VMD Plugin Highlights

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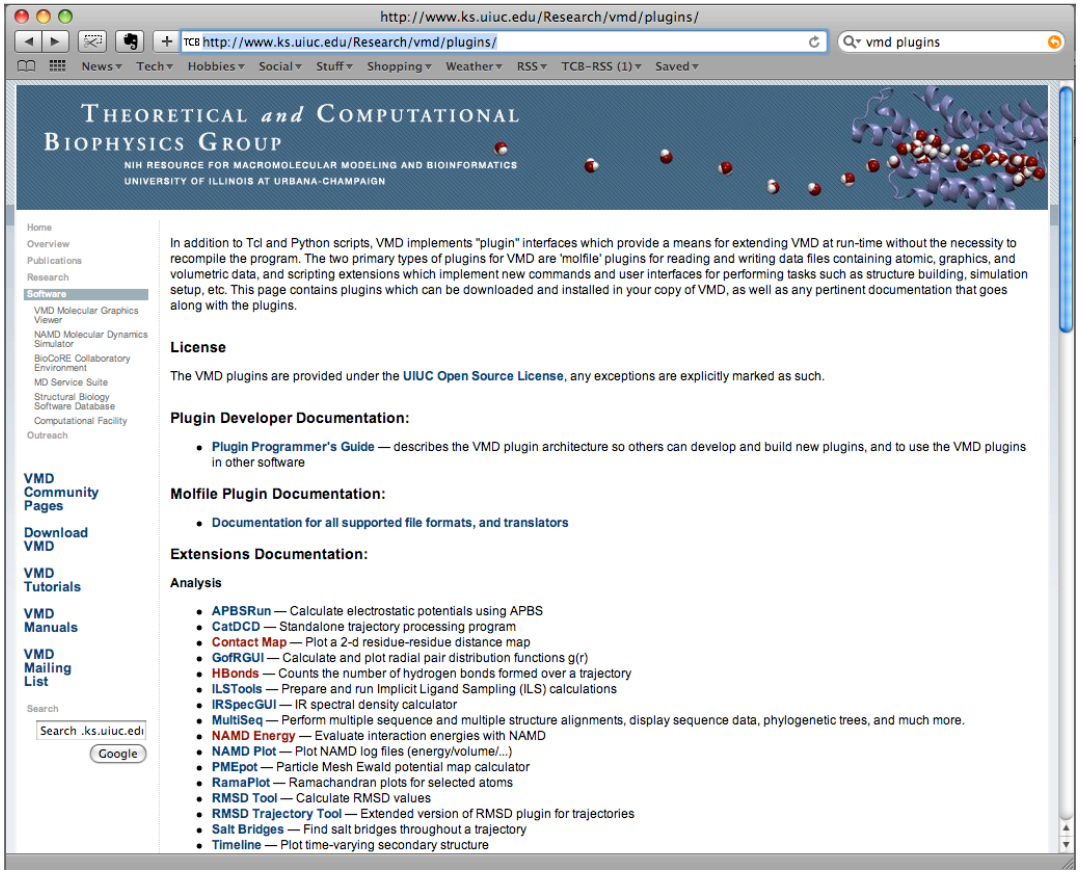
Plugins: The Molecular Modeling Toolbox

- Extensive library of plugins comes with VMD: See Extensions Menu
- Some are text only, many have text and graphical modes
- Write your own in Tcl/Tk
- Third-party plugins



