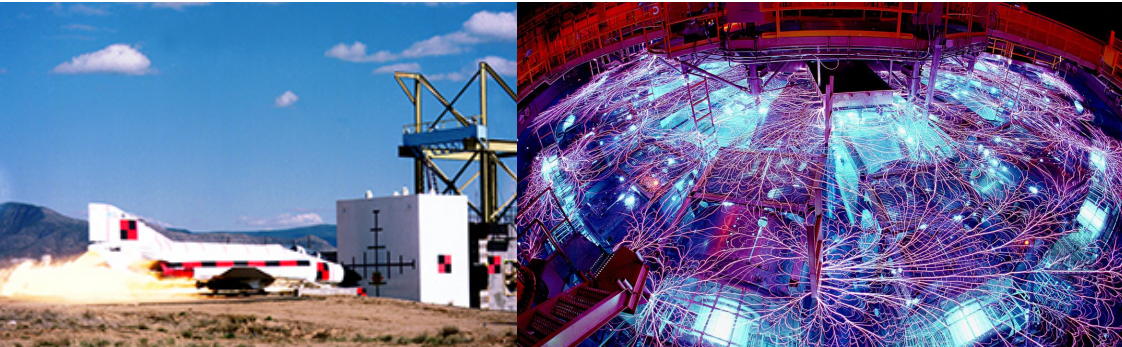*Exceptional service in the national interest*

Beginners Tutorial: Visualization

Mitchell Wood (mitwood@sandia.gov) , Sandia National Labs

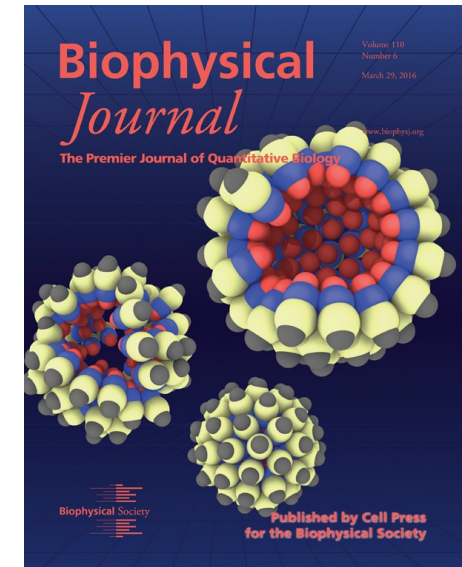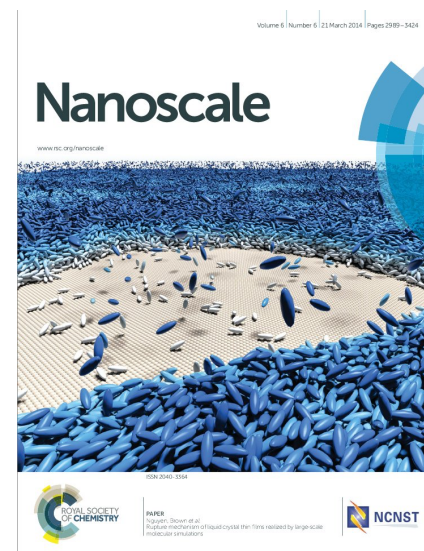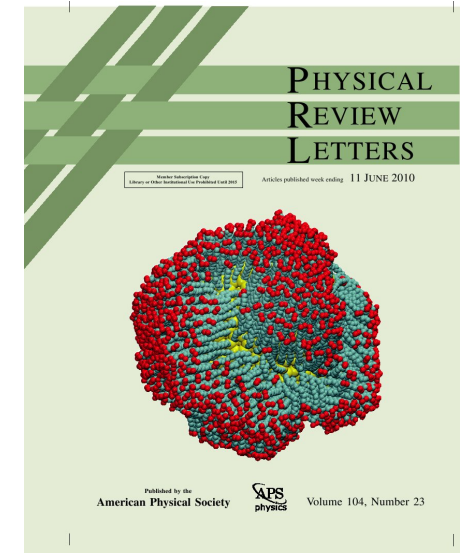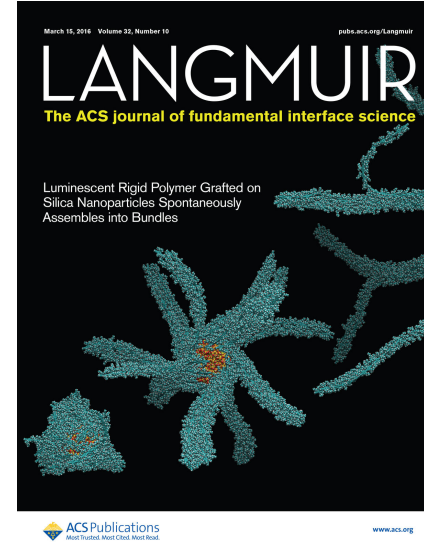5th LAMMPS Workshop and Symposium

