Visualization and Calculation of Electronic Structures

Amy Coddington
Nicholas Voshell

Advisors:

Dr. Yousef Saad

Dr. Suzanne Shontz

with help from Adam Jundt

Software

- PARSEC (Pseudopotential Algorithms for Real Space Eigenvalue Calculations)
  - Parallelized density functional theory code to calculate properties of electrons and electronic structure in molecules
- RSDFT (Real Space Density Functional Theory code)
  - Simplified version of PARSEC written in MATLAB
- PVOX (PARSEC Visualization Toolbox)
  - Tool for visualizing PARSEC output

Modeling Electronic Structures

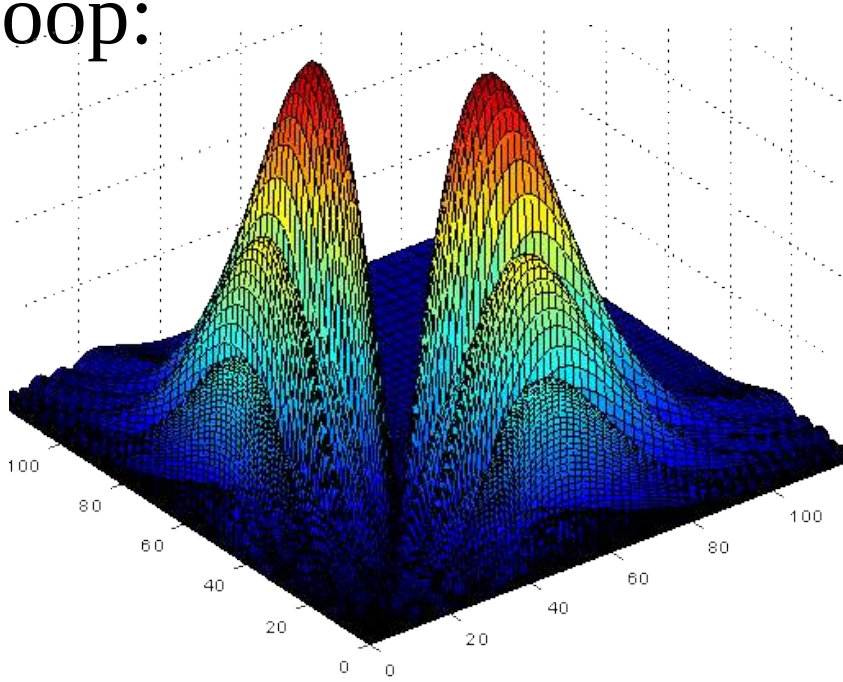
- Uses the Kohn-Sham formulation of Schrodinger equation

$$\left(\frac{-1}{2}\nabla^2 + V_{ion} + V_{XC} + V_H\right)\Psi = H\Psi = E\Psi$$

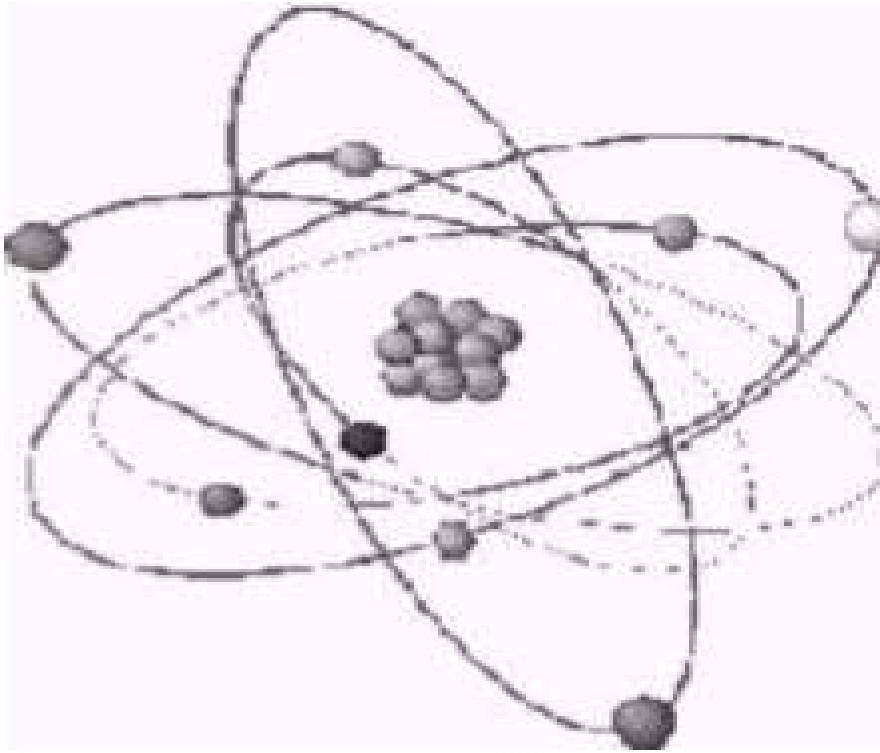
- Takes advantage of multiple simplifications
  - Electron potential determined by overall charge density rather than individual electron interactions
  - Assume inner electrons are closely bound to nuclei which do not move

