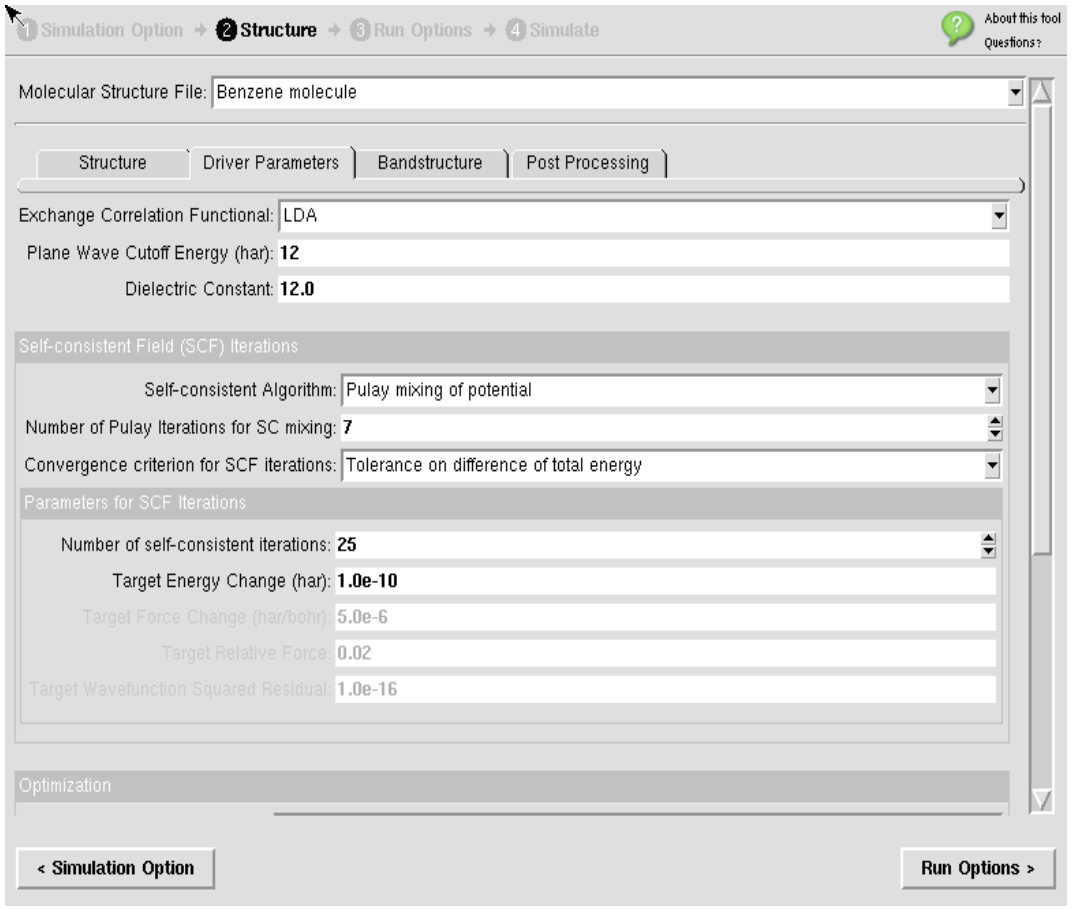
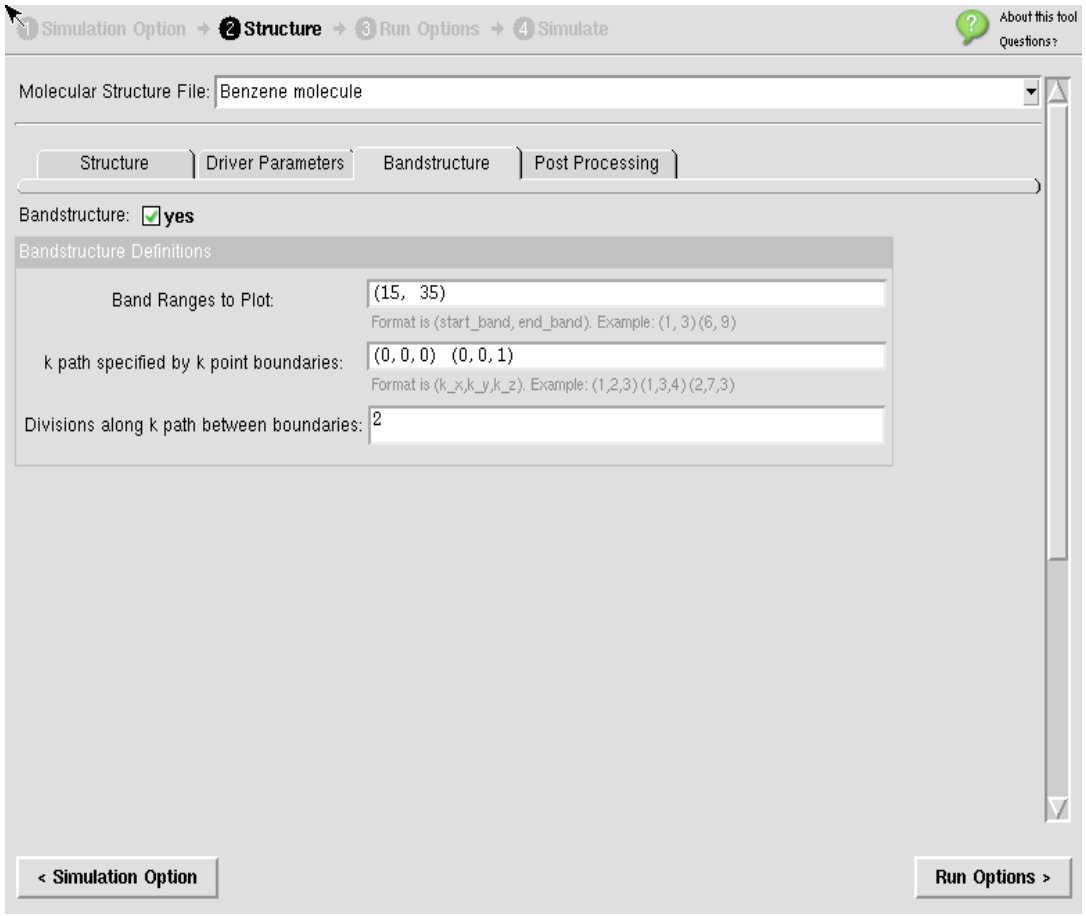
Second input phase: Structure II



