PVOX: The PARSEC vizualization toolbox

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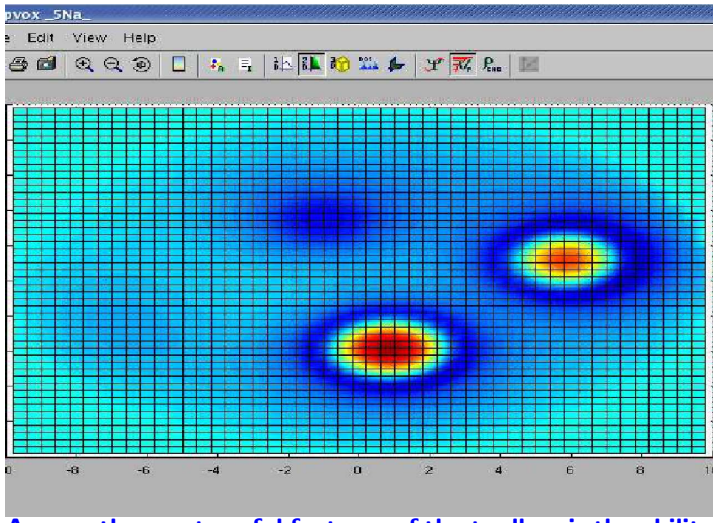
Background. PARSEC (Pseudopotential Algorithms for Real Space Energy Calculations) is a real-space code for electronic structures calculations developed by our group in the last 10 years. The code runs on parallel platforms (using MPI) and uses state of the art techniques in both Density Functional Theory and numerical methods for eigenvalue calculations. As the code is maturing it has become mandatory to provide interactive tools both for entering various options and data and for exploiting the output. In summer 05, three undergraduate interns. Lee Ballard, Micheal Frasca, and Nicholas Voshell, developed PVOX for performing various vizualization tasks from the output.

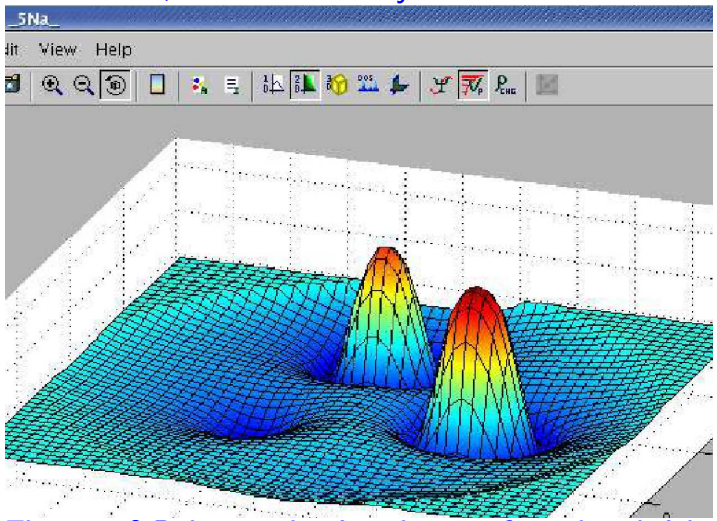
Approach. The matlab graphics interface was used for implementing the toolbox. The developers used many features of the latest version of matlab for this purpose. PVOX reads the output files from PARSEC and offers options in form of icons to the user. For example, the user can "browse" through slices of the various wavefunctions A few of the features of PVOX are illustrated below.

What we learned. This has been an excellent experience which provided the opportunity to work with outstanding students. The tool was developed in a very short period and will be quite useful to the group.

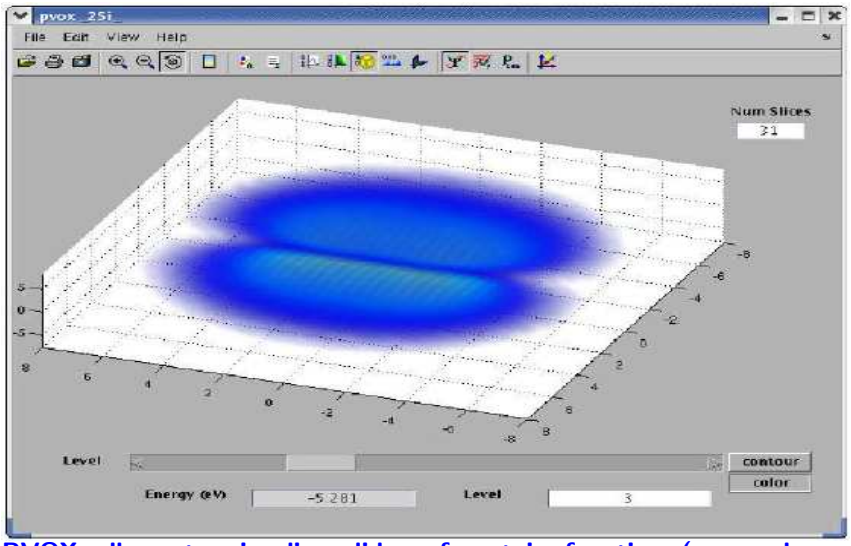
The icons used by PVOX. Each triggers a new item to be visualized. For example the rightmost button will show the atom locations while the icon ρ_{CHG} (next to last) will show the charge density.