August 2017, Albuquerque NM

Why Bother With Vis?

- Communicating simulation results is not a trivial task, even between experts

- Debugging simulation crashes

- Mechanistic understanding a.k.a. the 'unplotable' data
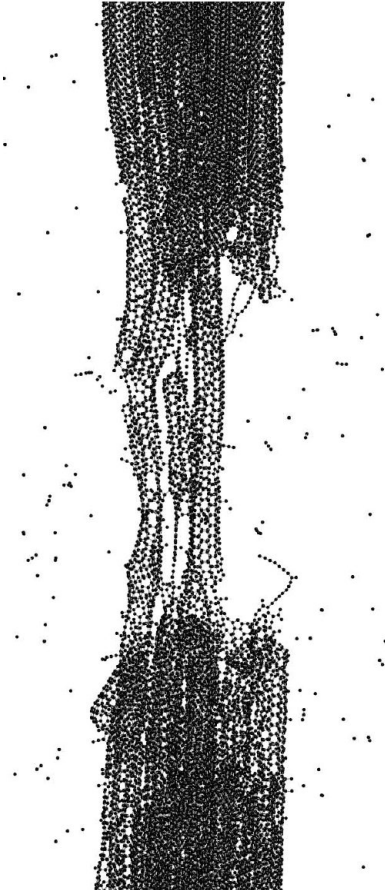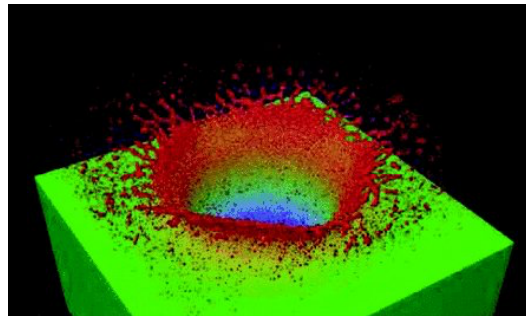
- Art?

- Exploration
  - Fast manipulation of structures
  - Multiple supported file formats

- Science illustration
  - Built-in analysis tools (rdf, FFT, etc.)
  - High quality renderings
  - Scene manipulation

- Artistic or features (covers, websites, etc.)
  - Unusual styles, property mappings
  - "photoshopping"
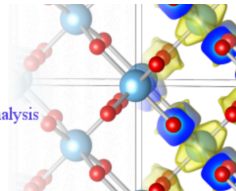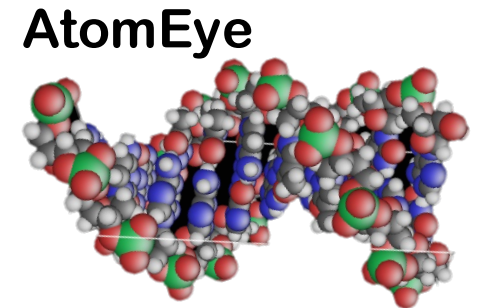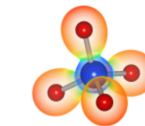
And many more…

Overview and Use Cases for VMD

- Open source code available at http://www.ks.uiuc.edu/Research/vmd/
- No compiling needed, binaries distributed for all platforms
- Has both a visual UI and scripting interface (great for batch processing)