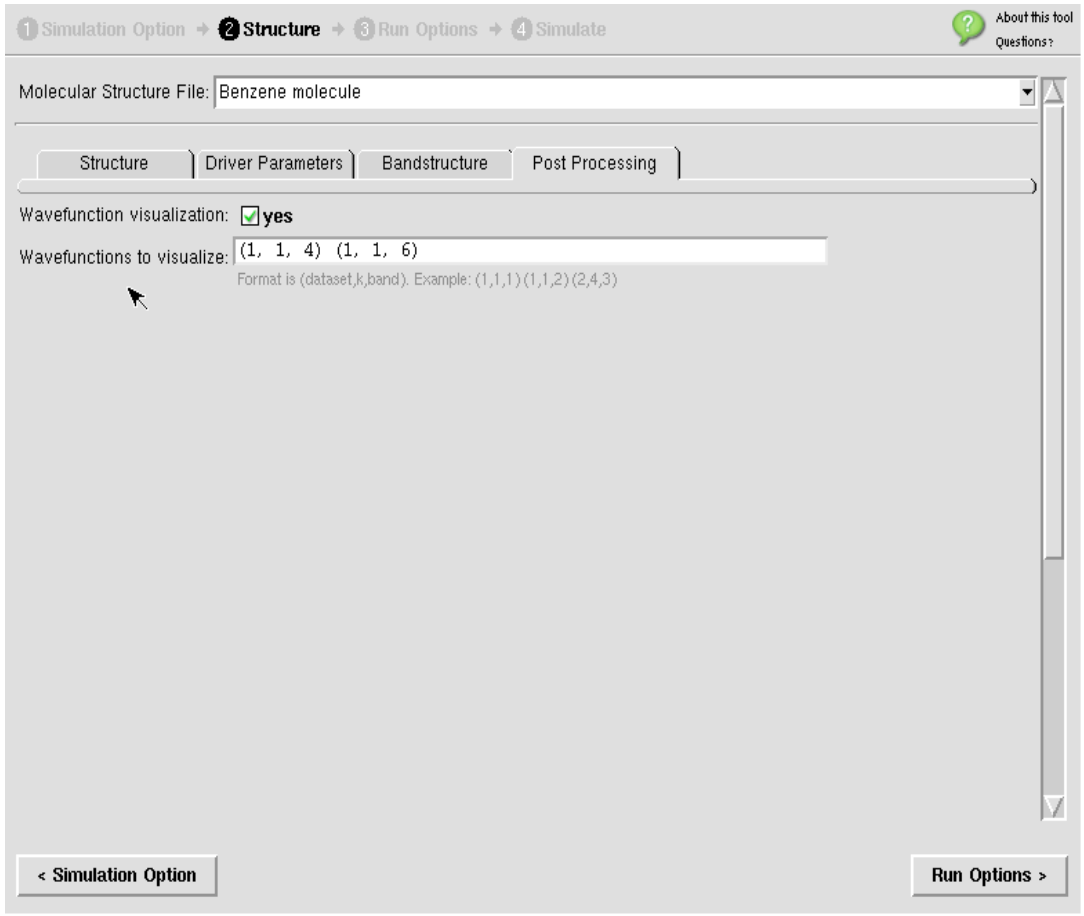
- Choose the algorithms used for DFT calculations as well as the convergence criteria.
- Each of these options deserves its own guide. Please see the references on the last page of this guide for more information.