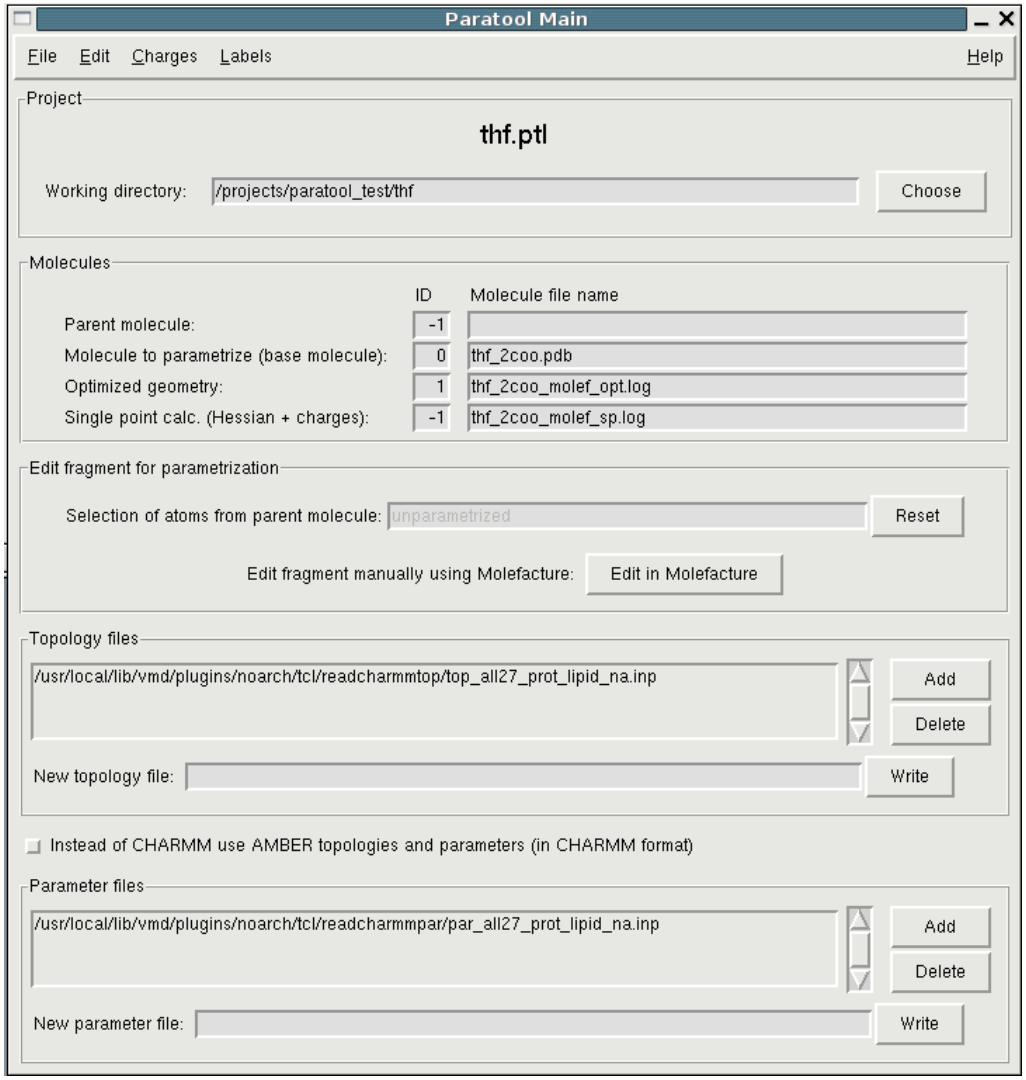
http://www.ks.uiuc.edu/Research/vmd/plugins/

