Force Field Explorer

A Graphical User Interface to TINKER

August 2003, Version 1.1

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Introduction

Force Field Explorer is being developed to facilitate use of the TINKER suite of molecular modeling tools. Current features include:

- Visualization using common representations (wireframe, ball & stick, tubes, spacefill, etc.) with special features for force field specific parameters such as Lennard-Jones minima and partial charge magnitudes.
- An Editor for Keyword Files.
- TINKER trajectory playback.
- Setup and real-time visualization of modeling routines, including optimizations, molecular dynamics, simulated annealing, Monte Carlo, etc.

Current Release and Future Plans

This is the second release of Force Field Explorer, v. 1.1. Major improvements over the initial release include:

- Communication between Force Field Explorer and TINKER has been automated.
- A shell window has been added which creates the potential for complete scripting control over Force Field Explorer.

Future goals include tighter coupling to the TINKER suite of modeling routines. We hope to add editing commands and support for other file types. Additionally, intuitive visualization techniques for results obtained using the AMEOBA potential are under development.

Installation

Force Field Explorer can be installed using the following directions (links to all required downloads are in the Table below).

1. Install JRE 1.4.2 and Java3D 1.3 (or higher)

   First, install Java version 1.4.2.
   Second, install Java3D version 1.3.1
   Linux users must copy the Java3D package into the top level Java directory before installing.

2. Install TINKER v. 4.1

   Download and install the TINKER v. 4.1 Distribution.
   Download or build TINKER Binaries.

3. Configure environment variables

   Edit the "ffeenv" file found in the TINKER/ffe directory for your platform such that it corresponds to your TINKER and JRE install directories.
   On Windows, the result should be pasted into the autoexec.bat file (usually found at c:\autoexec.bat).
   On Linux, the resulting file should be sourced from your login script.

Windows	Linux
Java 1.4.2 (JRE version without NetBeans)	Java 1.4.2 (JRE version without NetBeans)
Java3D 1.3.1 (JRE OpenGL version)	Java3D 1.3.1 (JRE version)
TINKER 4.1	TINKER 4.1

Supported Platforms

Supported platforms currently include Linux and Microsoft Windows. HP-UX, Solaris and SGI-IRIX will eventually be supported after further testing. We are currently considering porting the Java3D portion of Force Field Explorer to the Xith3D scenegraph that uses the JOGL wrapper for OpenGL calls. This would allow Force Field Explorer to run on MacOSX. The time frame on this is somewhere between next week and six months from now...

Bugs

Poor video card drivers can sometimes result in Force Field Explorer hanging your computer, although rarely with newer Xfree86 releases. If this should happen, try to find the latest drivers for your platform/video card combination. Should you happen to perform some command that causes a Java stack trace to be dumped to the console, please copy the output and forward it to us.

Acknowledgments

Most of the work on Force Field Explorer has been done by Michael Schnieders, a 3rd year graduate student with Jay Ponder. A significant contribution was also made by Zhiguang "Frank" Gao over the summer of 2002. The Force Field Explorer logo is courtesy of Pengyu Ren and shows an optimized AMEOBA gas phase water dimer. Special thanks go out to Alan Grossfield for offering many helpful suggestions. We would also like to thank Eric Reiss for making available his modified version of some Java3D Behaviors and Pat Niemeyer for his work in developing the BeanShell scripting framework. Needless to say, this tool (and the fun of creating it) exists due to the support of Jay Ponder.

Menu Descriptions

- **File**

  - Open
    An attempt is made to open any selected file as if it were a TINKER *.xyz file. Archive files are detected and their entire contents read in for play back.

  - Merge
    Merge two TINKER *.xyz files into one. At least two systems must be selected in the Tree view, at their respective root nodes. No attempt is made change atom type numbers if the systems use different force fields.

  - Save As
    Saves the active *.xyz file under a different name. Saving changes to archive files is not yet supported.

  - Close
    Close the active *.xyz file.

  - Close All
    Close all open files.

- **Selection**

  - From Tree
    - Select
      Select all the atoms below the currently selected node on the Tree, coloring them as specified using the "Selection Color" menu item.
    - Clear
      Clear all the currently selected atoms

  - From Graphics
    - Selection Level
      Specifies how many are atoms are selected when clicking over systems rendered to the Graphics window:
      - Atom
        Select one atom
      - Bond
        Select a bond, multiple selections on the same atom cause iteration through bonds the selected atom contributes to.
      - Angle
        Select an angle, multiple selections on the same atom cause iteration through angles the selected atom contributes to.

- Dihedral
  Select a dihedral, multiple selections on the same atom cause iteration through dihedrals the selected atom contributes to.
- Group
  Select one group/residue
- Molecule
  Select all atoms covalently bonded to the current atom
- System
  Select all atoms in the system

- Clear
  Clear all the currently selected atoms

♦ Selection Color
Choose the color for selected atoms.

