

LAMMPS User Workshop
Albuquerque, NM
5 August 2015

LAMMPS Users' Workshop Beginner's Tutorial Visualization of results

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Albuquerque, NM



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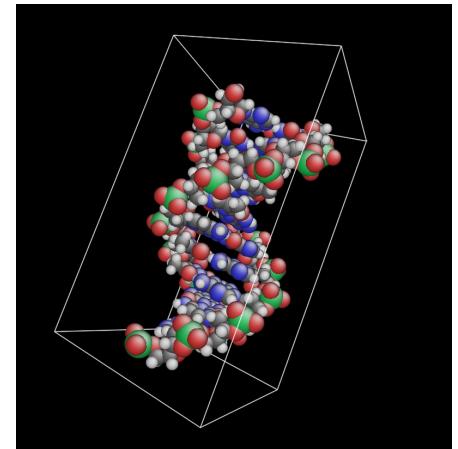
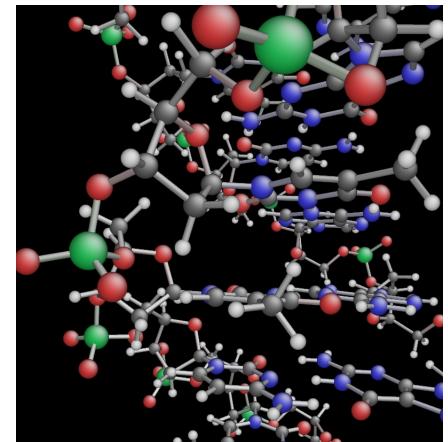


Agenda

- 8:30 – Welcome and agenda: Matt Lane, Sandia
- 8:35 – General LAMMPS overview: Aidan Thompson, Sandia
- 8:50 – Download, build, and run LAMMPS: Matt Lane, Sandia
- 9:10 – Basic output post-processing: Aidan Thompson, Sandia
- 9:25 – Visualization of results: Matt Lane, Sandia
- 9:40 – Break
- 9:50 – LAMMPS input scripts, syntax and rules: Steve Plimpton, Sandia
- 10:15 – LAMMPS capabilities - force fields, ensembles, fixes and computes, load-balancing, on-the-fly viz, GPU acceleration
- 10:45 – Hands-on– simple examples that come with LAMMPS
- 11:00 – Break
- 11:10 – Case study 1
 - Interatomic potentials and KIM: Ryan Elliott, Univ of Minnesota*
- 11:40 – Case study 2
 - Monitoring chemical reactions using on-the-fly molecular species analysis: Ray Shan, Sandia*
- 12:00 – Lunch

Major visualization tools

- **AtomEye (v3 released in 2012)**
 - li.mit.edu/Archive/Graphics/A/
 - Ju Li, MIT
 - Simple interface, versatile, unusual features
 - Source and Binary: Linux, Unix and MacOS
- **LAMMPS internal visual dump**
 - lammps.sandia.gov
 - Steve Plimpton, Sandia National Labs
 - Simple runtime generation, data conservation
 - Compile-time add on
 - Source only
- **Ovito (v2.5.0 released in July 2015)**
 - www.ovito.org
 - Alexander Studowski, Darmstadt University of Technology
 - Open source and freely available, reads LAMMPS dumps
 - Source and Binary: Linux, Windows and MacOS
- **VMD (v1.9.2 released December 2014)**
 - www.ks.uiuc.edu/Research/vmd/
 - Univ. of Illinois Urbana-Champaign
 - Huge palate of styles, fast, great GUI, reads LAMMPS dumps
 - Source and Binary: Linux, Windows and MacOS
- **Paraview and others**



Visualization goals

Exploration

- quick and easy images*
- no data conversion necessary*
- highly automated processing*

Science illustration

- built-in analysis tools (rdf, FFT, etc.)*
- smooth quality renderings*
- slice and cutaway*

Artistic or featured (covers, websites, etc.)