vmd-l@ks.uiuc.edu

http://www.ks.uiuc.edu/Research/vmd/mailing_list/

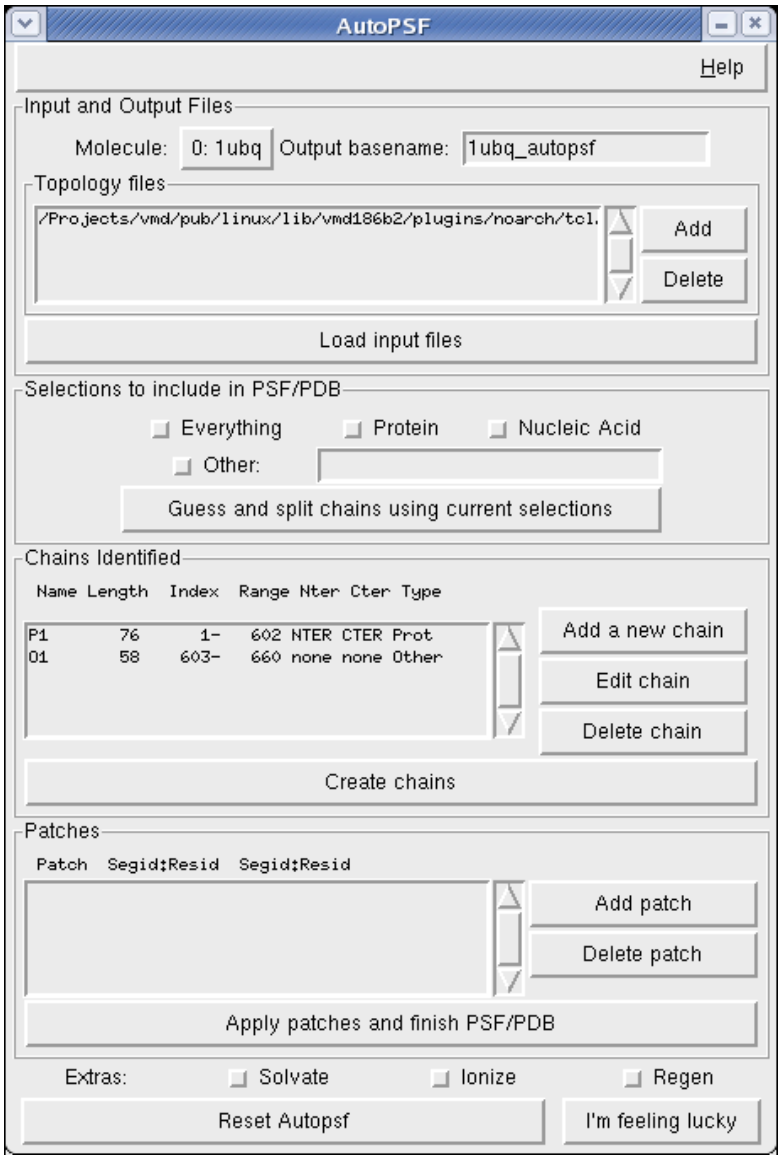
Build a molecule

- Molefacture — small structure builder
- Inorganic Builder — Build devices
- MergeStructs — Merge multiple structures
- Paratool — Calculation of force field parameters
- CGTools — Transform structures between coarse-grain and all-atom representations



