LAMMPS Users’ Workshop Beginner’s Tutorial

Welcome!

Matt Lane
Steve Plimpton
Aidan Thompson
Stan Moore
Ray Shan

Ryan Elliott
Univ. of Minnesota

LAMMPS User Workshop
Albuquerque, NM
5 August 2015

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