Aneesur Rahman

- 864 Lennard-Jones atoms on CDC 3600 computer
- 780 timesteps, 45 sec/step
- Irving Langmuir Prize - 1977
- American Physical Society (APS) Computational Prize is named in Aneesur’s honor

1927-1987
What’s new in LAMMPS

Steve Plimpton  
Sandia National Labs  
sjplimp@sandia.gov

4th LAMMPS User Workshop  
August 2015 - Albuquerque, NM
Thanks

- **Paul Crozier** has “died” (ok, took a management position)
- **Jeff Greathouse, Matt Lane, Stan Moore, Ray Shan, Aidan Thompson** - co-organizers
- **Phyllis Rutka and Val Romero** - administrative support
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  - **Eduardo Bringa** (Argentina)
  - **Stephen Foiles** (Sandia)
  - **Andres Jaramillo-Botero** (Caltech)
  - **Fabio Pavia** (EPLF and Ansys, Switzerland)
  - **Jim Larenztos and Brian Barnes** (ARL)
  - **Gary Grest** (Sandia)
  - **Christoph Kloss** (DCS Computing, Austria)
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- DOE/NNSA ASC - funding for facility/equipment rentals
- Materials Design - providing lunches!
- Scienomics - providing snacks and drinks!
Social activities

2 dinners & tram ride:

3 recreational choices:
Thanks to our user community

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- Please talk to LAMMPS developers whenever/wherever you can find us. Or just send us an email.
New interatomic potentials (pair styles)

- **Comb3** with polarization effects
  - U Florida groups of Sinnott and Phillpot
  - metals, oxides, hydrocarbons
- **Ziegler-Biersack-Littmark (ZBL)**
  - Stephen Foiles and Aidan Thompson (Sandia)
  - strong short-range repulsions
  - can be added to other potentials via pair hybrid
- **Peridynamics**
  - Rezwanur Rahman talk (Fri 8:30 AM), UT Austin
  - new viscoelastic and elastic/plastic models
- **Soft segmental repulsive potential (SRP)**
  - Tim Sirk (ARL)
  - prevents bond-crossing in DPD polymer chains
- **QEq** charge equilibration
  - Ray Shan talk (Wed 2:15 PM), Sandia
  - matrix and damped dynamics methods via fix qeq
  - can be added to other potentials (ReaxFF,COMB,etc)
  - with coul/streitz and EAM, enables Streitz-Mintmire potential
New “quantum-accurate” potentials

- Goal is to be as good as DFT for some systems, at a fraction of the cost
- Derived from “big data” archives of DFT results

**QUIP**
- Albert Bartok (Cambridge U)
- Interface to their QUIP MD code
- Variety of potentials including GAP

**SNAP**
- Aidan Thompson talk (Thu PM breakout A1), Sandia
- New potential for tantalum
Two polarization models

In addition to fix qeq (fluctuating charge) and COMB3 pair style ...

- **Adiabatic core/shell model**
  - Hendrik Heenan (Technical University of Munich)
  - CORESHELL package
  - crystalline materials

- **Thermalized Drude dipole model**
  - Alain Dequidt (Clermont University, France),
    with Julien Devemy and Agilio Padua
  - USER-DRUDE package
  - molecular systems and fluid states

- **Helpful docs**
  - doc/Section_howto.html: 24, 25, 26
  - doc/tutorial_drude.html
Two path-integral MD (PIMD) options

- Quantum MD via Feynman path integral method for quantum effects like tunneling
- One atom $\Rightarrow$ ring polymer of $P$ quasi-beads, equivalent to QM partition function

**Fix pimd** command

- Chris Knight & Yuxing Peng (U Chicago)
- uses multi-replica partitioning within LAMMPS
- scales nicely to large systems and machines

**Fix ipi** command

- Michele Ceriotti (EPFL)
- i-PI Python package performs PIMD
- LAMMPS called as client (via sockets) to compute forces/energies
Acceleration packages

- **Kokkos package**
  - Christian Trott, Stan Moore, Ray Shan (Sandia)
  - support for GPUs, Xeon Phi, OpenMP
  - 31 pair styles, some bonded styles, no PPPM (yet)
  - Stan talk (Thu 9:30 AM)

- **Intel package**
  - Mike Brown talk (Wed 3:15 PM), Intel
  - support for Xeon Phi, optimization for Intel CPUs
  - 5 pair styles, no PPPM (yet)

- **GPU package**
  - Mike Brown and Trung Nguyen (ORNL)
  - support for GPUs
  - 43 pair styles, PPPM

- **USER-OMP package**
  - Axel Kohlmeyer (Temple U)
  - 103 pair styles, 29 fixes, PPPM, Verlet & rRESPA
  - most bonded styles and PPPM variants

- **USER-CUDA package** being deprecated for Kokkos
All packages now usable via one build command

Example:
```bash
Make.py -p gpu -gpu mode=single arch=31
-o gpu -a lib-gpu file mpi
```

Use same input script with any package:

Example:
```bash
mpirun -np 48 -ppn 12 lmp_gpu -sf gpu -pk gpu 2
-in in.script
```
USER-DIFFRACTION package