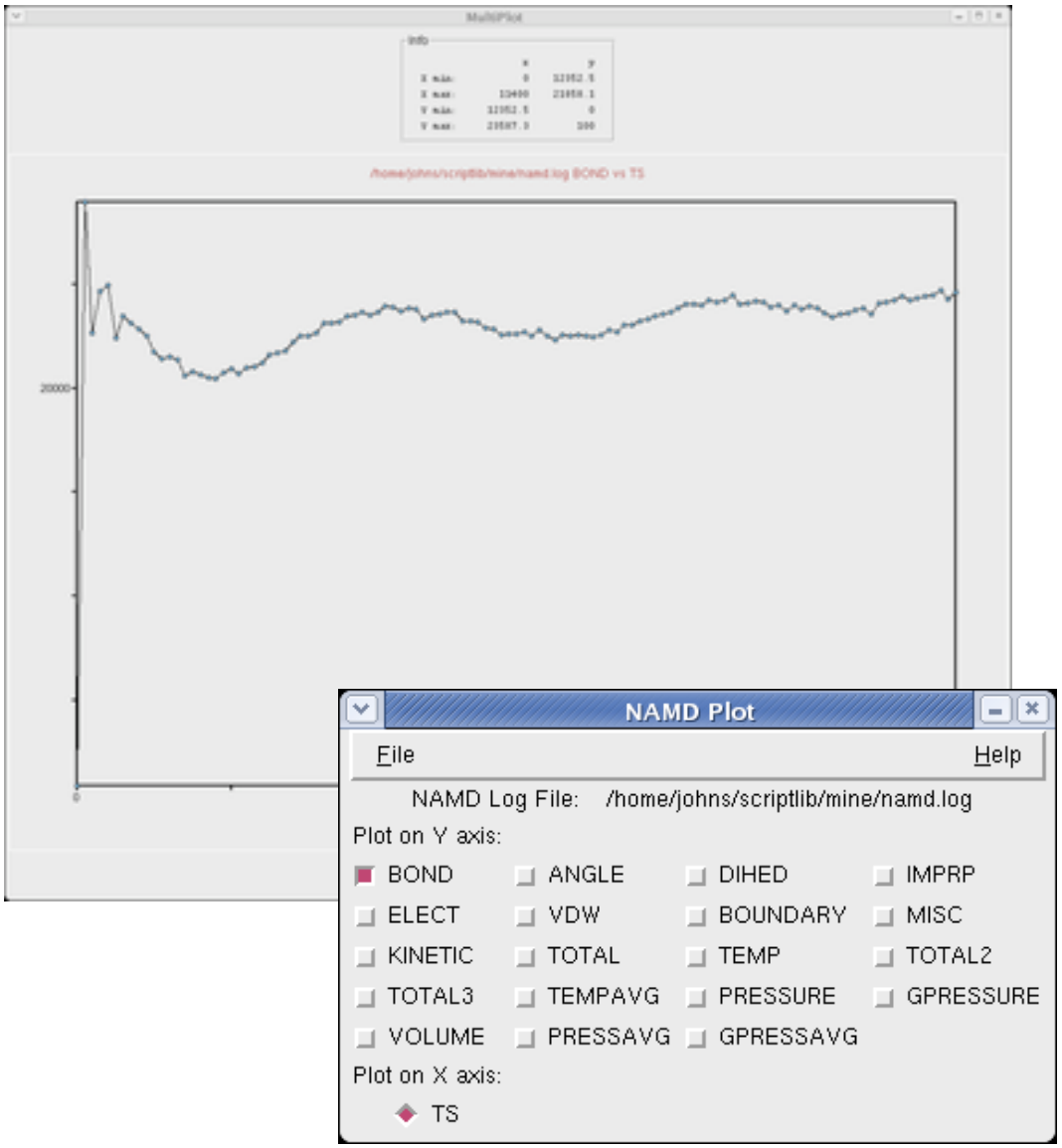
Prepare the System

- PSFgen — Build structures for use with NAMD
- AutoPSF — Automatic PSF structure building tool
- Solvate — Add water to a structure
- AutoIonize — Add sodium or chlorine ions to a structure for simulation



