Interatomic Potentials in LAMMPS

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Recently Added Potentials

- **COMB potential (Generation 2)**
  Tzu-Ray Shan (U Florida), talk on Tues PM metal and semiconductors and their oxides

- **Embedded ion method potentials (EIM)**
  Xiaowang Zhou (Sandia), ionic compounds combo of Li, Na, K, Rb, Cs, F, Cl, Br, and I

- **C++ version of ReaxFF**
  Metin Aktulga (LBNL), talk on Wed PM can be faster than Fortran version by 2-3x

- **Electron force field (eFF)**
  Andres Jaramillo (Caltech), explicit electron dynamics in extreme conditions
Recently Added Potentials

- **AIREBO potential bug fixes**
  Marcel Fallet & Steve Stuart (Clemson), one more bug-fix, upgrade is imminent

- **Mishin ADP potential**
  Chris Weinberger (Sandia) & Chandra Veer Singh (Cornell) angular-dependent EAM for metals and alloys

- **Dreiding potential**
  Tod Pascal (Caltech) hydrogen bonding for solvated biomolecules

- **New Peridynamics potentials**
  Mike Parks & Stuart Silling (Sandia), talk on Wed PM fracture at the meso and continuum scales
Upcoming Potentials

• Core/shell potential
  Mike Chandross (Sandia), zero-order model for polarization, uranium and other nuclear fuel materials

• COMB potential (Generation 3)
  Tzu-Ray Shan (U Florida), more materials with polarization effects

• MGPT potential
  from John Moriarty & Jaime Marian (LLNL), tantalum and other transition metals

• BOP potential
  Xiaowang Zhou and Don Ward (Sandia) High-accuracy potential for semiconductors
LAMMPS Potential benchmarks

<table>
<thead>
<tr>
<th>Potential</th>
<th>System</th>
<th>Atoms</th>
<th>Timestep</th>
<th>CPU</th>
<th>LJ Ratio</th>
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<tbody>
<tr>
<td>Granular</td>
<td>chute flow</td>
<td>32000</td>
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<td>FENE bead/spring</td>
<td>polymer melt</td>
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<td>Lennard-Jones</td>
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<tr>
<td>Tersoff</td>
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<td>SPC/E</td>
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<td>AIREBO</td>
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Compute Cost of Interatomic Potentials Growing Exponentially

Compute cost of LAMMPS potentials versus publication date

Drivers
- Cycles are cheap
- Availability of quantum calculations ($N < 100$)
- Qualitative accuracy no longer enough

http://lammps.sandia.gov/bench.html#potentials
Challenges with Complex Potentials

• How to Implement in LAMMPS?
  – Rewrite code from scratch (REBO)
  – Integrate existing serial code (ReaxFF)
  – Access via general API (KIM)

• How to Validate LAMMPS Version?

• How to Handle New Versions?
How to Fit Potentials to New Materials?

• Automated fitting procedures exist for certain classes of materials and potentials (EAM)
• More commonly, good fits can be obtained only by gurus (Baskes, van Duin)
• Combination of nonlinear optimization and physical intuition
• Increasing interest in automated machine-learning approaches
  – Splines
  – Genetic programs
  – Multi-objective optimization
  – Neural networks
  – Series expansions
GAP Approach for Interatomic Potentials

GAP: A systematic, informatics approach
- Based on QM and mathematics rather than empiricism.
- Local density around each atom expanded in 4D hyperspherical harmonics, analogous to Fourier series
- Atomic configurations described by bispectrum of lowest-order coefficients in series
- Preserves universal physical symmetries: invariance w.r.t. rotation, translation, permutation
- Gaussian process (GP) regression used to interpolate energy of QM configurations
- 100-1000x more expensive than MEAM
- Far cheaper than QM, linear scaling
- Can trade performance and accuracy

Diamond: Force errors for GAP fitted to DFT. Adding higher-order GAP coefficients systematically increases accuracy
Bartok et al., PRL 104 136403 (2010)
GAP Potential for Beryllium

Beryllium

Working with GAP developers, fitting directly to forces and energies from high-temperature DFT MD simulations of small systems (from Mike Desjarlais, 1640)

- Initial fit to:
  - ambient HCP
  - high-pressure BCC and liquid
- Accurately reproduced that data
- Problems with:
  - ambient elastic constants
  - high-pressure HCP
- Need to refit with more data