ReaxFF in LAMMPS

New LAMMPS features briefs

LAMMPS Users' Workshop @ CSRI

Thursday, Feb 25, 2010, 11:15 a.m.

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The ReaxFF Interatomic Potential

Developed by Adri van Duin:

van Duin ACT, Dasgupta S, Lorant F, Goddard WA, *J. Phys. Chem A.* 105 9396 (2001) (183 citations up to Feb 2010)

Describes bond formation and charge transfer in condensed phases, especially organics

Bonded interactions generated on-the-fly, based on distance-dependent bond-order functions.

Bond-orders adjusted to compensate for atomic over/under-coordination

Atom charges computed using electro-negativity equalization i.e. minimizing quadratic function in *N* charges (Coulombic plus ionization energies)

$$E_{System} = E_{bond} + E_{over/under} + E_{lp} + E_{pen} + E_{coa} + E_{hb} + E_{tors} + E_{conj} + E_{val} + E_{vdW} + E_{Coul}$$
$$= E(\text{bond-order}) + E(\text{non-bond}) + E(\text{charge equilibration})$$

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ReaxFF MD Codes

reac.f (van Duin)

- Serial FORTRAN code written
- integrates parameter optimization and MD
- Not optimized for CPU or memory
- *N <10^4*

GRASP (Thompson)

- Spatial parallel C++
- Uses optimized versions of reac.f subroutines to bond-orders, energies.
- Charge equilibration using sparse parallel CG method.
- Exactly matches reac.f.
- *N ~ 10^7*

USC Code (Nakano, USC)

- Spatial parallel.
- *N ~ 10^9*

ParallelReax (Aktulga, PurdueU)

- Spatial Parallel C
- Dynamic memory. Fast.
- Carefully validated against reac.f
- *N ~ 10^7*

LAMMPS (Thompson and Cho) Similar to GRASP implementation

LAMMPS II (Aktulga): in progress

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ReaxFF in LAMMPS

Command Syntax

```
pair_style reax 10.0 1.0e-5
pair_coeff * * ffield.reax 3 1 2 2
```

(1 ReaxFF index for each LAMMPS type)

Potential Files

ffield.reax.mattsson: general-purpose hydrocarbon parameterization

Mattsson *et. al,* "First-Principles and Classical Molecular Dynamics Simulation of Shocked Polymers," *Phys. Rev. B* 81 054103 (2010).

ffield.reax.budzien: PETN

Budzien, Thompson, and Zybin, "Reactive Molecular Dynamics Simulations of Shock Through a Single Crystal of Pentaerythritol Tetranitrate," *J. Phys. Chem. B* 113 13142 (2009).

ffield.reax.rdx: nitramines (RDX/HMX/TATB/PETN)

Zhang, van Duin, Zybin, and Goddard, "Thermal Decomposition of Hydrazines from Reactive Dynamics Using the ReaxFF Reactive Force Field," *J. Phys. Chem. A* 113 10770 (2009).

ffield.reax.cho: c/h/o combustion force field November 2006

Chenoweth, van Duin, and Goddard, "ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation," *J. Phys. Chem. A* 112 1040 (2008)

We hope to add Water, SiO2, and CNT to this list soon.

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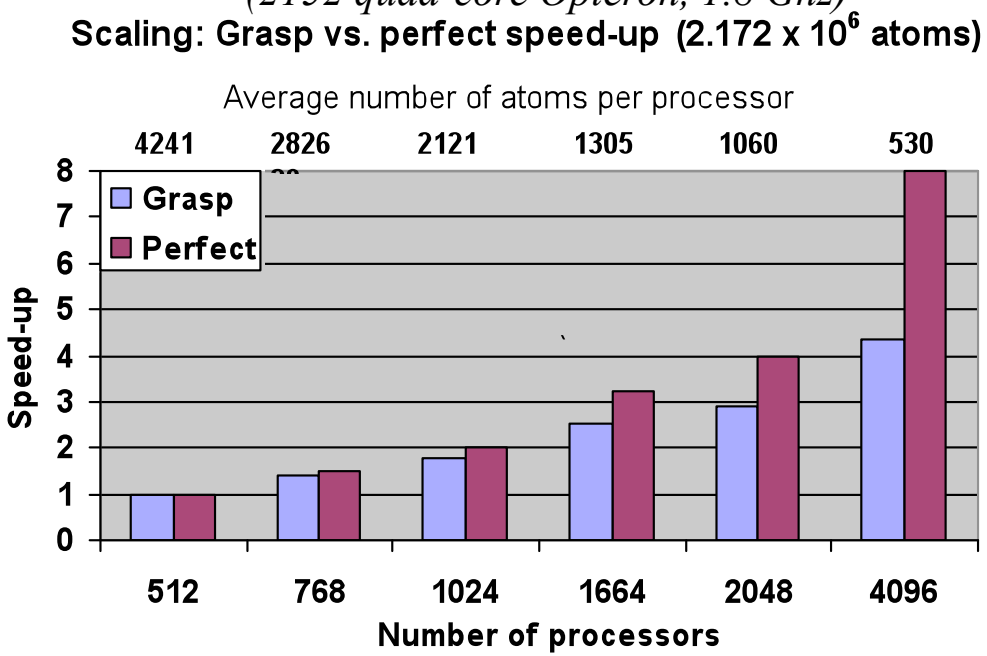
Parallel Scaling of ReaxFF in GRASP/LAMMPS