Calculations: $H\Psi = E\Psi$

- Becomes an eigenvalue problem where E is a scalar, H is a matrix, and Ψ is a vector
- Unfortunately H depends on Ψ, so the problem becomes more complex
- Designed with self consistent loop:
  - Guesses Ψ and calculates H
  - Use that H to generate Ψ
  - Repeat until results are within tolerance



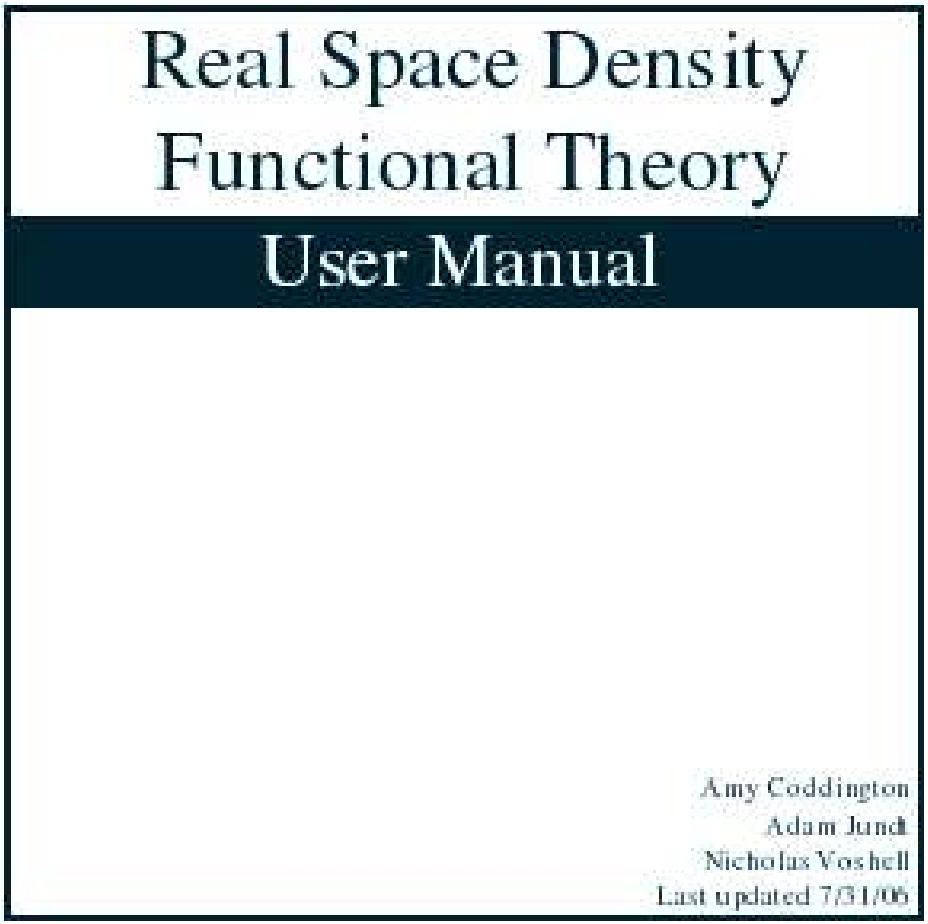
RSDFT vs. PARSEC



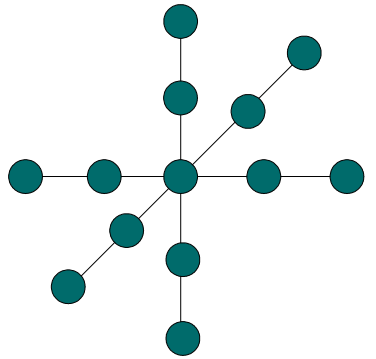
- PARSEC is written in Fortran
  - Conceptually complex algorithms and data structures to take advantage of multiple processors
  - Can be used to accurately model large structures
  - 10+ years of effort and thousands of lines of code
- RSDFT is written in MATLAB
  - Designed for use in prototyping and education
  - RSDFT can currently only be used for small systems of atoms and is not as accurate
  - Under a year of effort and hundreds of lines of code

Overview of work done on RSDFT

- Added higher-order finite difference approximations to the Laplacian
- Implemented more accurate pseudopotential approximations
- Created manual for users of RSDFT