➢ **View**

♦ Center
- System
  Remove any rotations/translations that have been applied to the selected system.
- Graphics
  Remove any zoom/rotation/translation that has been applied to the entire scene.

♦ Drag System
Specify how systems are selected for rotation/translation.
- Below Mouse
  The system below the mouse in the Graphics panel is moved.
- Active
  The System whose node is currently selected in the Tree is moved.

♦ Rotate System About
- Selection
  This sets the center of rotation of the active system to the geometric center of the atom(s) selected by Graphical picking.
- Center
  Reset the center of rotation of the active system to its geometric center.

♦ Capture Graphics
Capture the Graphics panel to an image file of the format specified under Format. The resolution of the image is exactly the number of pixels in the 3D window.

♦ Format
Select the format for image capture. Available formats currently include:

- JPEG
- PNG

♦ Background Color
Select the background color for the Graphics scene.

➢ **Graphics**
While a graphics change is being rendered, one additional graphics command will be cached. Other commands are ignored while the 3D view catches up. Changes are applied to all atoms below the currently selected node in the Tree View.

♦ Style
- Wireframe
- Spacefill
- Invisible
- Ball & Stick
  Slow for large systems (more than a few thousand atoms)
- Tube
  Slow for large systems (more than a few thousand atoms)
- RMIN
  Similar to Spacefill, but the sphere radii are set to the Lennard-Jones minima for the given atom

♦ Color
- Atom
  By atomic number
- Group
  By residue type
- Molecule
  By molecule
- System
  By system

♦ Polygon
- Fill
  Fill rendered polygons
- Points
  Render only vertices
- Lines
  Render edges between vertices

♦ Toggle Hydrogens
Show/Hide hydrogen atoms

♦ Preferences – Radius

A scale factor applied to all rendered spheres and cylinders.

- Preferences – Wireframe Thickness
  This specifies the thickness of wireframe representations in pixels.

- Preferences – Detail
  Changes the number of vertices used in creating spheres and cylinders. More vertices (a higher number on the slider) creates a smoother appearance, but slower rotations.

Tools

- Measure
  Measure various geometric quantities writing output to the console:
  - Distance
    Measure the distance between two atoms (angstroms)
  - Angle
    Measure the angle formed by three selected atoms (degrees)
  - Dihedral
    Measure the dihedral formed by four selected atoms (degrees)

- Trajectory
  Trajectory commands control visualization of TINKER archive files. Only one archive file can be played at a time.
  - Play
    Iterate through frames at the requested Rate, or as fast as possible if the requested Rate can not be achieved.
  - Stop
    Stop play back.
  - Rate
    Set the playback frame Rate, only values between 1 and 199 are accepted. Note that rate and frame numbers currently can not be set until the trajectory is played at least once.
  - Frame
    Choose the displayed snapshot.

- Simulation

  - Connect
    - Local
      Attempt is made to connect to an executing TINKER job on the machine where FFE is running.
    - Remote
      Attempt to connect to an executing TINKER job on the machine specified by the the IP address entered in the “Remote Adress” dialog.

- Release
  End communication with an executing TINKER job. A connection to one executing simulation at a time is currently supported. To form a new connection the current simulation must be released.
- Port
  Specify the port through which FFE and TINKER communicate. The default is 2000.
- Remote Address
  Specify the remote IP address that FFE will use to connect to a remote simulation.

➢ **Window**

♦ Show
- Tree
  Show/Hide the Tree view.
- Toolbar
  Show/Hide the Toolbar.
- Graphics Axis
  Show/Hide the Axis used to rotate the entire scene in the Graphics window.
- Console
  Show the command line Console.

♦ Resize Windows
This resets the bars that separate GUI components to their default relative sizes. This is helpful because some sizing operations are not allowed as a result of the 3D window being "Heavy Weight" while the Tree is "Light Weight". Specifically, attempting to drag the separator between the Tree and Graphics windows is not possible. The "<" and ">" buttons on the Force Field Explorer toolbar can also be used to change the relative size of the Tree and Graphics components.

♦ Look & Feel
Controls the Java skin mechanism.
- Java
  This is the default appearance and should be consistent across platforms.
- System
  This appearance should resemble that of the native platform.

➢ **Help**

A help menu has not been implemented yet, sorry. Hopefully this manual is answers any questions.

♦ About
This displays our logo and contact information.

Description of Force Field Explorer Components

Tree

The Tree is a structural hierarchy of each system, used for navigating through systems and making selections. When Force Field Explorer opens a TINKER coordinate file, it attempts to groups atoms into covalently bonded groups. Within a covalent group it searches for protein/nucleic acid backbone patterns and if found further groups atoms into residues. This is done even in the absence of a sequence file. Furthermore, all waters are grouped together, as are ions. For example, after rendering an entire membrane system in Spacefilling mode, selecting the "Water" node and choosing Wireframe gives result shown in Figure 1.