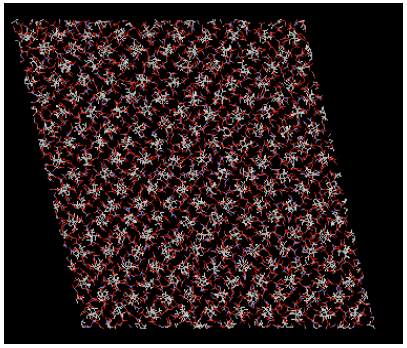
Non-Bond, Bond-Order and Bonding
- Computationally expensive
- Short-Range
- Local Communication
- Load-balancing issues

Jade (ERDC): Cray XT-4

(2152 quad-core Opteron, 1.8 Ghz)



Charge Equilibration
- Distributed CG implementation
- *Implemented distributed sparse matrix multiply*
- *Low computation and communication cost*
- *Small part of overall force time up to N ~ 10^6*
- *Requires global communication*
- *Could be a problem for larger N*



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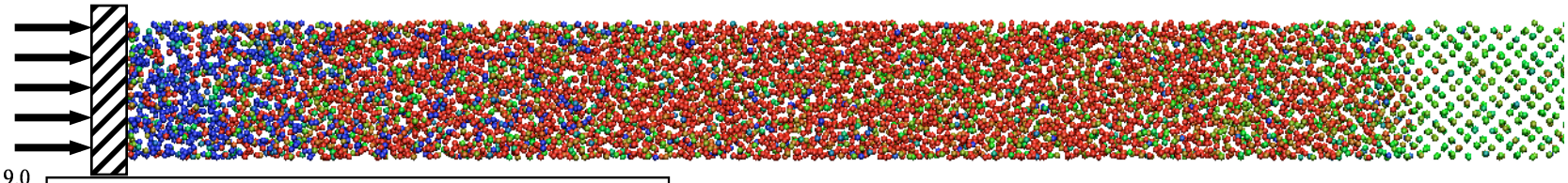
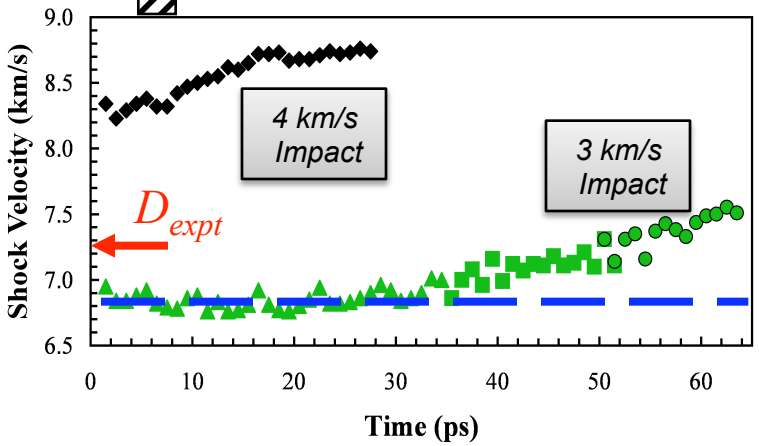
Atomistic Energetic Modeling