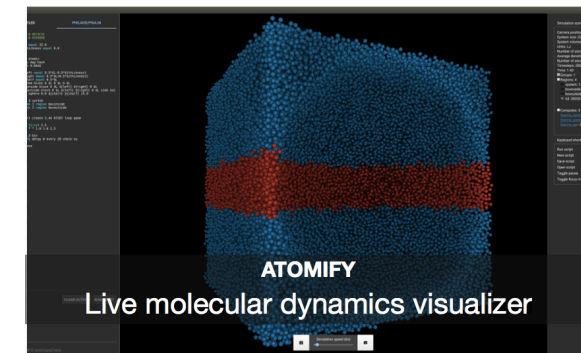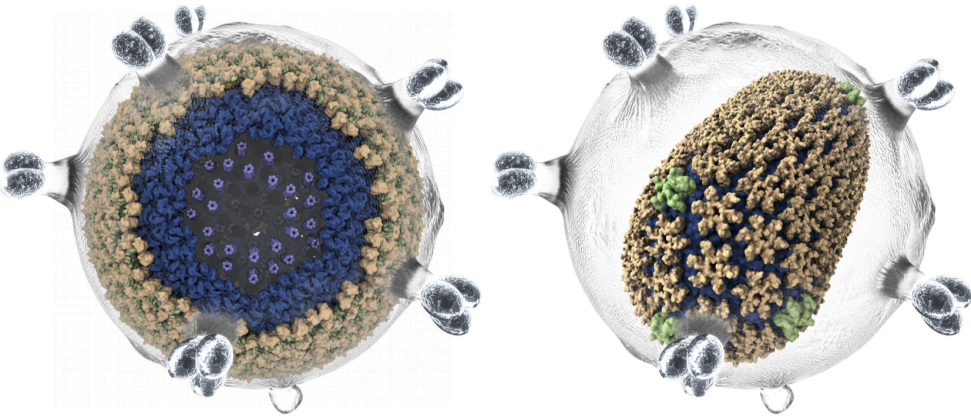VMD rendering of the immature retroviral lattice for Rous sarcoma virus (left) and the mature HIV capsid(right).

"Chemical Visualization of Human Pathogens: The Retroviral Capsids" Juan R. Perilla, Boon Chong Goh, John Stone, and Klaus Schulten. SC 2015, Austin, TX.
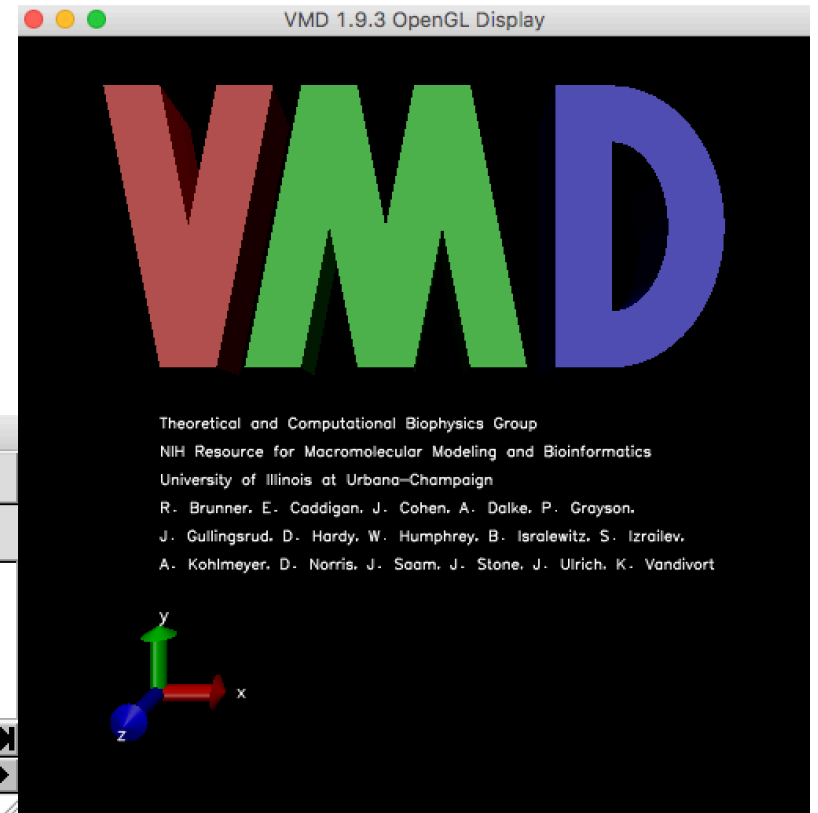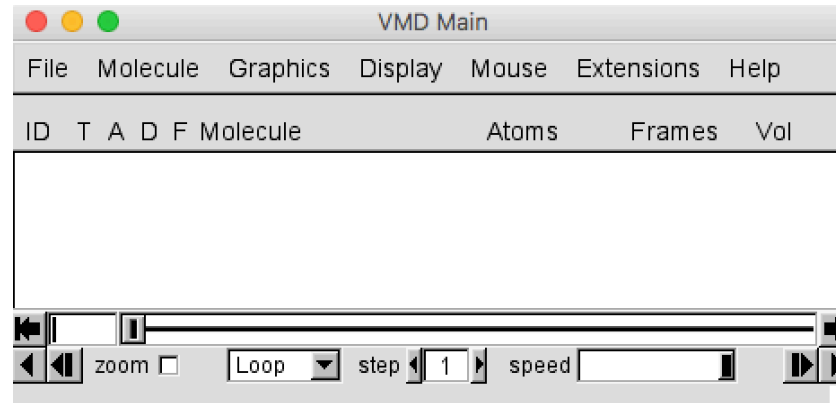
Overview and Use Cases for OVITO