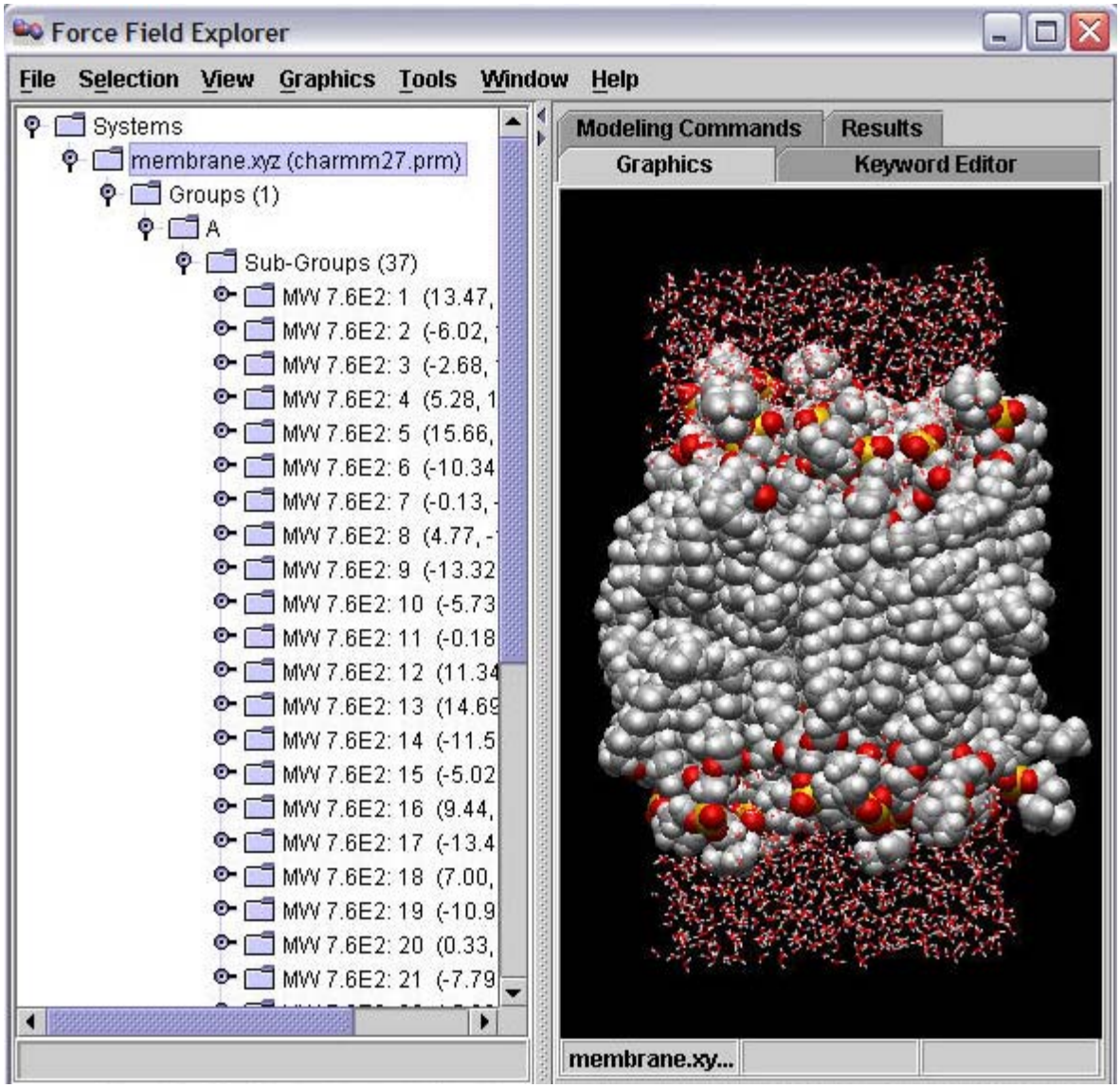

Figure 1. The membrane system has been highlighted in the Tree View. The current rendering was created by choosing Spacefill for the entire system, then selecteing the Water node (not shown) and choosing Wireframe.

Graphics

Dragging the Graphics Axis component performs a rotation about the origin of the entire scene. This is useful for manual docking of two systems. For example, after positioning each system individually in the X-Y plane by dragging them with the mouse, a rotation about the Y-axis allows orientation in the Y-Z plane.