Second input phase: Structure III



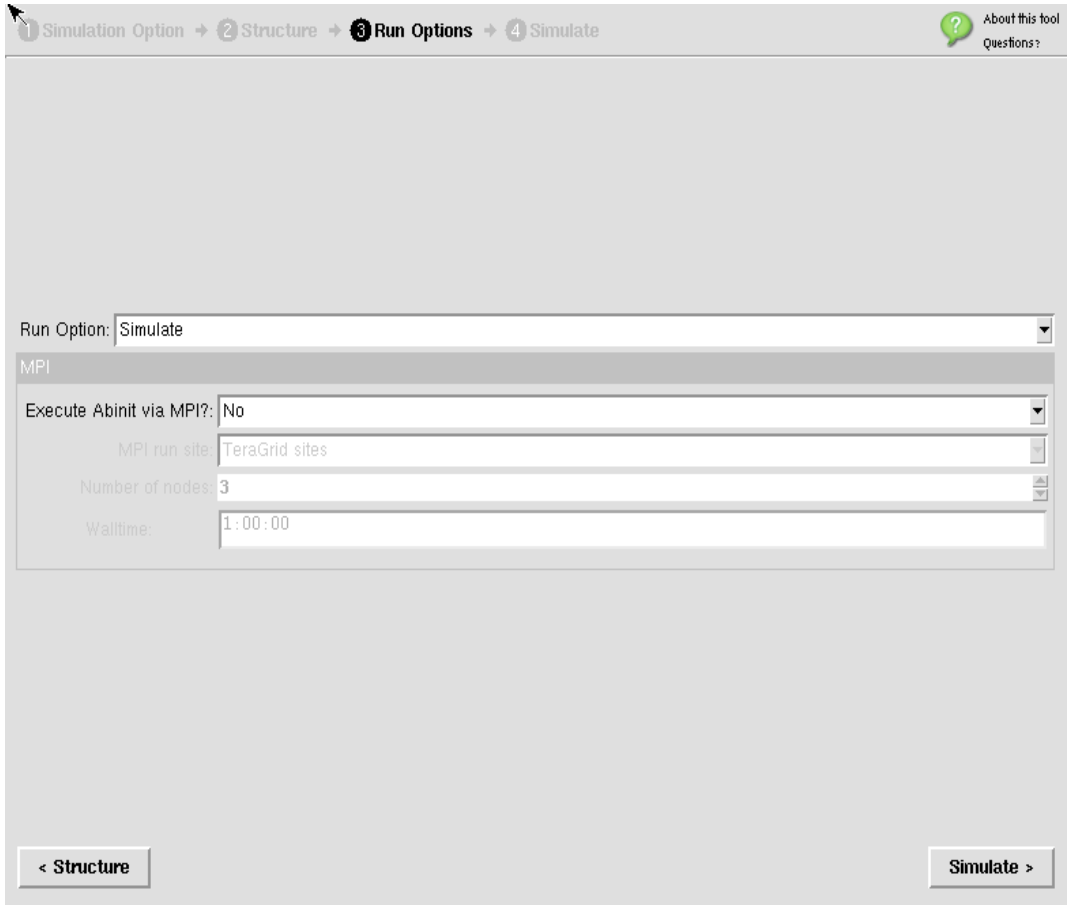
- ABINIT can calculate the band structure of a system.
- Specify which bands to calculate and plot, as well as the *k*-point range.