OVITO
Open Visualization Tool

- Open source code available at OVITO.org
- No compiling needed, binaries distributed for all platforms
- Prepare structures, analyze and render simulation data from one intuitive program.
- Has both a visual UI and scripting interface (great for batch processing)

Modelling Simul. Mater. Sci. Eng. **18** (2010) 015012   A Stukowski

1. File import   2. Color coding   3. Selection   4. Delete selected   5. Slice
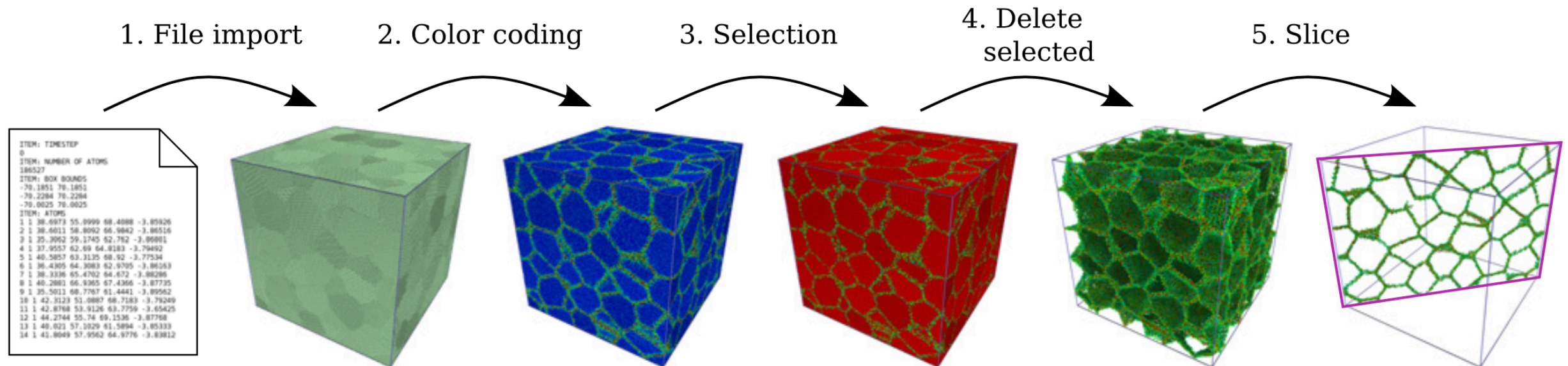
Distinguishing Between VMD and OVITO

VMD — Visual Molecular Dynamics

OVITO — Open Visualization Tool

- Best for biological systems

- LAMMPS dump formats: atom, dcd, xtc, xyz, write_data

- Needs local files

- Atom-level properties need script input, see http://www.ks.uiuc.edu/Research/vmd/script_library/

- Long standing user base, forum support

- Best for metals, condensed matter

- LAMMPS dump formats: atom, cfg, xyz, hdf5, custom, compressed files, write_data

- Local or remote(sftp) file locations

- Atom-level properties in dump file can be used as coloring schemes

- Support through Alex Stukowski and his group, smaller user base