∇^2 Laplacian approximation

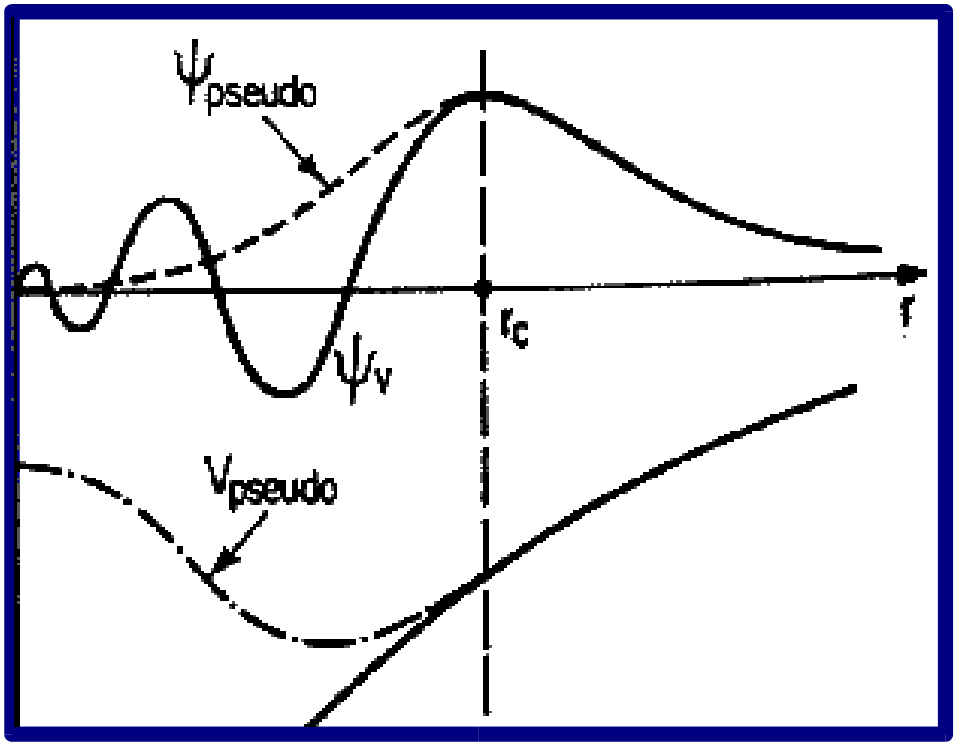


- High-order finite difference methods from Bengt Fornberg
- Represent Laplacian as a linear term in neighboring wavefunction values
- Presently only uses neighbors in orthogonal directions

Order	Pos -4	Pos -3	Pos -2	Pos -1	Pos	Pos +1	Pos +2	Pos +3	Pos +4
2				1	-2	1			
4			-1/12	4/3	-5/2	4/3	-1/12		
6		1/90	-3/20	3/2	-49/18	3/2	-3/20	1/90	
8	-1/560	8/315	-1/5	8/5	-205/72	8/5	-1/5	8/315	-1/560

Pseudopotentials

- Electronic properties dominated by valence electron distribution
- Generally, the inner electrons are confined to small regions
- Pseudopotential approximates ion core potential (nucleus, inner electrons) for easier computation



Pseudopotential Approximations

- First approximation (ionic potential outside, constant inside)

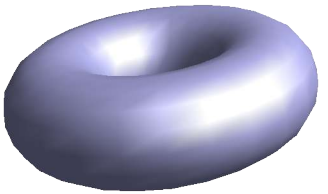
$$w(r)=\begin{cases}\dfrac{-Z}{r} & r>R\\ A & r<R\end{cases}$$

- The Shaw pseudopotential adds more details, yielding a new formula:

$$w(r,\theta,\phi)=\frac{-Z}{r}-\sum_{0}^{l_0}\left[\Theta(R_l-r)*\left(A_l-\frac{Z}{r}\right)*P_l(r,\theta,\phi)\right]$$

$$\Theta(R-r)=\begin{cases}1 & if\ r<R\\ 0 & if\ r>R\end{cases}$$

Spherical Harmonics



- P operator includes spherical harmonics.

$$P_l(r,\theta,\phi)=\sum_{m=-l}^{l}|Y_{m,l}(\theta,\phi)><Y_{m,l}(\theta,\phi)|$$

$$Y_{m,l}(\theta,\psi)=g_l(\cos\theta)*e^{m*\phi}$$

(g is the Legendre polynomial)

- The operation of P on the wavefunction can be described as:

$$P_l\Psi=\sum_{m=-l}^{l}[Y_{m,l}(\theta,\phi)\iint Y^{*}_{m,l}(\theta',\phi')*\Psi(r,\theta',\phi')\delta\theta'\delta\phi']$$