Second input phase: Structure IV



- ABINIT can also create wavefunction visualizations.
- Specify which wavefunction images to generate.

Third input phase: Run Options



- ABINIT can run serially or in parallel.
- Specify which type of run, and, if parallel, the number of processors on which to run and the maximum run time.

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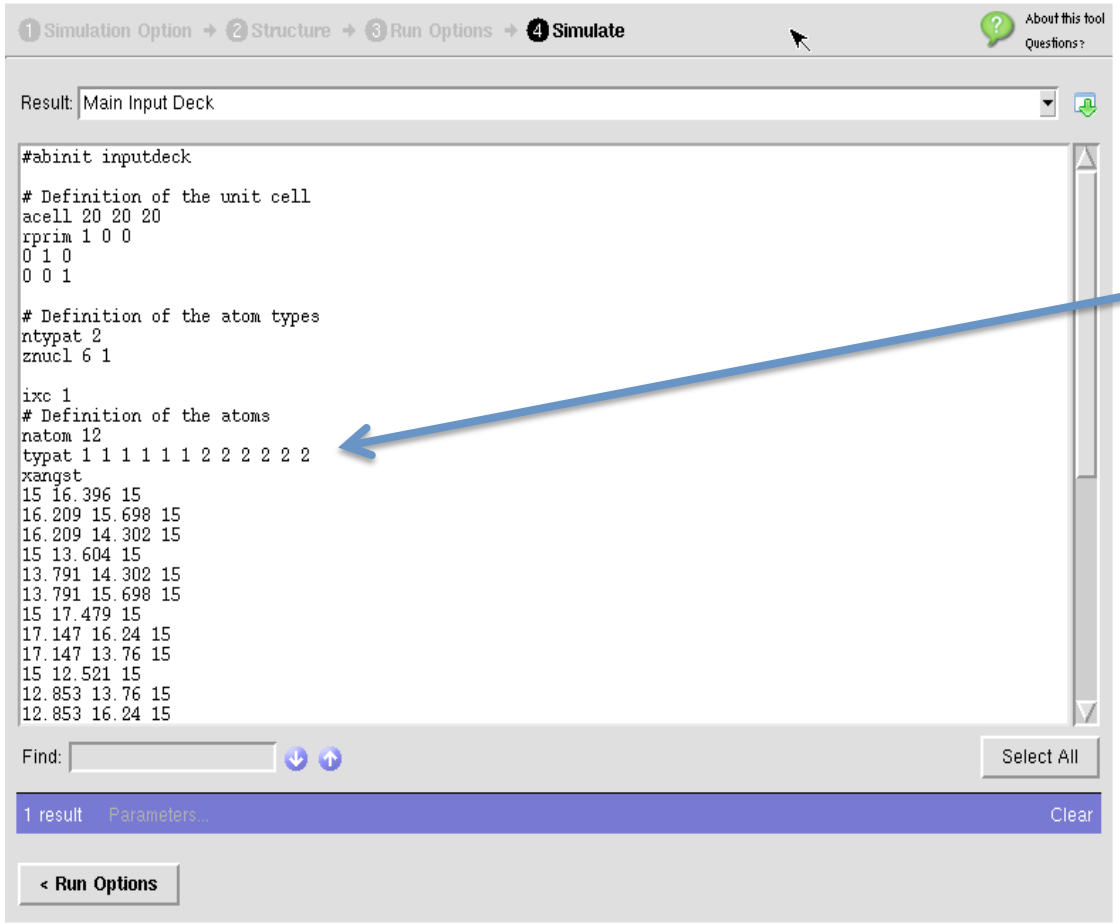
What if you just hit Simulate?



- The default run is a simulation of a benzene molecule.
- An ABINIT input deck is generated from the options chosen in the GUI.
- The default run also generates a plot of total energy over the simulation, the electron density, one wavefunction, and the final molecular structure.