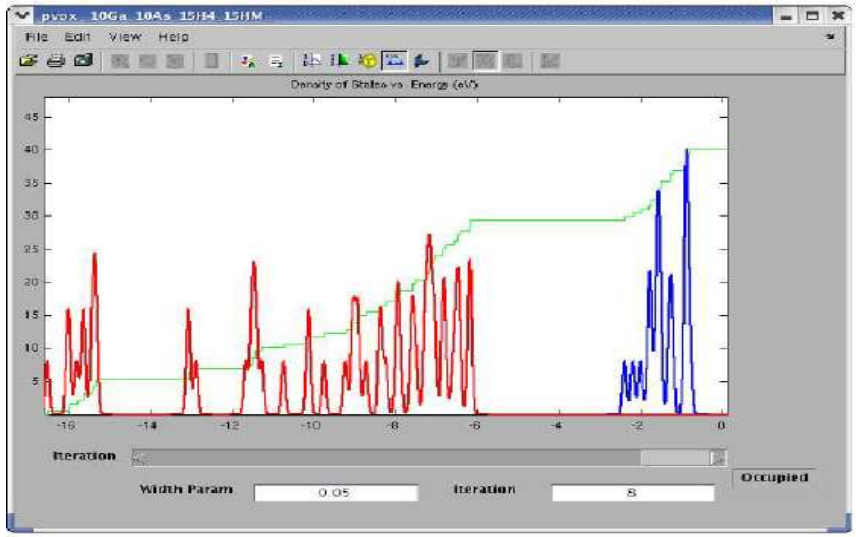
Among the most useful features of the toolbox is the ability to visualize 2-D slices of the data (e.g., potential). Planes are XY slices, with Z selected by the user.



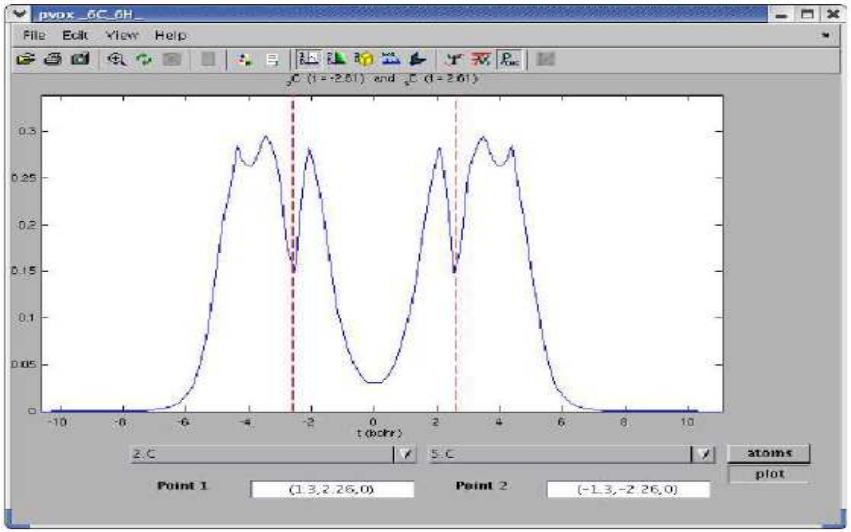
The same 2-D data can be viewed as a surface where height and color to show the data



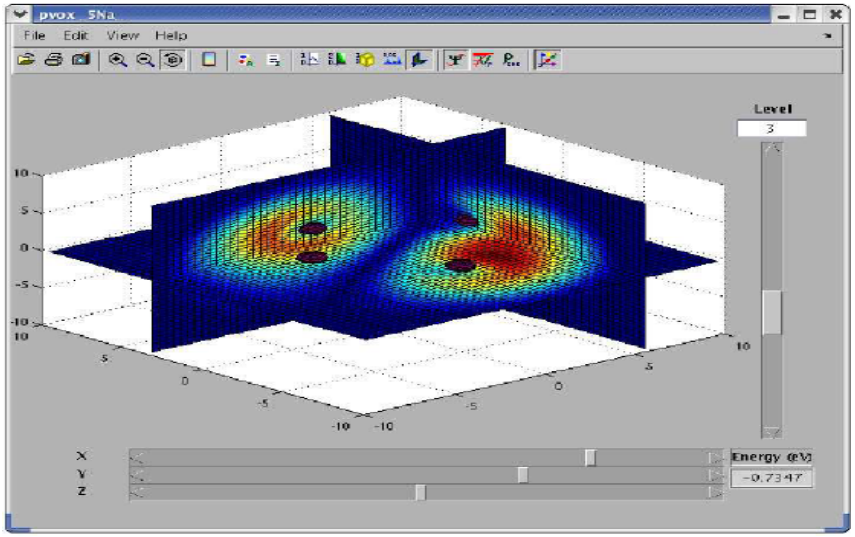
PVOX allows to visualize slides of certain function (e.g. charge density) by exploiting color and transparency.



This shows the density of states with the color red indicating the occupied states and blue the unoccupied ones.



The user can probe into a given function (e.g. Charge density) in space along arbitrary user-defined lines.



The user can select planes and slide through the charge density (for example) in any direction.