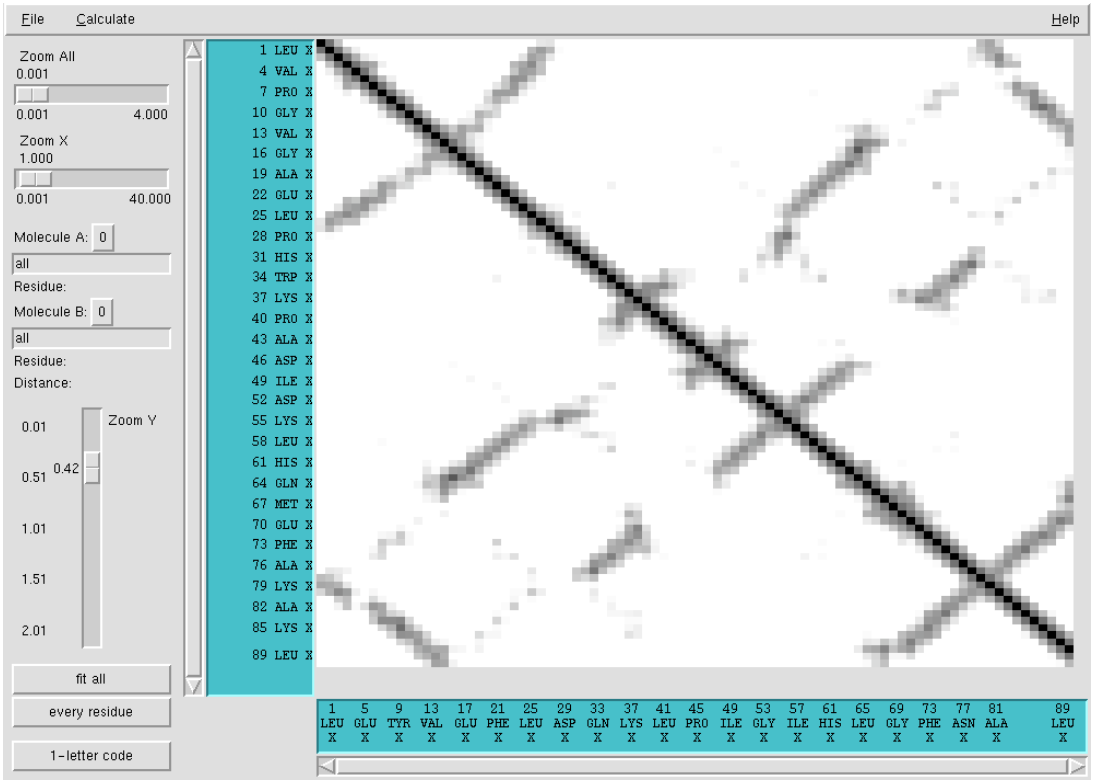
Post-Processing

- TkConsole — A better console
- CatDCD — Trajectory processing
- PBCTools — Tools for manipulating simulation data with periodic boundary conditions
- NAMD Plot — Plot NAMD log output
- RamaPlot — Ramachandran plots
- RMSD Trajectory Tool — Calculate RMSD values for trajectories



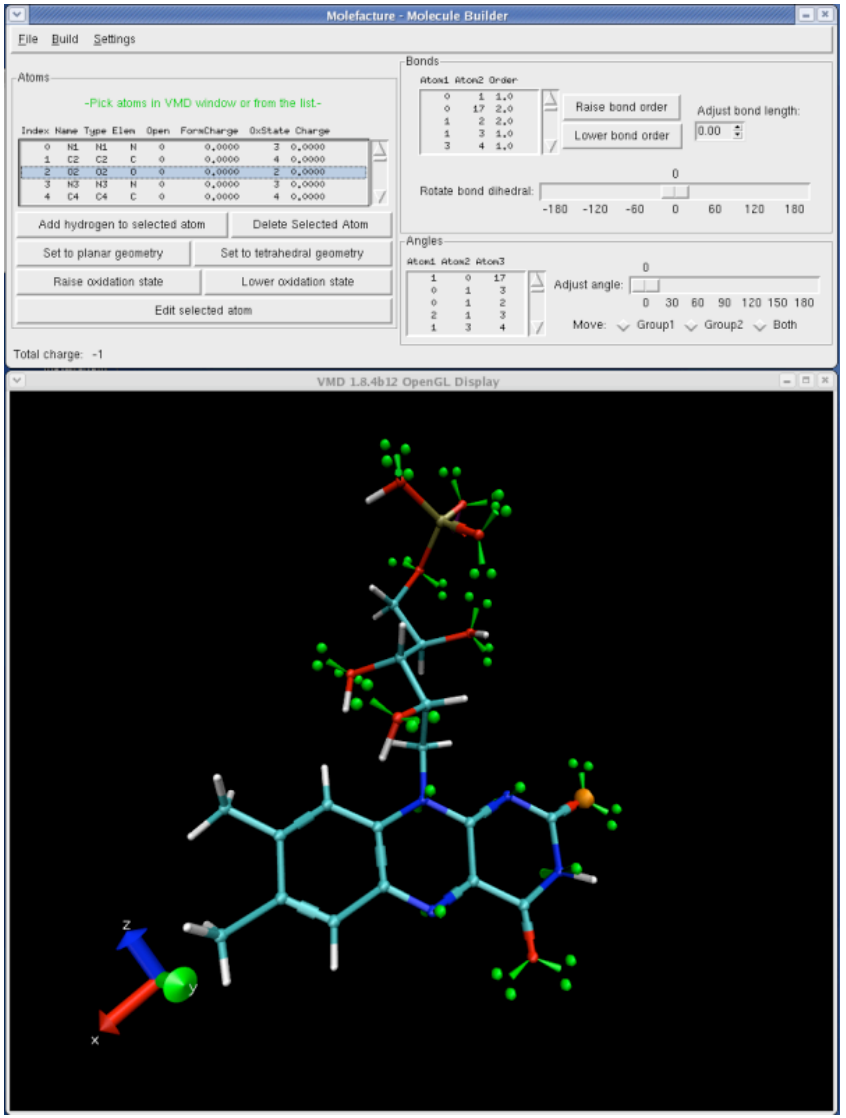
Analysis

- Contact Map — Plot a 2-d residue-residue distance map
- HBonds — Counts hydrogen bonds formed over a trajectory
- Salt Bridges — Find salt bridges throughout a trajectory
- NAMD Energy — Evaluate interaction energies
- PMEpot — Particle Mesh Ewald potential map calculator
- Timeline — Plot time-varying secondary structure