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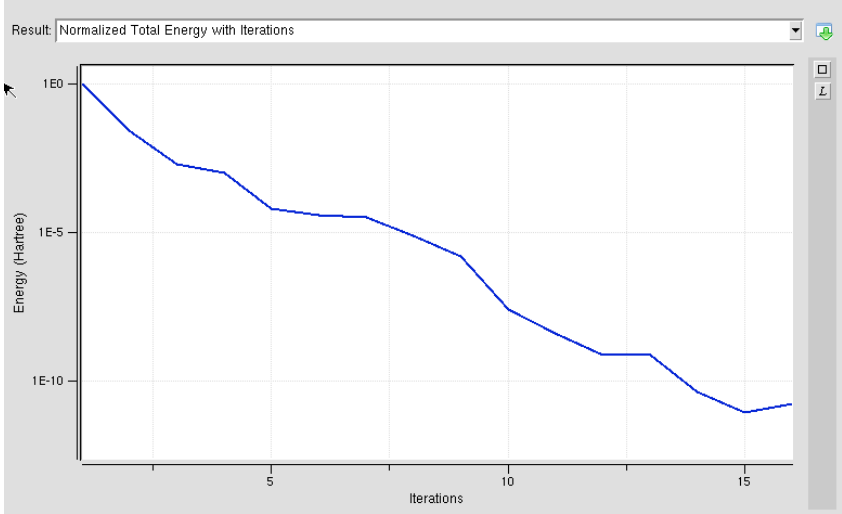
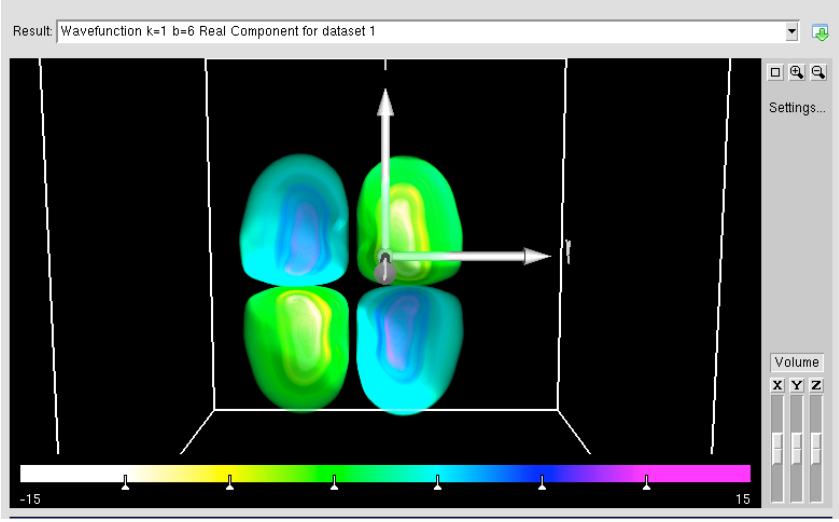
What happens if you just hit Simulate? Default outputs

Total energy, which decreases to convergence during the simulation



Specific wavefunction(s) chosen in the Structure input phase



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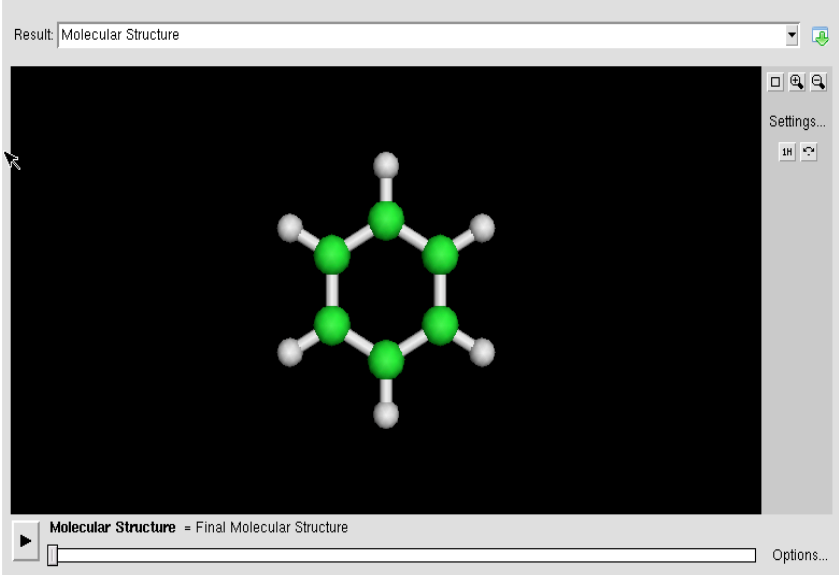
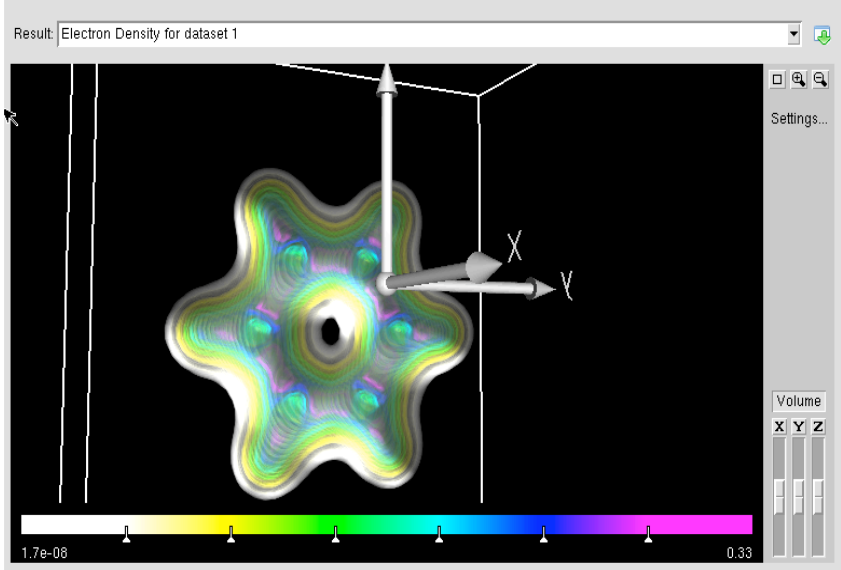
What happens if you just hit Simulate? Default outputs

