Interatomic Potentials in LAMMPS

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Sandia National Laboratories

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National Nuclear Security Administration

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 bio-molecules

- **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**

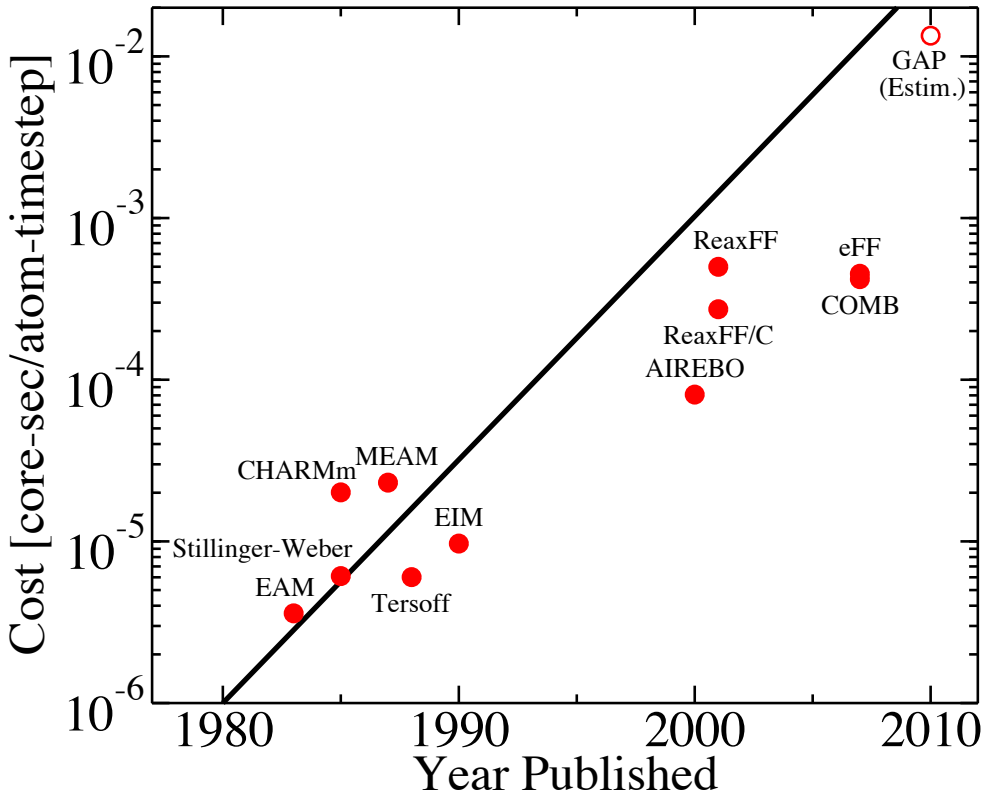
  Xiaowang Zhou and Don Ward (Sandia) High-accuracy potential for semiconductors

LAMMPS Potential benchmarks

Potential	System	Atoms	Timestep	CPU	LJ Ratio
Granular	chute flow	32000	0.0001 tau	5.08e-7	0.34x
FENE bead/spring	polymer melt	32000	0.012 tau	5.32e-7	0.36x
Lennard-Jones	LJ liquid	32000	0.005 tau	1.48e-6	1.0x
DPD	pure solvent	32000	0.04 tau	2.16e-6	1.46x
EAM	bulk Cu	32000	5 fmsec	3.59e-6	2.4x
Tersoff	bulk Si	32000	1 fmsec	6.01e-6	4.1x
Stillinger-Weber	bulk Si	32000	1 fmsec	6.10e-6	4.1x
EIM	crystalline NaCl	32000	0.5 fmsec	9.69e-6	6.5x
SPC/E	liquid water	36000	2 fmsec	1.43e-5	9.7x
CHARMM + PPPM	solvated protein	32000	2 fmsec	2.01e-5	13.6x
MEAM	bulk Ni	32000	5 fmsec	2.31e-5	15.6x
Peridynamics	glass fracture	32000	22.2 nsec	2.42e-5	16.4x
Gay-Berne	ellipsoid mixture	32768	0.002 tau	4.09e-5	28.3x
AIREBO	polyethylene	32640	0.5 fmsec	8.09e-5	54.7x
COMB	crystalline SiO2	32400	0.2 fmsec	4.19e-4	284x
eFF	H plasma	32000	0.001 fmsec	4.52e-4	306x
ReaxFF	PETN crystal	16240	0.1 fmsec	4.99e-4	337x
ReaxFF/C	PETN crystal	32480	0.1 fmsec	2.73e-4	185x
VASP/small	water	192/512	0.3 fmsec	26.2	17.7e6
VASP/medium	CO2	192/1024	0.8 fmsec	252	170e6
VASP/large	Xe	432/3456	2.0 fmsec	1344	908e6

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?**

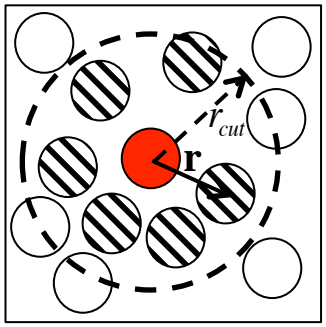
How to Fit Potentials to New Materials?