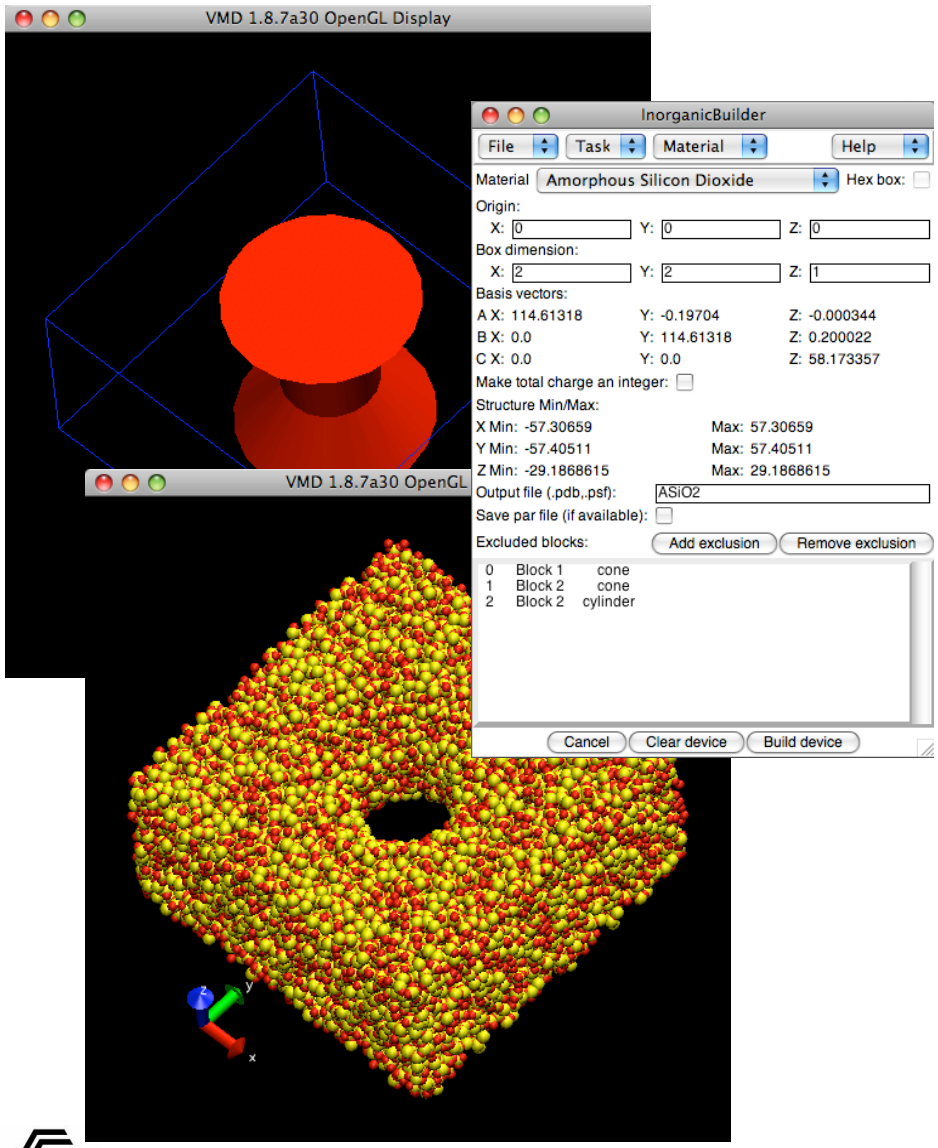


Molefacture: Assemble small molecules

- Edit molecules
- Add, delete, or manipulate their structure at atomic level
- Build new components from a library of common fragments.



