

LAMMPS User Workshop
Albuquerque, NM
5 August 2015

LAMMPS Users' Workshop Beginner's Tutorial

Welcome!

Matt Lane
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Aidan Thompson
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Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.



Goals for today

- **Start at square one and move quickly and coherently through to expert material.**
- **Combination of lecture and hands-on activity designed to get you going quickly with simple problems, while you develop your own simulations.**
- **Broadly sample what LAMMPS can accomplish, so that you can begin to think about how it applies to your own research ideas.**
- **Maintain “free time” so that you can network with each other and with staff to answer the questions your interested in.**

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

Group statistics

- **55 Attendees / 5 Staff**
- **Platform**
 - **26** Windows
 - **20** Macintosh
 - **5** Linux / Unix
- **Environment**
 - **lots** Academia
 - **10** Industry
- **Already running LAMMPS back home?**
 - **half** Semi-beginner