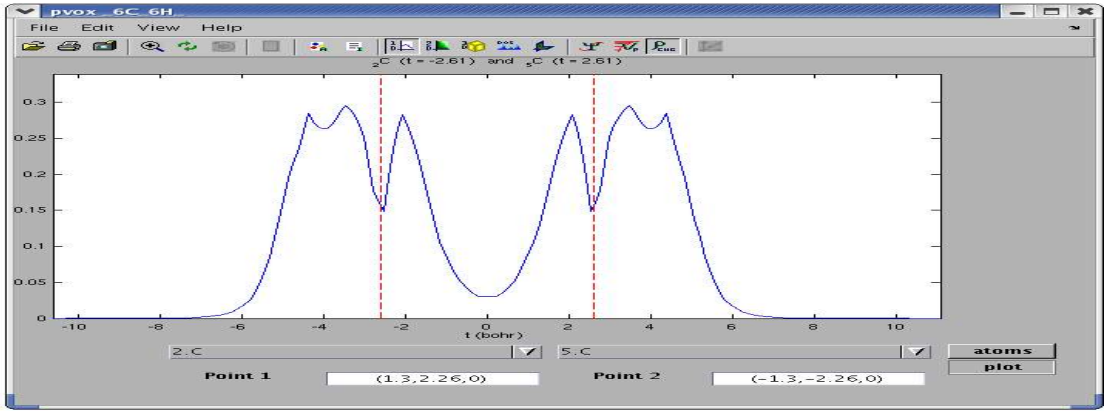
PVOX

- PARSEC Visualization Toolbox
- Written by interns last summer

  Nicholas Voshell
  Lee Ballard
  Michael Frasca

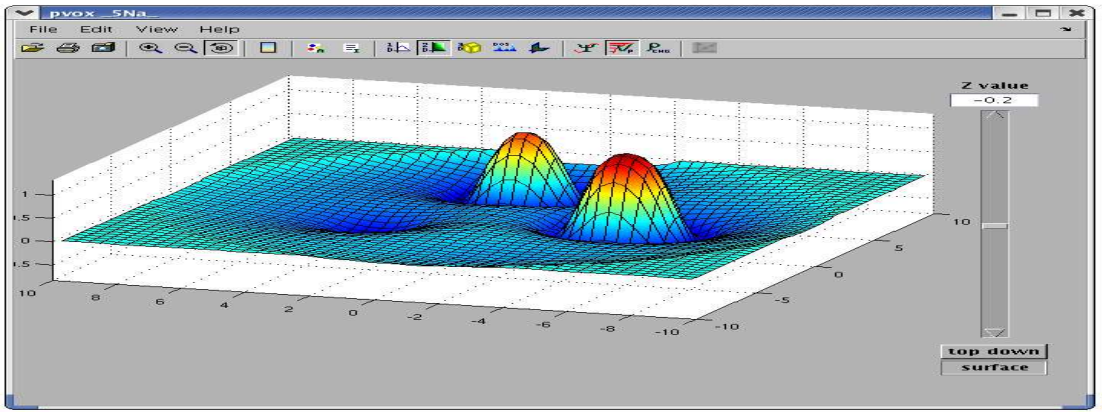
- Application written in MATLAB that shows different views of the wavefunction, electro-magnetic potential, and charge density