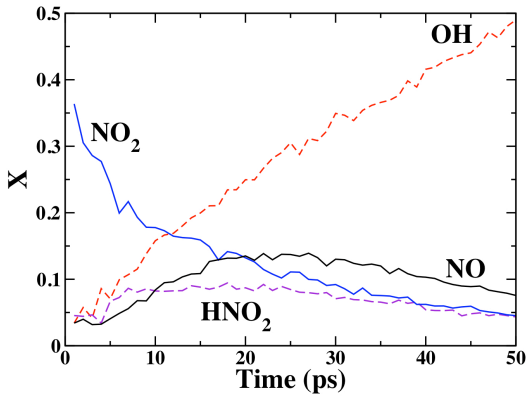
"Reactive Molecular Dynamics Simulations of Shock Through a Single Crystal of Pentaerythritol Tetranitrate," Joanne L. Budzien, Aidan P. Thompson, and Sergey Zybin, *J. Phys. Chem. B* 113 13142 (2009).





Identified three distinct regimes:

- *Deceleration (onset of endothermic reactions)*
- *Acceleration (onset of exothermic reactions)*
- *Steady State*



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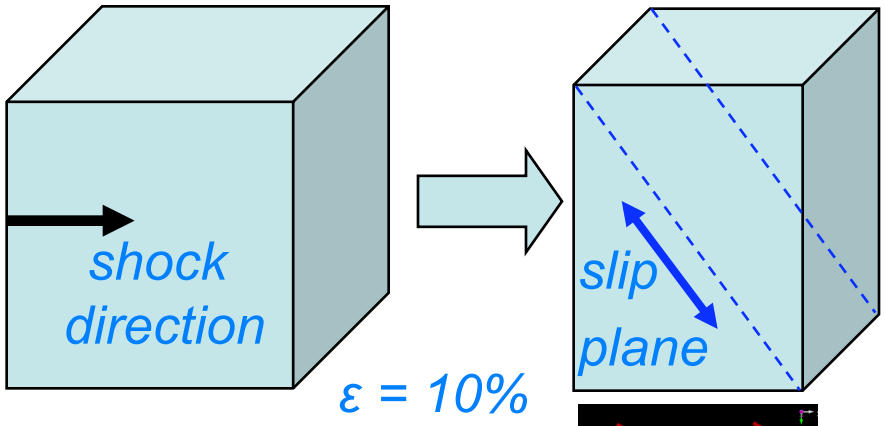
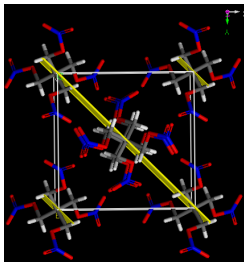
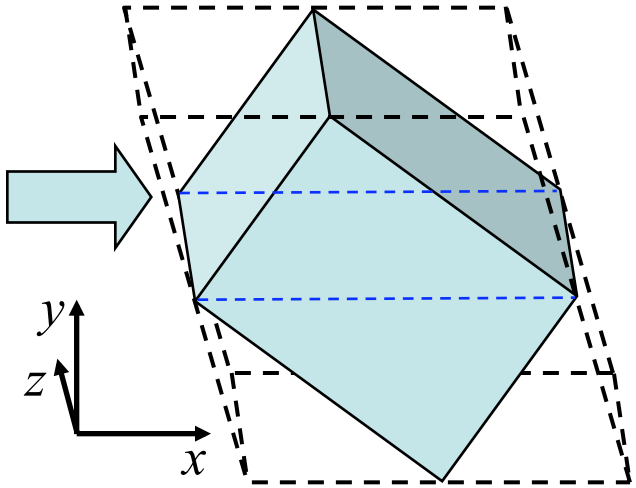
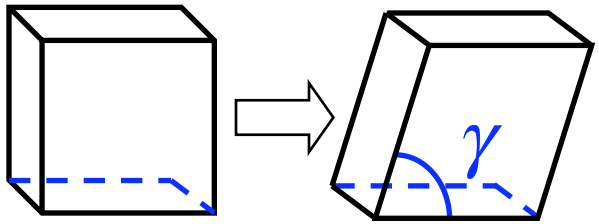
PETN Orientation-dependent Sensitivity







Dynamic Shear + Compression (DSC) simulation protocol:



Zybin, Goddard, Xu, van Duin and Thompson, *Appl. Phys. Lett.* (2010)