Exceptional service in the national interest





Beginners Tutorial: Visualization Mitchell Wood (<u>mitwood@sandia.gov</u>), Sandia National Labs 5th LAMMPS Workshop and Symposium

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Why Bother With Vis?



- 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"



ονιτο

Open Visualization Tool

sual Molecular Dynamics

And many more...



AtomEye

VESTA nalization for Electronic and STructural Analysis

Overview and Use Cases for VMD







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.

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- 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)



Theoretical and Computational Biophysics Group NIH Resource for Macromolecular Modeling and Bioinformatics University of Illinois at Urbana–Champaign

- R. Brunner, E. Caddigan, J. Cohen, A. Dalke, P. Grayson,
- J. Gullingsrud, D. Hardy, W. Humphrey, B. Isralewitz, S. Izrailev,
- A. Kohlmeyer, D. Norris, J. Saam, J. Stone, J. Ulrich, K. Vandivort





- 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



Distinguishing Between VMD and OVITO





- Best for biological systems
- LAMMPS dump formats: atom, dcd, xtc, xyz, write_data
- Needs local files
- Atom-level properties need script input, see
 <u>http://www.ks.uiuc.edu/Research/vmd/script_library/</u>
- 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