PVOX Functionality



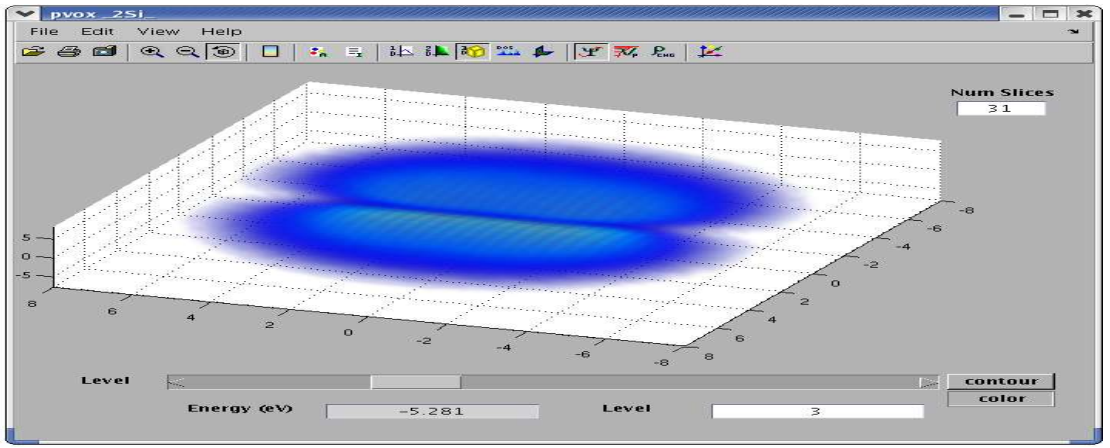
1D View

easily view wavefunction, charge density or potential



2D View

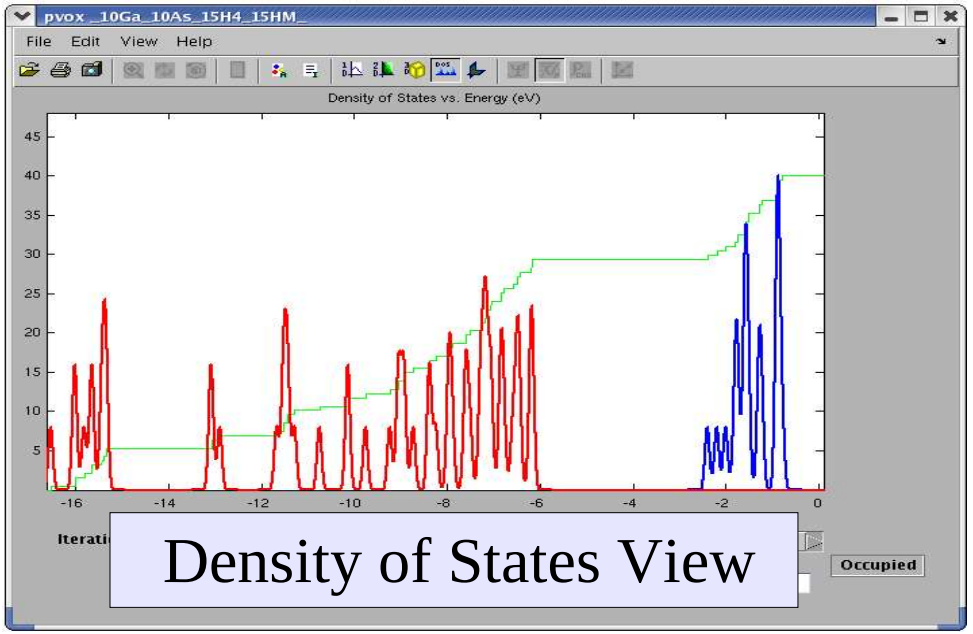
view XY slices of the data with user-defined Z