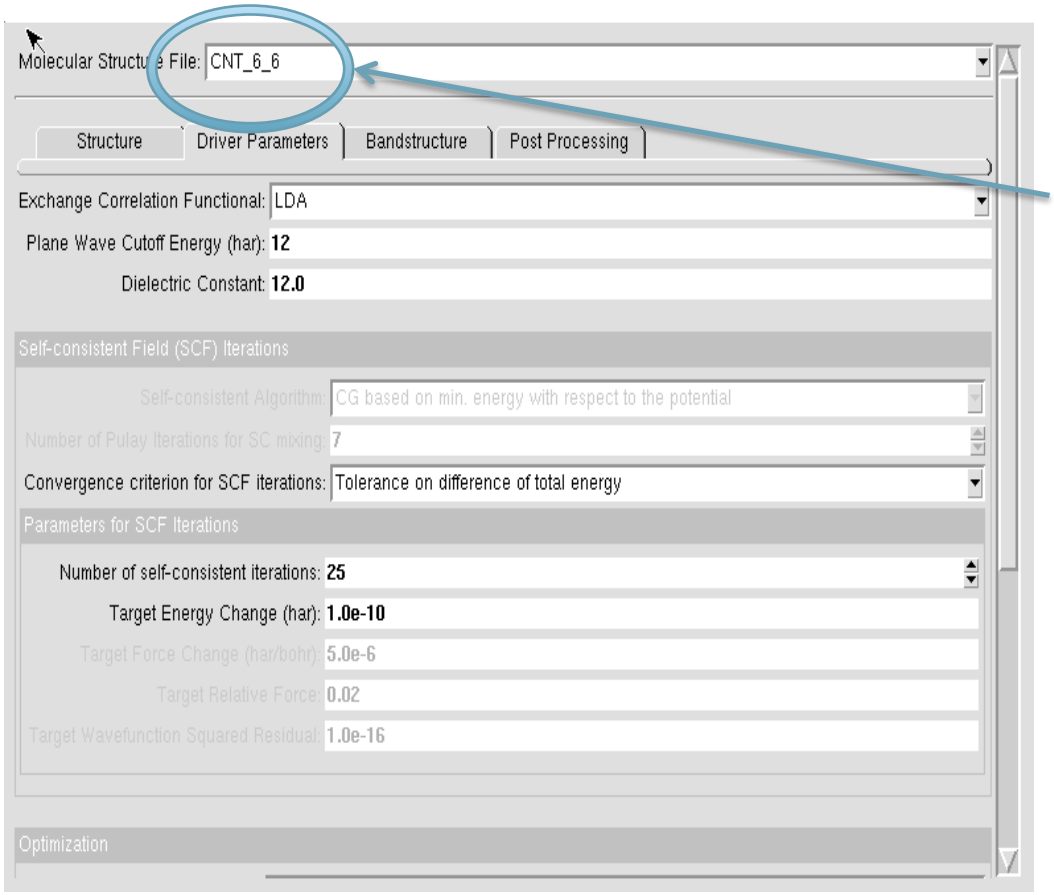
Molecular structure



Electron density



Another preloaded example: (6,6) Carbon nanotube



- Select CNT_6_6 structure file in the Structure phase.
- We can also enable wavefunction visualization and band structure calculation here.