- unusual styles*
- color and refined rendering*
- “photoshopping”*

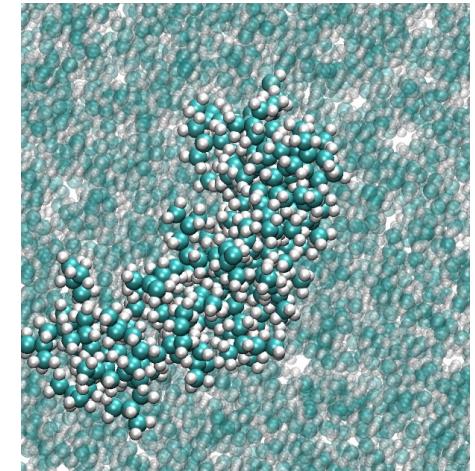
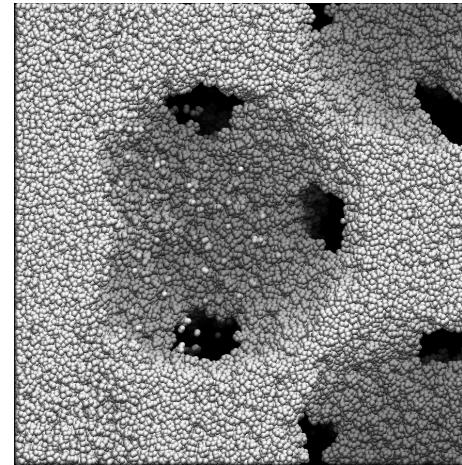
Video

- efficient trajectory handling*
- temporal trajectory or rotation/perspective movies*
- multiple format saves*

Visualization goals

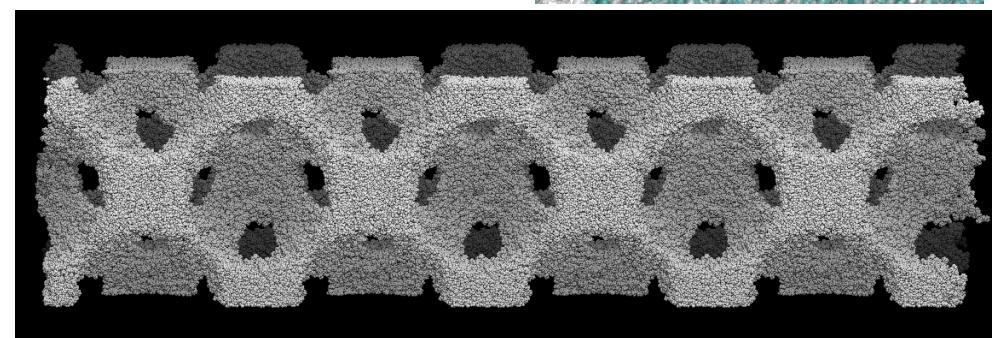
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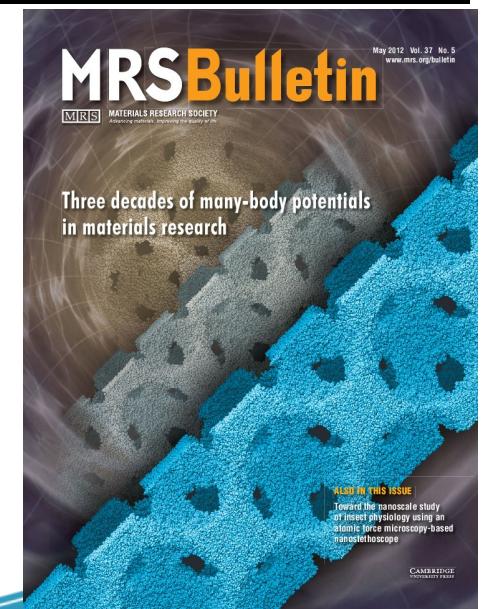
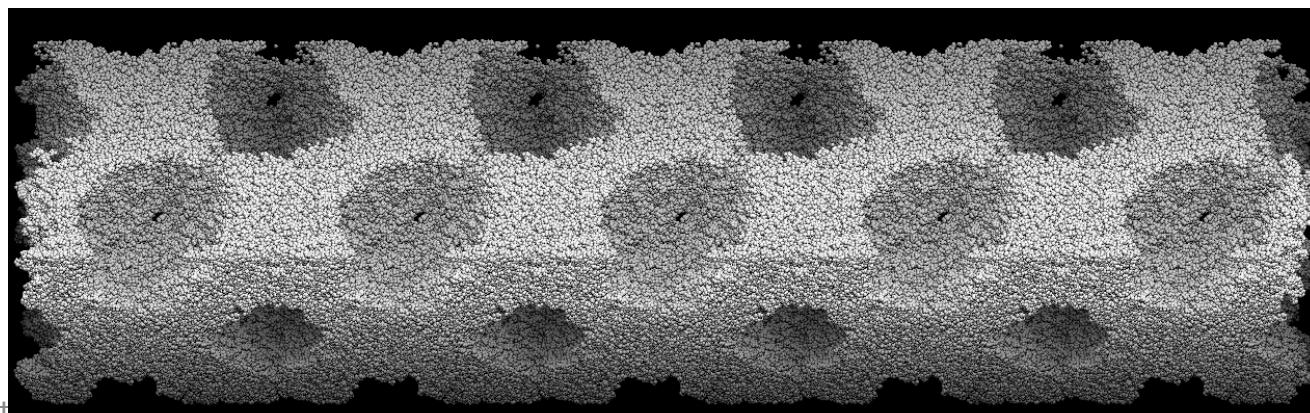