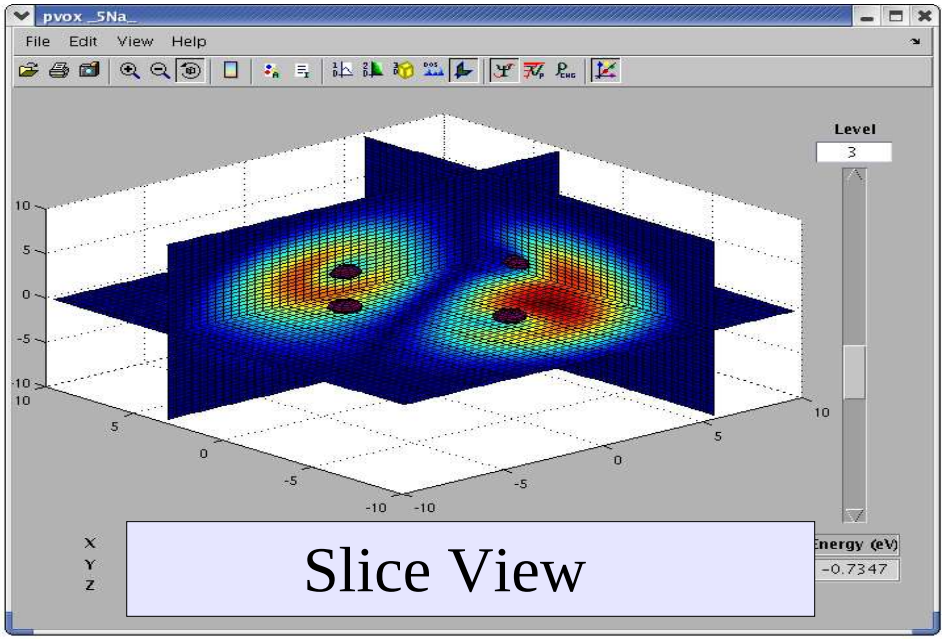
3D View

view based on color and transparency, contour view also available

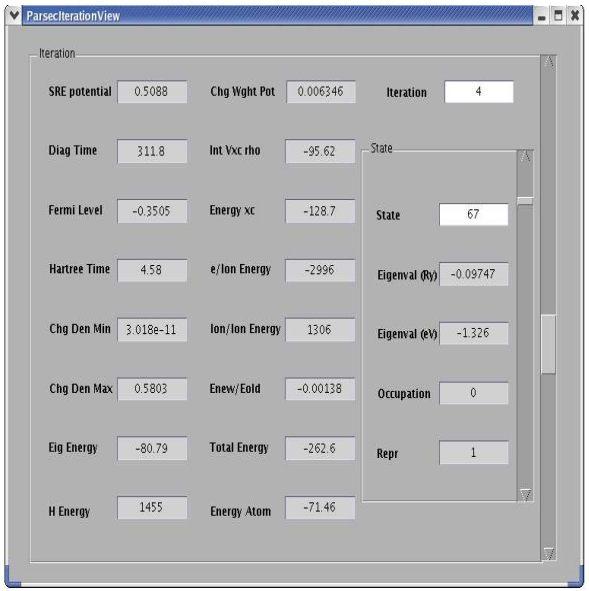
PVOX Functionality Continued



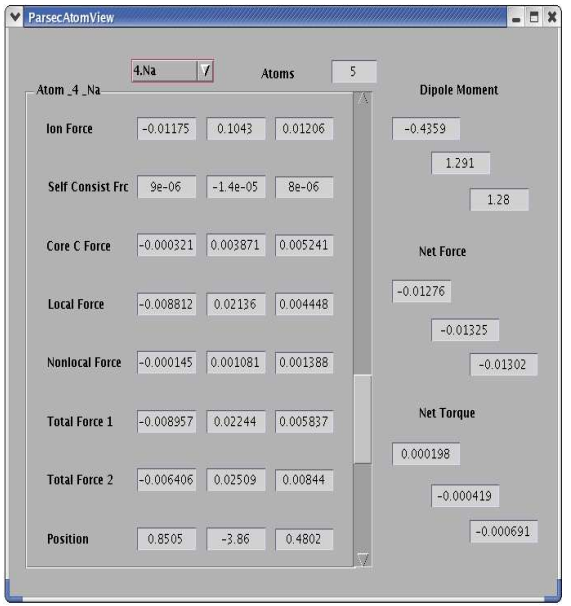
Density of States View



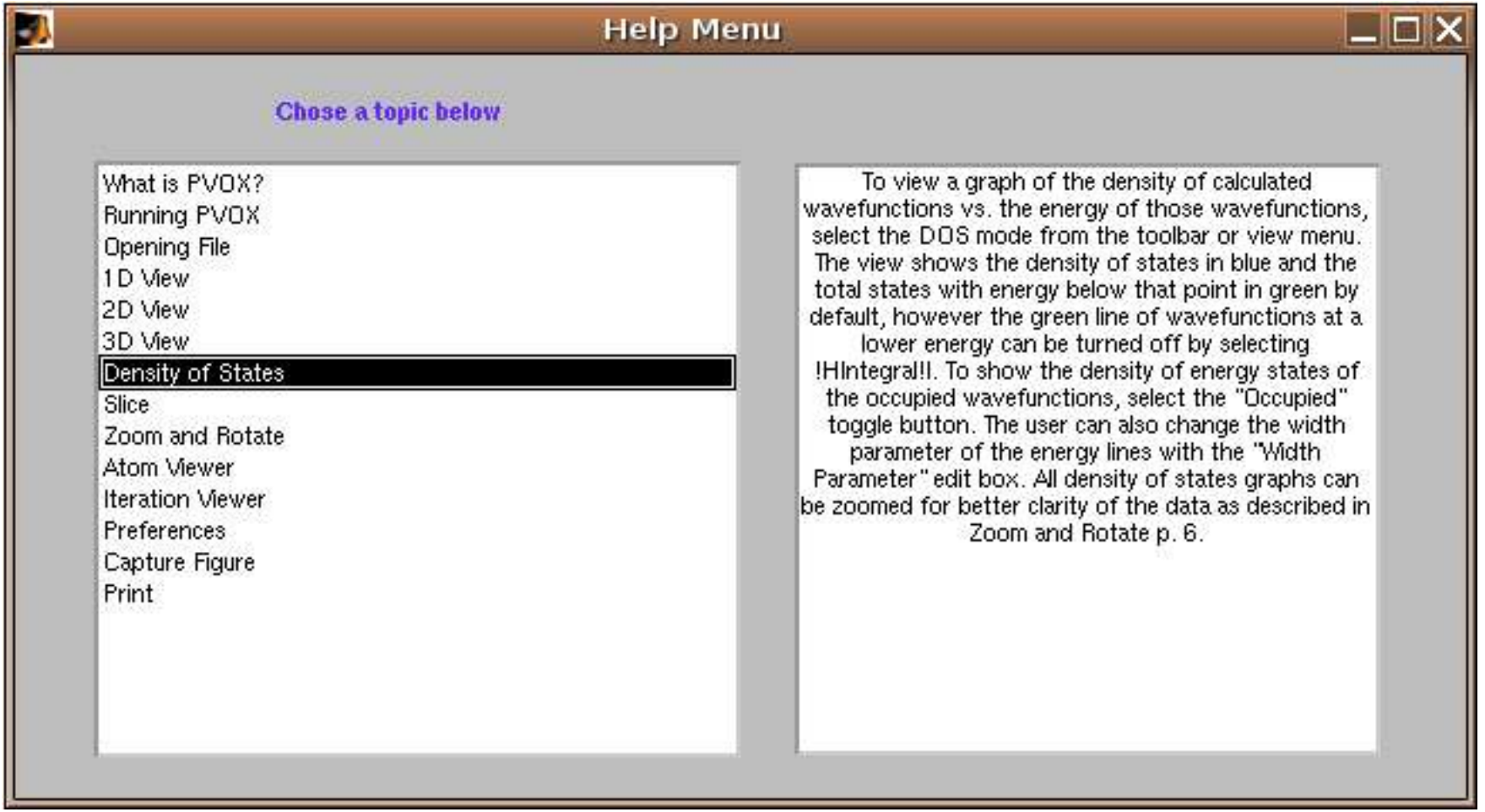
Slice View