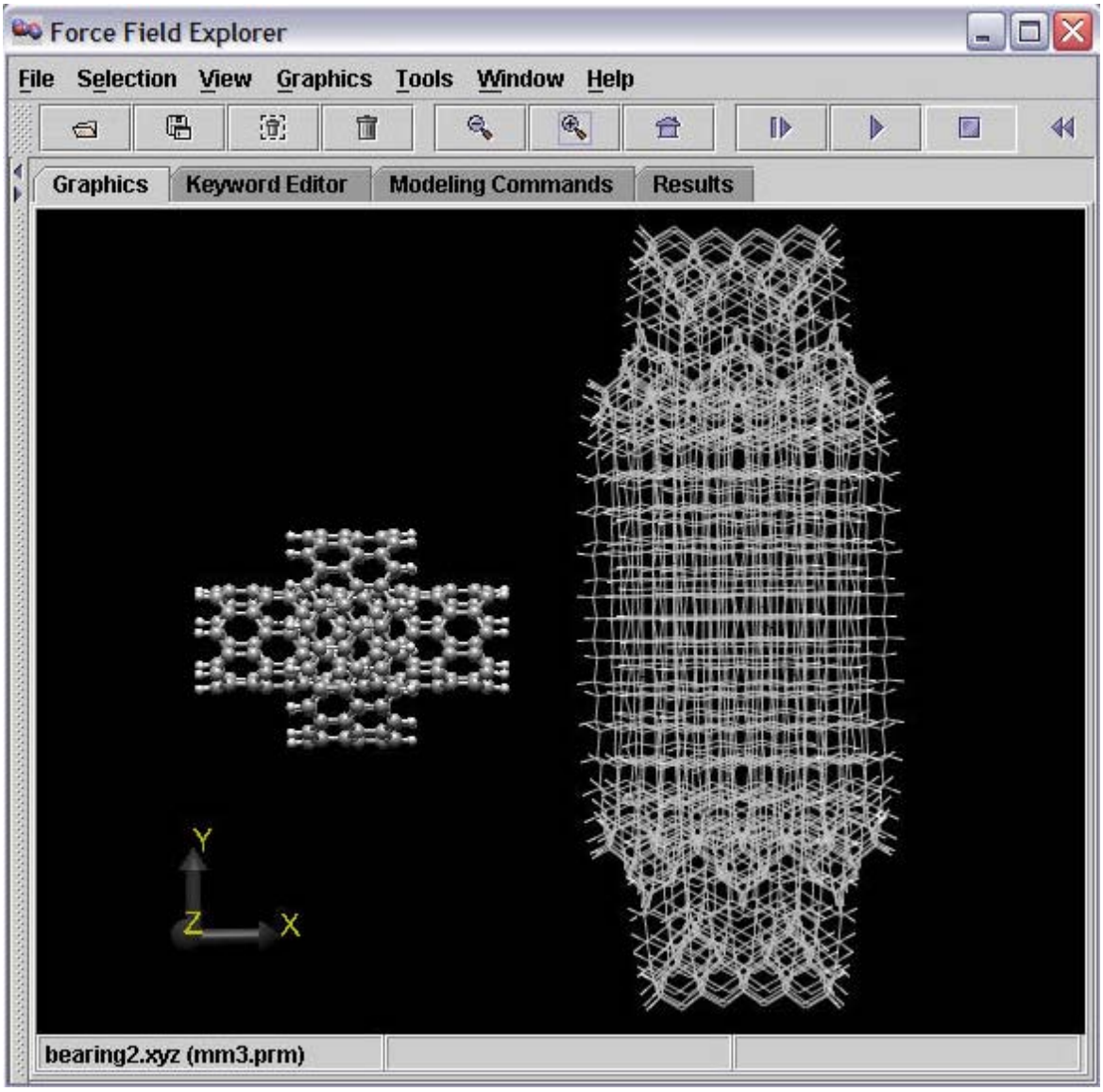

Figure 2. Dragging the Axis causes the entire scene to rotate about the global origin.