Inorganic Builder: Build nanodevice models



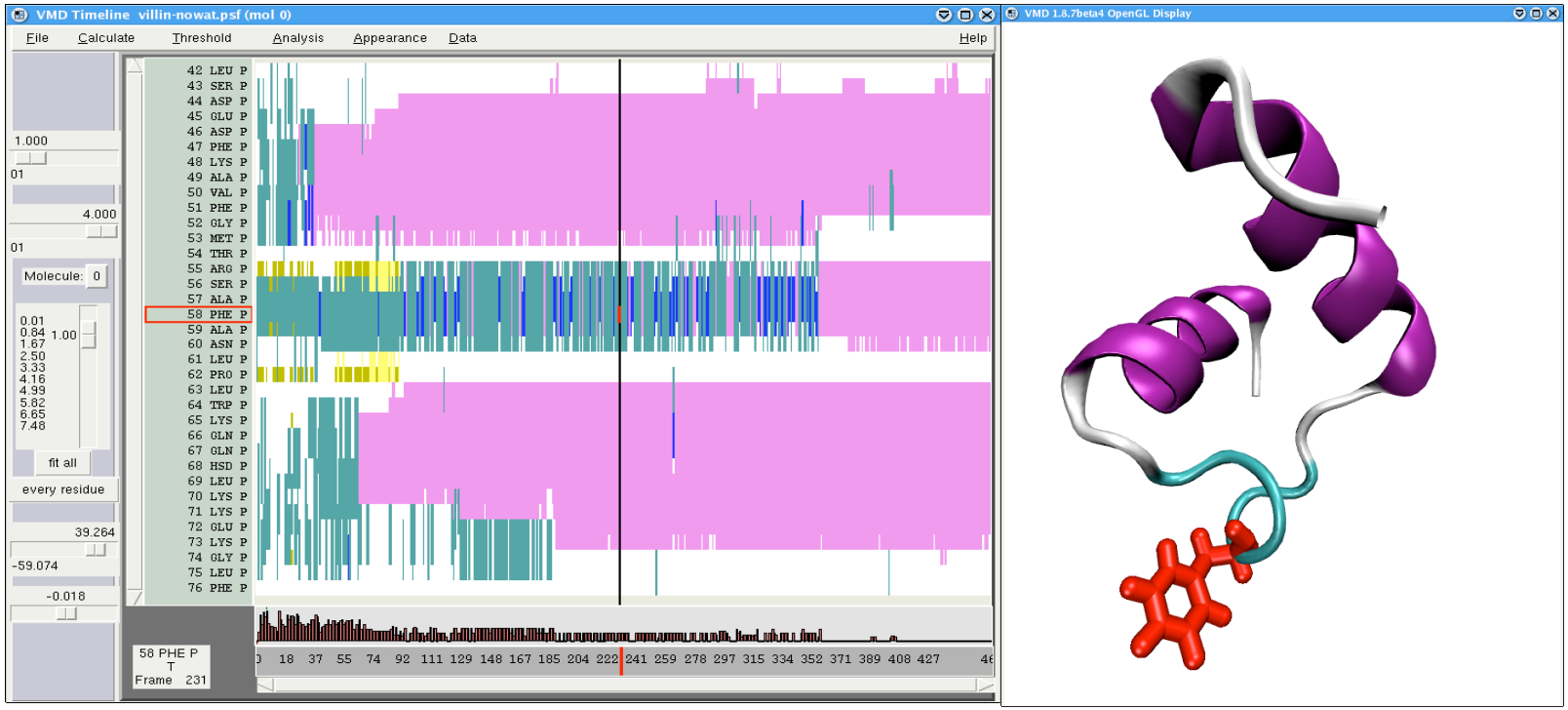
Goal: Provide a fast way to build device models for evaluating prototype designs

InorganicBuilder Plugin

- Design device model geometry
- Bond search: type/distance based
- Extract surface atoms
- Add biomolecules
- Solvate model
- Library of common materials
- Extensible material list

Timeline: a tool to locate events in MD trajectories

Events during 7 µs villin headpiece folding



Per-residue secondary structure: villin headpiece folding from a fully denatured state.
7µs simulation; 654 atoms; over 1 million frames to examine

VMD **Timeline plug-in**: graphing and analysis tool to identify events in an MD trajectory

- a single picture shows changing properties across entire structure, entire trajectory.
- explore time vs. attribute (per-residue or per-selection) linked to molecular structure
- many analysis methods available; user-extendable

End