Iteration and atom data viewers allow users to examine calculation results

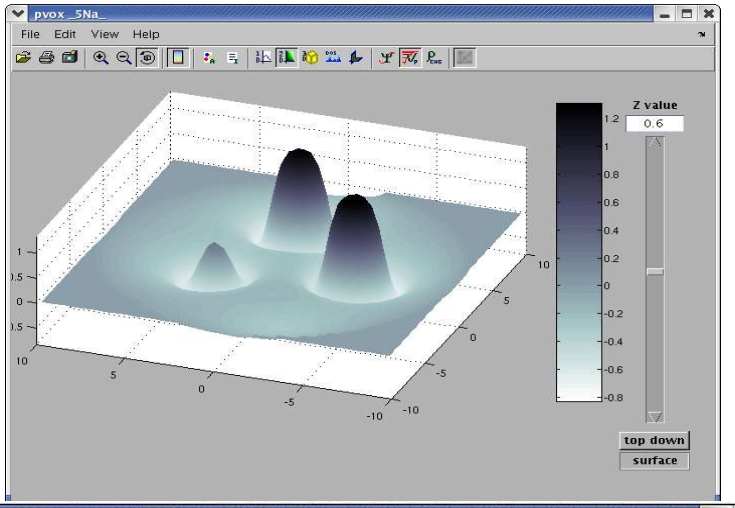


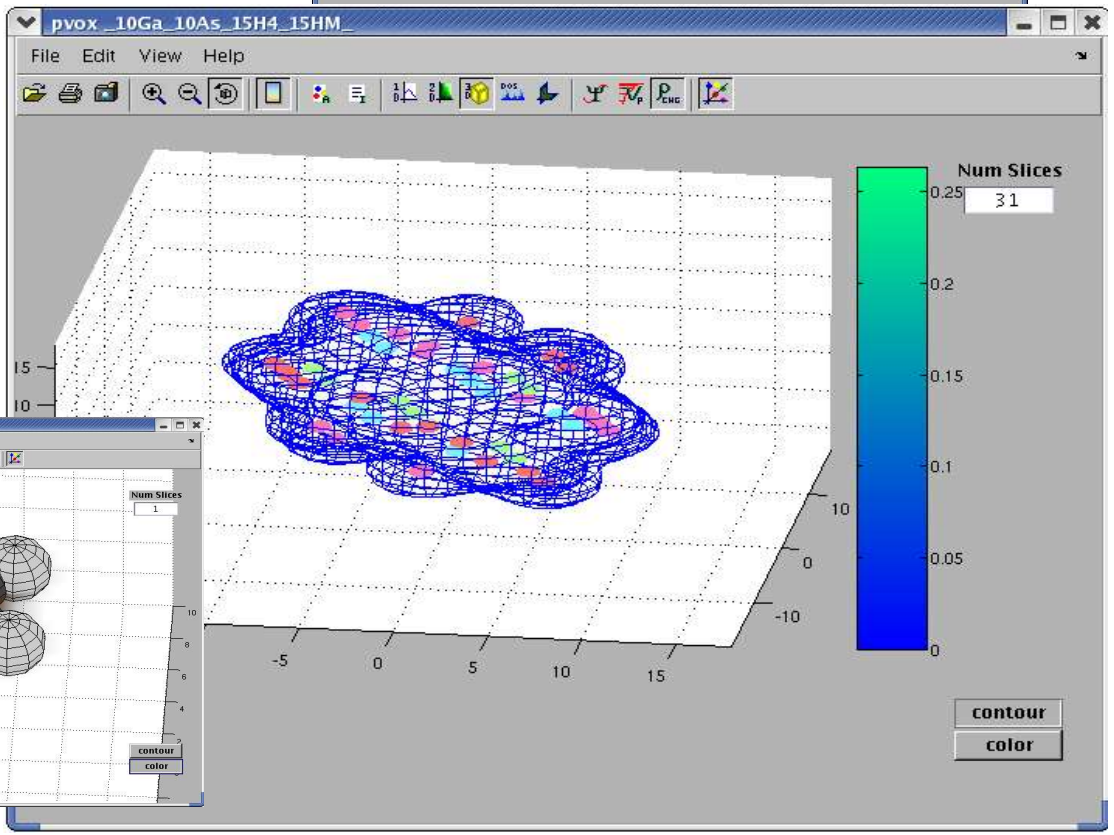
Help Browser

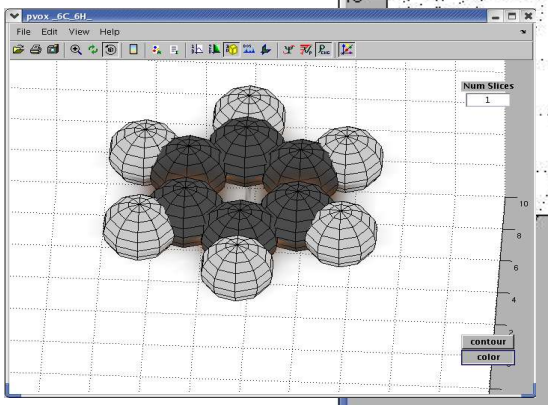


Preferences

- Atom color / size
- Colormap
  - Select from standard MATLAB colormaps
  - Invert colormap
- Grid lines
- Contour values
- Draw mode