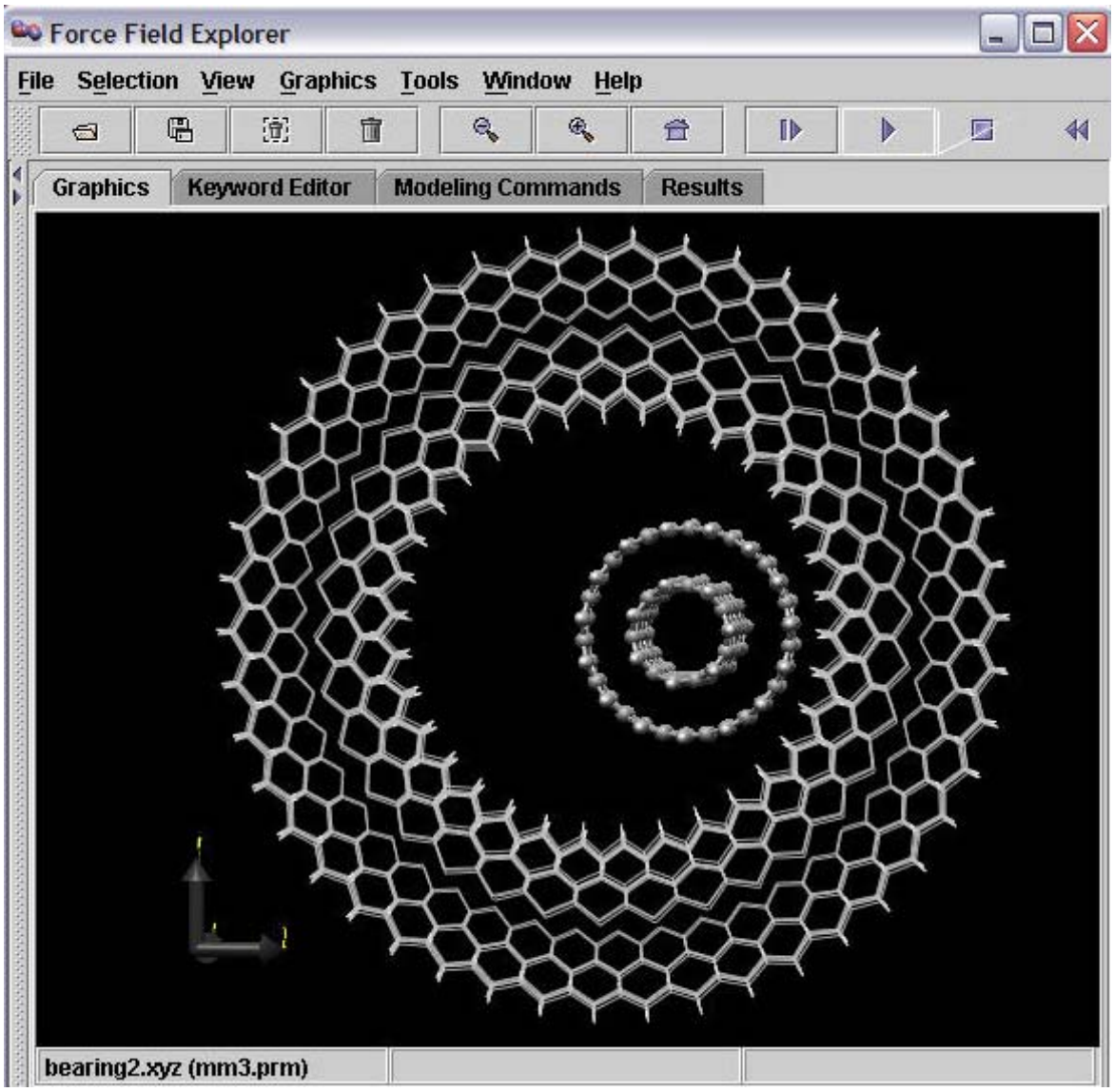

Figure 3. Global rotations are useful for manual docking of two or more systems.

Keyword Editor

The Keyword Editor facilitates modification of keyword files that control various aspects of TINKER calculations. If a Modeling Command is executed on a system, the corresponding Keyword File is automatically saved. Modifications can also be saved at any time using one of the save buttons. Any text or keywords that Force Field Explorer does not recognize are considered "Comments" and are appended to the end of saved key files. As an example, all of the keywords needed to define the TIP3P water model for use in TINKER are shown below.