- 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

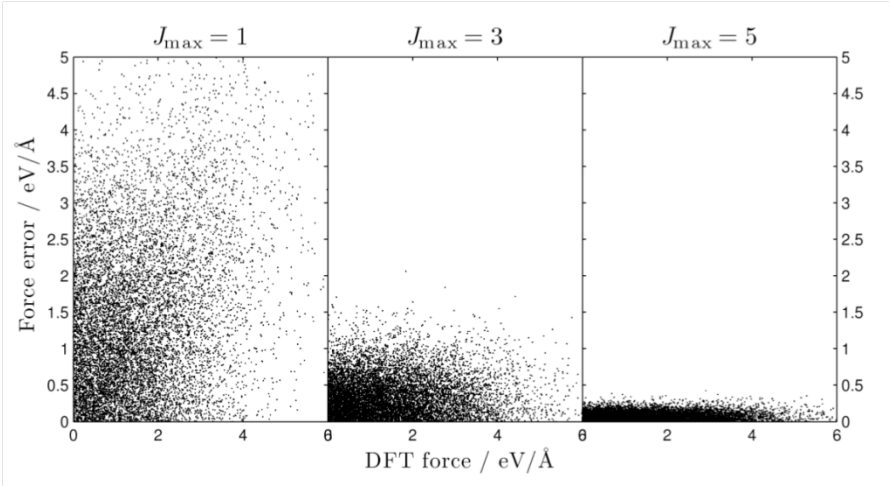
GAP Approach for Interatomic Potentials

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



$$\rho(\mathbf{r}) = \sum_{j=0}^{\infty} \sum_{m',m=-j}^{j} c^{j}_{m',m} Y^{j}_{m',m}(\theta,\phi,\omega)$$

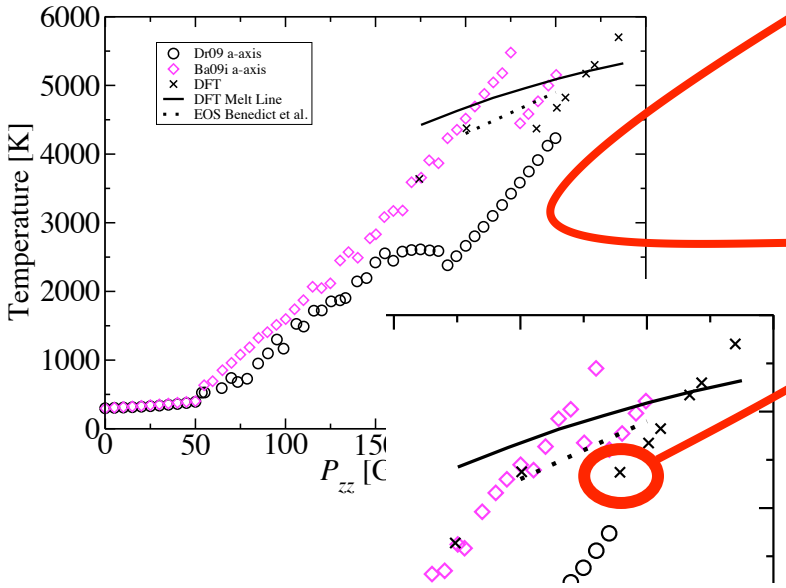


Diamond: Force errors for GAP fitted to DFT. Adding higher-order GAP coefficients systematically increases accuracy
Bartok et al., *PRL* **104** 136403 (2010)

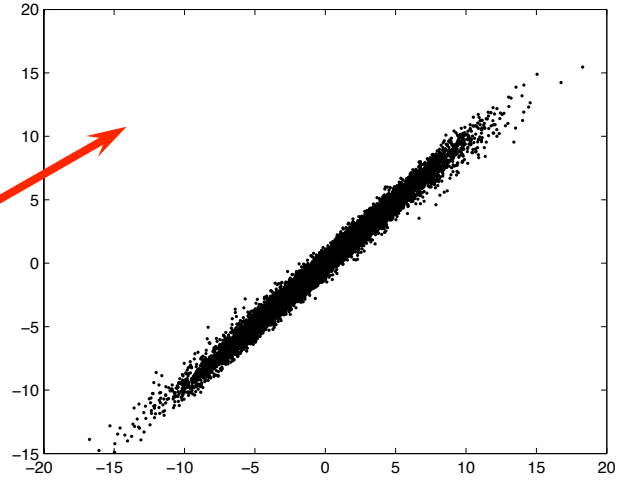
GAP Potential for Beryllium

Beryllium

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



GAP Forces versus DFT Forces for Liquid Be at 5,000 K, 250 atoms



- 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