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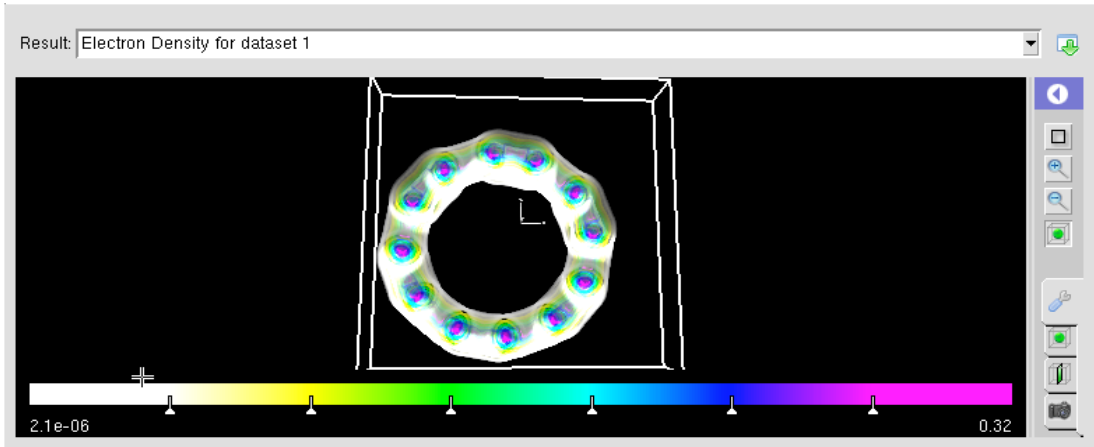
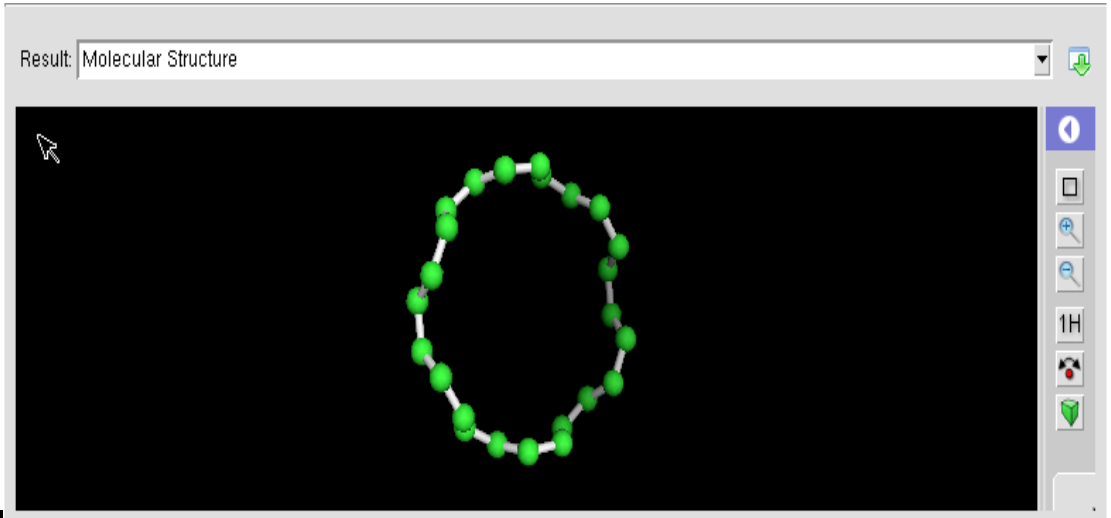
Carbon nanotube outputs