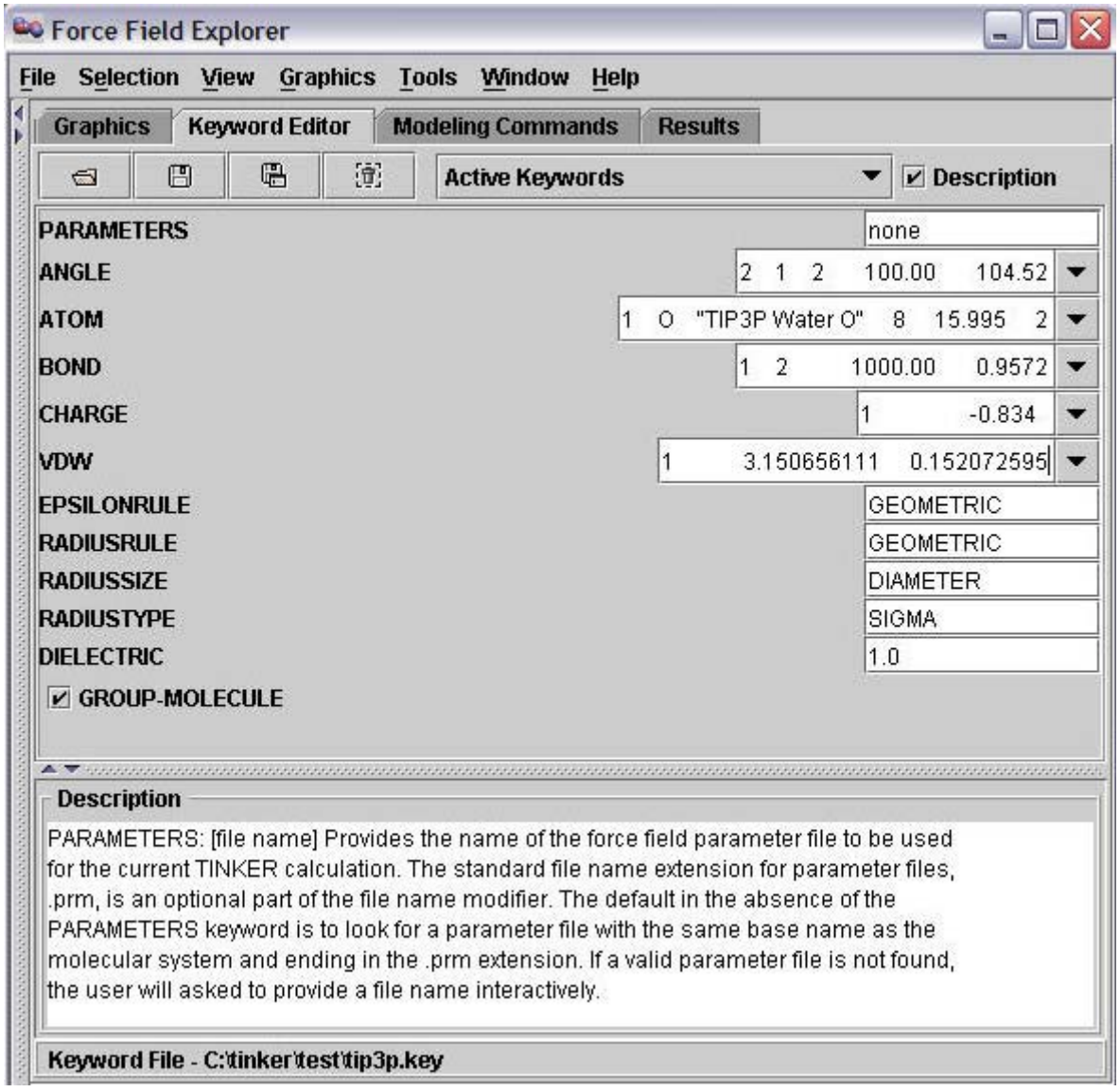

Figure 4. The Keyword Editor is displaying all the keywords needed to define the TIP3P water model for use in TINKER.

Modeling Commands

The Modeling Commands component of Force Field Explorer allows launching of many of the TINKER programs. After selecting a routine and configuring its modifying arguments, selecting the "play" button starts the job running. If the job will modify the coordinates of the system, FFE will automatically connect to the routine and show progress interactively. If the job completes before Force Field Explorer is exited, the textual results in the log file are loaded into the Results component. If Force Field Explorer exits while jobs are running, they continue in the background unless explicitly killed by the user.

As an example, after loading "crambinx.xyz", a unit cell of a crambin crystal structure into Force Field Explorer, the minimize command can be selected (Figure 5). The minimization progress is shown graphically until the operation completes, then a textual log is loaded and displayed.