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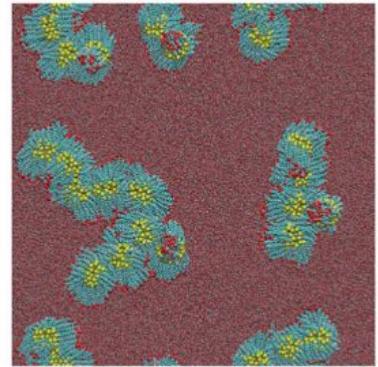
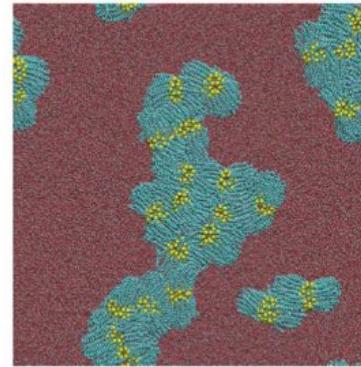
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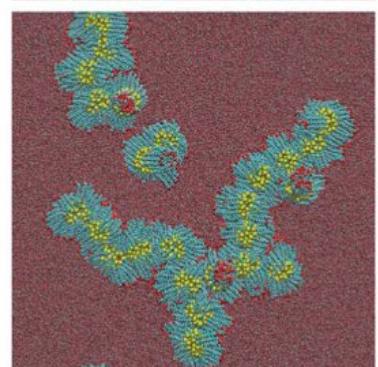
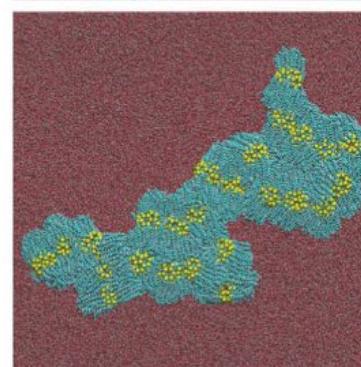
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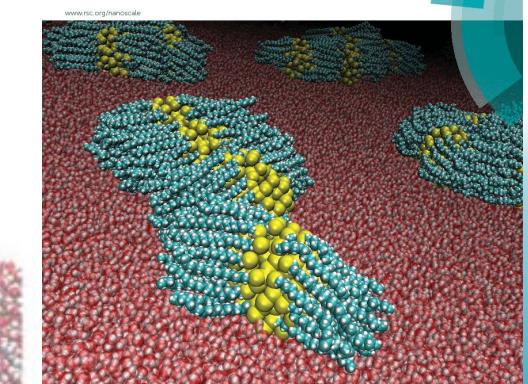
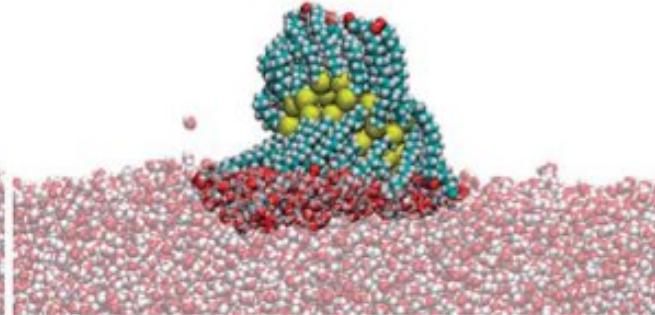
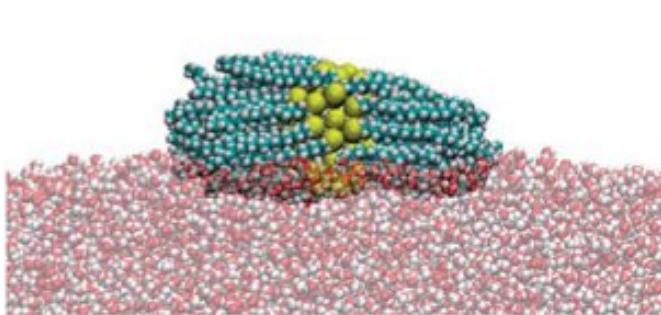


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Tools for extracting meaning from noise

Crystal structure (centro-symmetry, common neighbor analysis, coordination number) , grain boundaries, dislocations

DXA analysis Alex Studowski

Property color maps (temperature, per-atom stress, velocity, etc.)

Continuous color maps

Slices and cutaways, suppression of “bulk” atoms

Atom selection/removal by location, proximity, type, or property

Radial distribution functions, diffraction patterns, displacement vectors, etc.