- Shawn Coleman talk (Thu 9:45 AM), ARL
- Compute X-ray and electron diffraction patterns
- Bulk Ni example:

VisIt package for visualization
USER-LB package for Lattice-Boltzmann

- Colin Denisston group (U Western Ontario)
- Venkat Bala poster (Fri 10:30 AM), UWO
- Particles in background Lattice-Boltzmann fluid
- MD particles influenced by hydrodynamic forces

- Biopolymer filtration, Phys Rev Lett 112, 118301 (2014)
- GPU version for LB now available (contact Colin)
USER-SMD package = SPH for solids

- Georg Ganzenmueller (Ernst Mach Institute, Germany)
- Stable, quadratic convergence, various material models
Other new user packages

- **USER-FEP package**
  - Agilio Padua (Universite Blaise Pascal Clermont-Ferrand)
  - free-energy perturbation with soft potentials
  - fix adapt/fep command and several pair styles

- **USER-QMMM package**
  - Axel Kohlmeyer (Temple U)
  - couple LAMMPS with DFT using Quantum Espresso
  - LAMMPS performs MD algorithm, BC, constraints, etc
  - QE called to compute QM forces (subset of atoms and procs)
  - could be generalized to other DFT codes

- **USER-QTB package**
  - Yuan Shen, Tingting Qi, and Evan Reed (Stanford)
  - quantum nuclear effects (low temperatures, heat capacity)
  - fix qtb and fix qbmsst commands
Monte Carlo options

MC only, or MC moves interspersed with MD
Paul Crozier (Sandia), Aidan Thompson talk (Fri 9:15 AM)

- **Fix gcmc command**
  - Atomic/molecular insertions/deletions, rotate, displace
  - Supports all pair styles, KSpace
  - Local or global energy evaluation

- **Fix atom/swap command**
  - Metropolis MC for surface relaxation
  - Swaps atom types, displaces atoms

- **Fix tfmc command**
  - Kristof Bal (U Antwerp, Belgium)
  - Force-biasing to enable longer timescales
  - E.g. chemical vapor deposition onto surface
New **molecule** command reads molecule template file
- coords, atom types, bond topology (angles, dihedrals, etc)
- center of mass, moment of inertia
  for overlapping finite-size particles

**Input to other commands:**
- `create_atoms` (with molecules)
- molecule insertion: `fix gcmc`, `fix deposit`, `fix pour`
- `fix rigid/small`

**See doc/molecule.html for details**
Invoke Python code from your input script

In addition to Python scripts calling LAMMPS ...

- New **python command** defines a Python function
  - Function can be in-lined in input script or in a file
  - Pass LAMMPS variables to Python, values returned
  - Associate function with **python-style variable**
  - Python function invoked whenever variable is evaluated
    - Immediate in input script (parameter for command)
    - Every N steps during a simulation when fix requests it
  - Function can **callback** into LAMMPS (e.g. grab atom coords)

- **Why?**
  - Make input script into a **real programming language:**
    complex looping, branching, etc
  - Compute values more complex than LAMMPS variables allow
  - Easier way to add functionality than C++ coding
    - assuming it’s not a time-critical operation

- See [doc/Section_python.html](doc/Section_python.html) for details
New chunk commands

- General way to compute quantities for subsets of atoms
- **Chunk** = atoms in spatial bin, molecule, same atom type, etc
- More generally, chunks can be set by any atom property, output of per-atom compute or atom-style variable
  - atoms in local clusters
  - atoms within velocity windows
  - atoms with similar potential energy
  - atoms with same local defect structure
- **Compute chunk/atom** assigns chunk ID to each atom
  - one-time or dynamically (e.g. as clusters change)
- **Compute */chunk** commands calculate per-chunk values
  - count, sum of atom property, COM, MSD, etc
- **Fix ave/chunk** time averages & outputs per-chunk values
- See doc/Section howto 23 for overview
Miscellaneous input/output enhancements

- **Read_data command**
  - can now be used multiple times
  - allows building of system, component by component
  - e.g. substrate, adsorbed molecule, solvent

- **Write_data command**
  - write out a data file for current configuration
  - replaces old restart2data program

- **MPIIO package** for parallel I/O
  - Paul Coffman (IBM)
  - read/write of dump and restart files
Load-balancing via RCB

- RCB = recursive coordinate bisectioning
- Assigns same number of (weighted) atoms per processor
- See balance and fix balance commands
- Often needed for coarse-grained models
  - DPD, SPH, Peridynamics, granular, etc

- Worked to reduce comm with 26 neighbors to 6+ (for 3d)
2d SPH “water” flowing over a dam
Georg Ganzenmueller (Ernst Mach Institute, Germany)
Load-balancing examples for soft and hard materials

2d SPH “water” flowing over a dam
Georg Ganzenmueller (Ernst Mach Institute, Germany)

Atomic microlattice of metal struts
Alex Stukowski (Tech Univ Darmstadt)
- star imbalance = 18x
- 13x speed-up for 21M atoms on 16K cores
Give us your input on LAMMPS development plans

- Come to **breakout A2** on Thurs PM
- Variety of topics will be discussed
- User ideas/feedback is welcomed
- Volunteer your expertise & coding effort
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