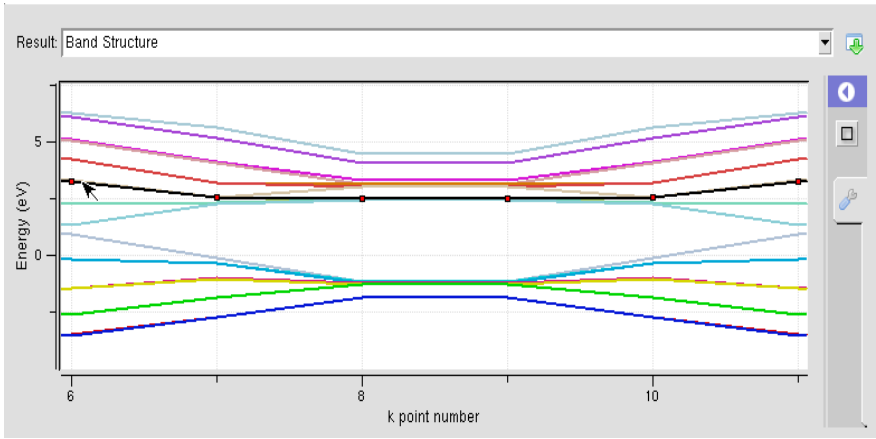
- Electron density



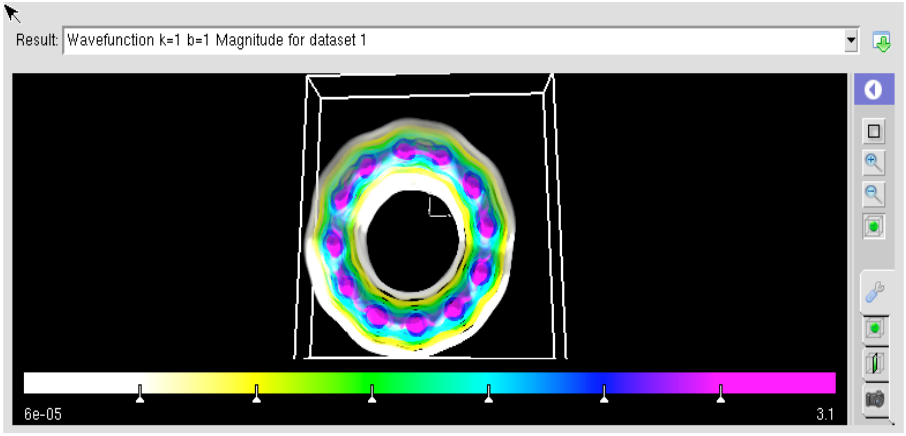
- Molecular structure

Carbon nanotube outputs II

Band structure



Wavefunction



Limitations of ABINIT

- The use of plane waves requires that all systems must be periodic. You may need to create a large supercell, using the scaling factors in the Structure phase, for non-periodic systems. The size of the supercell should be large enough to minimize interactions with periodic images of the system.
- Shifts in the k-point grid must be explicitly stated in the Structure phase. Other *ab initio* codes allow the user to specify, for example, a Monkhorst-Pack [see References] k-point grid.
- When running parallel (MPI) jobs at TeraGrid sites, we cannot currently retrieve job status from the remote sites. The status bar appears to hang while the parallel job runs remotely. This problem is a fundamental architecture issue with the queue systems used by TeraGrid sites. The nanoHUB engineers are working on other submission strategies.

References

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  - » Kohn, W.; Sham, L. J. (1965). "Self-consistent equations including exchange and correlation effects". *Phys. Rev.* ***140 (4A): A1133–A1138. doi:10.1103/PhysRev.140.A1133*** **(1998 Nobel Prize in Chemistry for DFT)**
  - » Local Density Approximation (LDA) for the exchange-correlation energy
    - ✓ D. M. Ceperley and B. J. Alder (1980). "Ground State of the Electron Gas by a Stochastic Method". *Phys. Rev. Lett.* ***45: 566–569. doi:10.1103/PhysRevLett.45.566***
    - ✓ Perdew, J. P.; Zunger, Alex (1981). "Self-interaction correction to density-functional approximations for many-electron systems". *Phys. Rev. B* ***23 (10): 5048–5079. doi:10.1103/PhysRevB.23.5048***
    - ✓ John P. Perdew and Yue Wang (1992). "Accurate and simple analytic representation of the electron-gas correlation energy". *Phys. Rev. B* ***45: 13244–13249. doi:10.1103/PhysRevB.45.13244***

References II

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  - » X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, Ph. Ghosez, J.-Y. Raty, D.C. Allan, "First-principles computation of material properties : the ABINIT software project", Computational Materials Science **25**, 478-492 (2002).
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