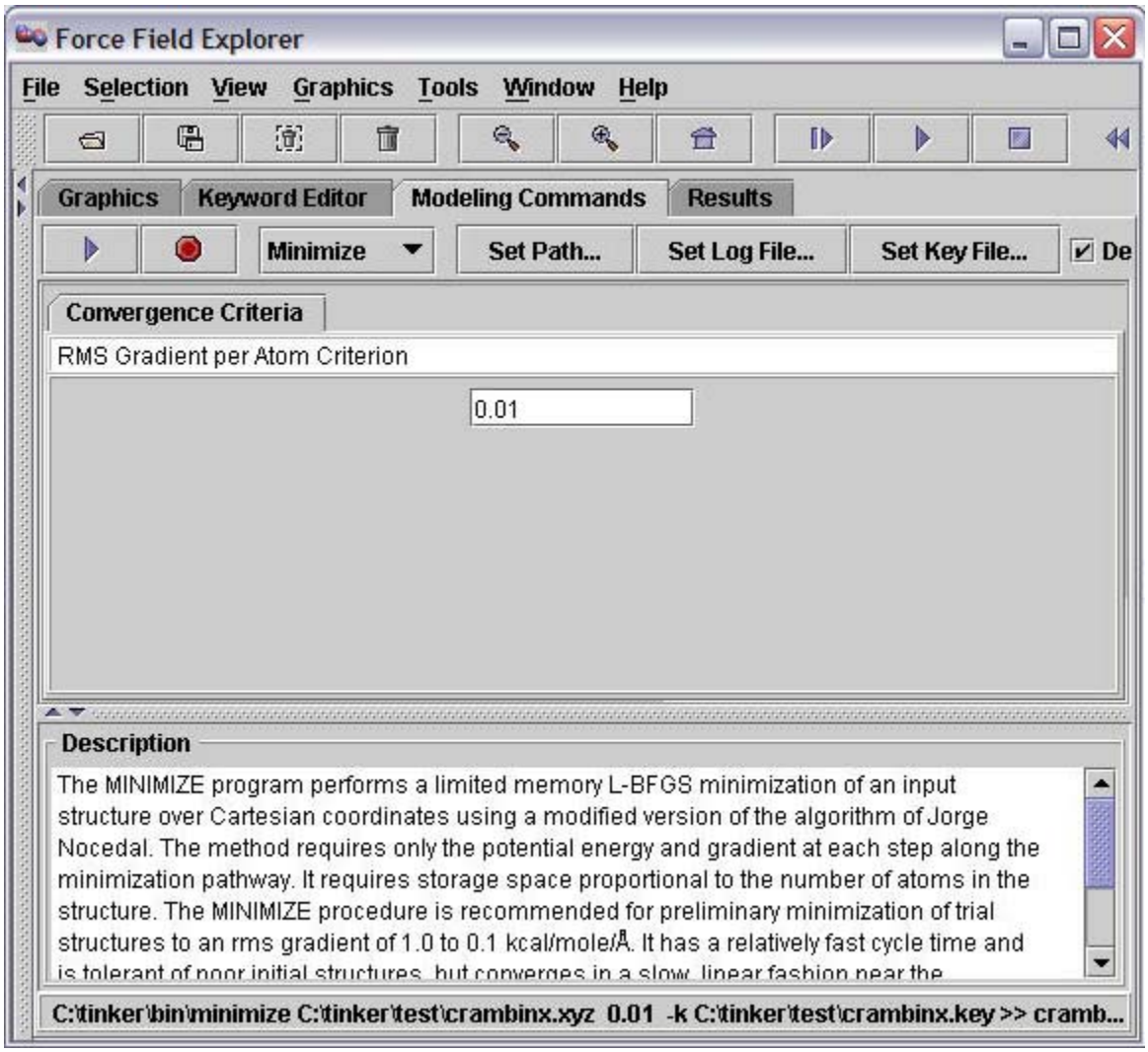

Figure 5. The Modeling Commands panel executes TINKER routines.

Results

The Results component is a simple text editor where output logged from TINKER routines is automatically loaded. It can also be used to edit any text file, for example TINKER *.xyz files or *.key files.

