

2017 LAMMPS User Workshop
Albuquerque, NM
1 August 2017

LAMMPS Users' Workshop Beginner's Tutorial

Welcome!

Aidan Thompson

Matt Lane

Steve Plimpton

Mitch Wood

Stan Moore

(many others)

**Sandia National
Laboratories,
Albuquerque, NM**



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: Mitch Wood, 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– examples that come w/ LAMMPS Aidan Thompson, Sandia
- 11:30 – Unstructured one-on-one exploration (until noon)

Group statistics

- **## Attendees / # Staff**
- **Platform**
 - **##** Windows
 - **##** Macintosh
 - **##** Linux / Unix
- **Environment**
 - **##** Academia
 - **##** Industry
- **Already running LAMMPS back home?**
 - **##** Semi-beginner