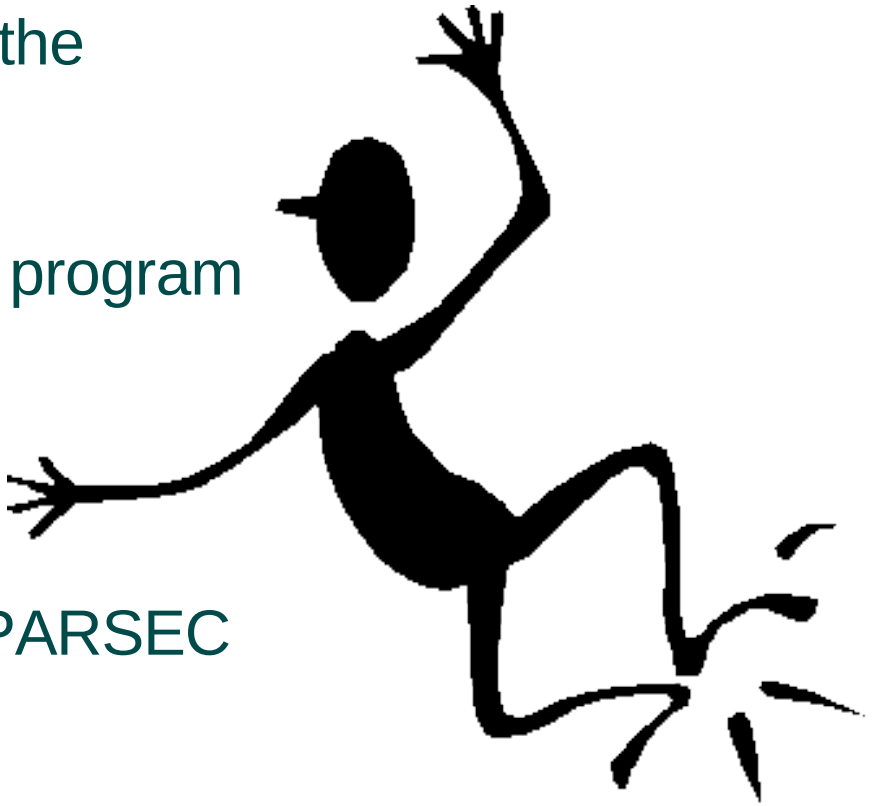






PVOX progress

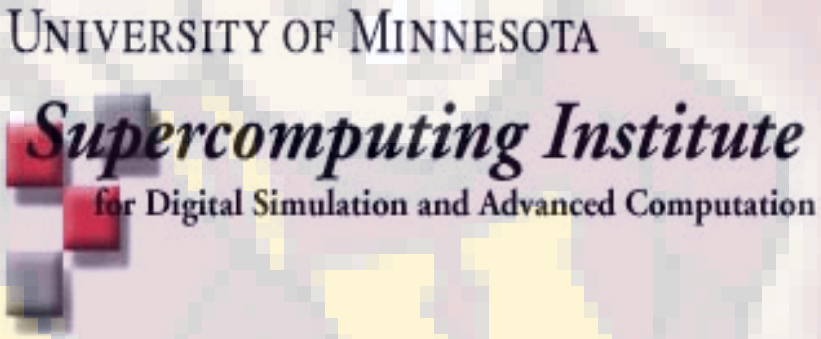
- Fixed colorbar in MATLAB R13 (version 6.5)
- Tested PVOX across various platforms and versions of MATLAB
- Added a troubleshooting guide to the documentation
- Added a help menu inside of the program
- Modified PVOX to read in RSDFT output
- Program has been requested by PARSEC users and will be available soon

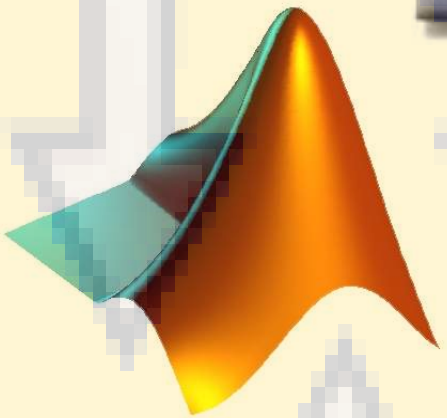


Potential Future Work

- Parallelize RSDFT code to increase performance
- Implement more accurate methods in RSDFT
- Improve 2D mode in PVOX to allow user-specified planes
- Provide PVOX support on Macintosh and Windows platforms

Any Questions?





Special thanks to our advisers Prof. Saad and Dr. Shontz, our colleague Adam Jundt, and MSI and ITAMIT