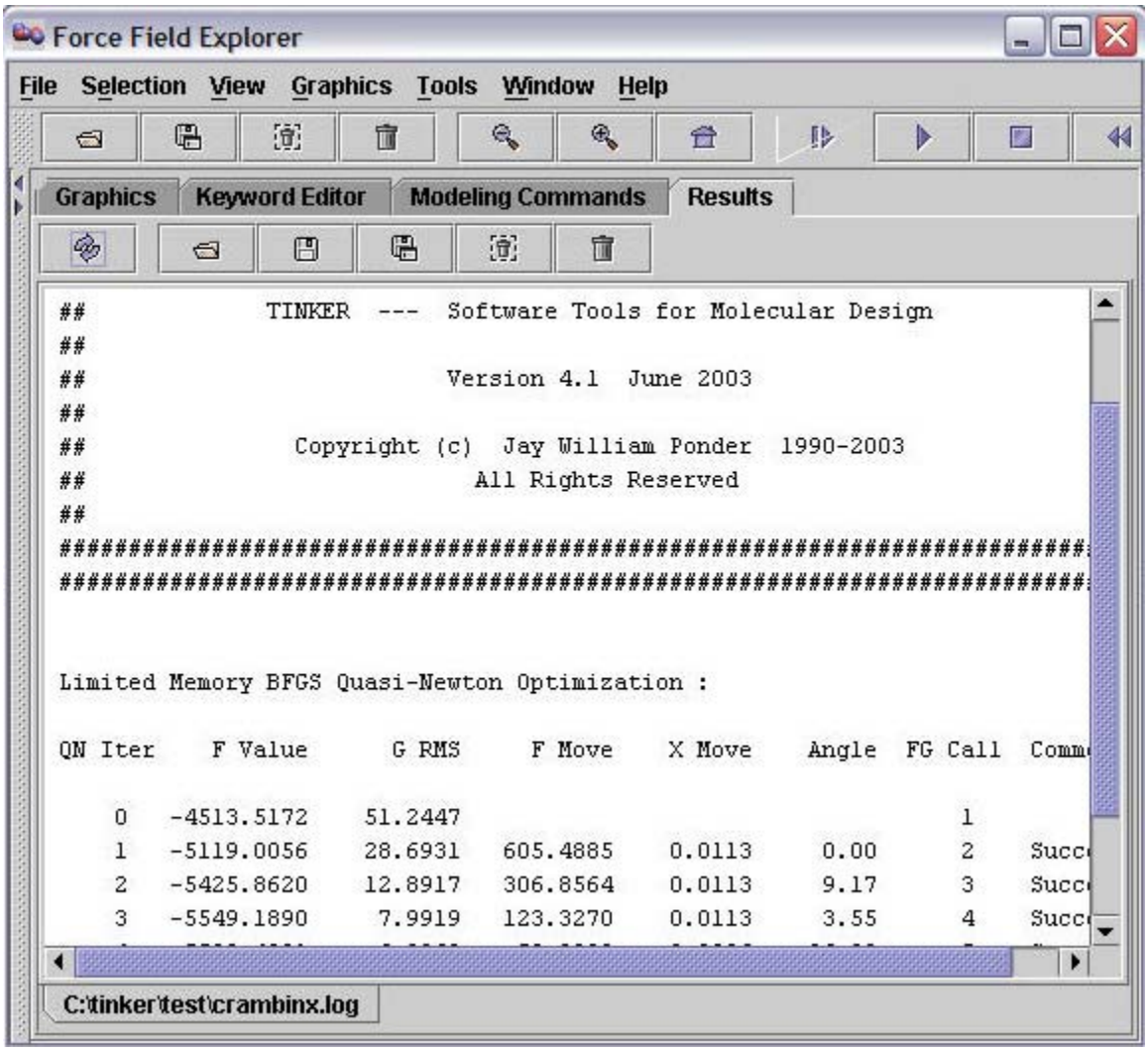

Figure 6. The Result panel shows output logged from TINKER routines.

An Example

Investigating various implicit solvation models implemented in TINKER using a DNA helix (AMBER force field) and the protein crambin (CHARMM force field). This example requires that you have installed a complete TINKER distribution

1. Force Field Explorer (FFE) has been tested extensively with the molecules included in the TINKER distribution, so that is a good place to start for an example *.xyz file to load. Once FFE has been started, choose open from the file menu and navigate to the tinker/test directory, then select bdna.xyz.
2. Expand the tree view on the left a few levels, and select strand (A) or (B). Then select Graphics->Style->Spacefill on the menu. One strand should now be displayed using the spacefill representation, while the other remains wireframe. In general, style, color, atom selections, etc. are applied to the atoms below the point selected in the tree view. Now select Graphics->Coloring->Partial Charge. The negatively charged phosphates should now be bright red, and positively charge nitrogen atoms dark blue. Atoms with smaller partial charges are a more lightly shaded red or blue.
3. Now open crambin.xyz. You can move molecules by clicking over them and dragging the mouse. One could, for example, move crambin and the DNA helix so they are not superimposed.
    - Left Mouse = Rotate
    - Right Mouse = Translate
4. To manipulate the entire scene, left-click on the XYZ axis in the lower left corner and drag the mouse. Additionally, clicking the middle button anywhere on the Graphics panel and dragging vertically results in the whole scene being zoomed in/out.
5. Now click the "Keyword Editor" tab. You will see the active TINKER keywords for crambin.xyz, loaded from the crambin.key file (or the active keywords for dna.xyz, if it was reselected as the molecules were dragged around). By alternately selecting nodes in the tree view that belong to DNA or crambin, respectively, the keywords being displayed will change to reflect the "selected/active" system. You should see that an implicit solvation model has been specified for both.
6. Now click on the "Modeling" tab. Choose the "Set Path" button to specify the directory where the TINKER executables are located. Make sure "e" from the Analyze options box is selected. Now click launch. As long as the path has been selected, Analyze will execute on the currently selected TINKER *.xyz file and the results will be posted to the "Results" tab when Analyze completes.
7. Changing the implicit solvation model can be done by returning to the "Keyword Editor" tab and entering one of the other choices described in the "Description" box displayed when the mouse is over the SOLVATE keyword. Navigate back to the "Modeling" tab and click Launch (the "e" option should still be selected). Changes to the Keyword file, in this case the SOLVATE keyword, are automatically saved when Launch is selected and before Analyze executes.

Returning to the "Results" tab, the new Analyze output should appear below any previous data in the log file.