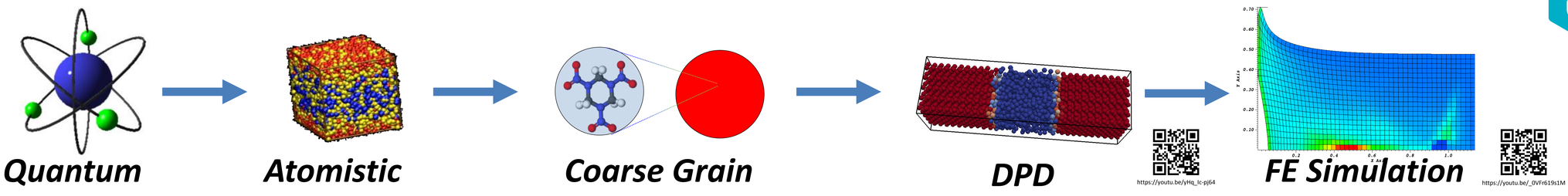
Parallelization, Acceleration, and Advancement of Dissipative Particle Dynamics (DPD) Methods

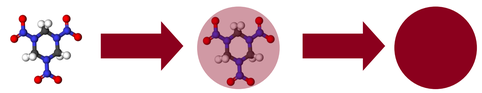
Timothy I. Mattox*[1], James P. Larentzos[1], Christopher Stone[2], Sean Ziegeler[1], John K. Brennan[3] and Martin Lísal[4]

[1] *Engility Corporation at the U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, U.S.A.*
[2] *Computational Science & Engineering, LLC, Chicago, IL 60622, U.S.A.*
[3] *U.S. Army Research Laboratory, The Rodman Materials Research Laboratory, Aberdeen Proving Ground, MD 21015, U.S.A.*
[4] *Laboratory of Aerosols Chemistry and Physics, Institute of Chemical Process Fundamentals of the ASCR and Department of Physics, J.E. Purkinje University, Ústí nad Labem, Czech Republic*

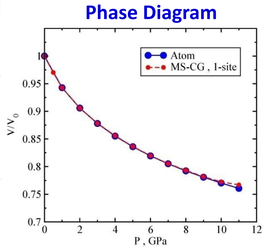


Coarse-Graining of RDX

Bottom-up coarse-graining (CG) from atomistic models is used to develop the meso-scale model. Properties which depend on intermolecular interactions, such as the phase diagram are well reproduced. However, properties which depend on the coarse-grained intramolecular degrees of freedom, such as the heat capacity, are underestimated. DPD-E provides a means to *recapture* these lost degrees of freedom.



Phase Diagram



Heat Capacity at 300 K

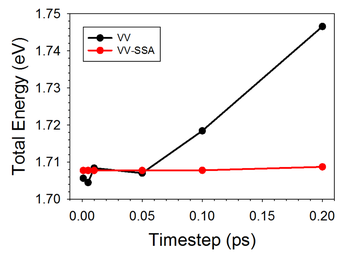
Source	C_p, J mol^{-1}K^{-1}
Experiment	232.54
CG-RDX	46.51

Gain Computational Speed by Removing Atomistic Detail

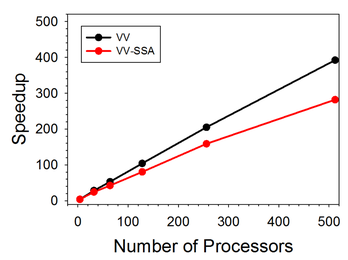
S. Izvekov, P.W. Chung, and B.M. Rice, *J. Chem. Phys.*, **135**, 044112 (2011).

Shardlow Splitting Algorithm (SSA)

- Split momenta integration into deterministic dynamics and stochastic dynamics
- Both can then be integrated using standard numerical integrators
- Readily extended to other DPD variants (not true for other integrators)
- Larger time steps allowable (~10-100x larger, with comparable energy conservation)



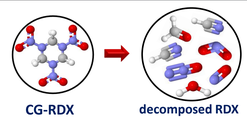
Energy diverges with original LAMMPS velocity-Verlet (VV) integrator



Lísal, Brennan, Bonet Avalos, *J. Chem. Phys.*, **135** (2011)

DPD with Chemical Reactions

- Add chemical reactivity to DPD method framework
- DPD Particle Microreactor: Reactions occur within or between DPD particle and NOT through bond breaking



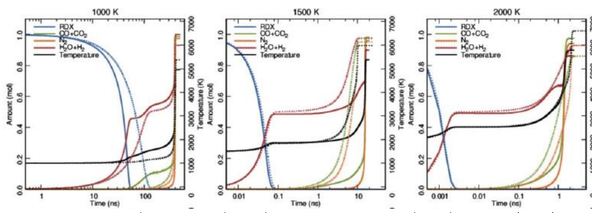
Step 1: Unimolecular Decomposition of RDX: endothermic

$$'RDX' \rightarrow 2CH_2O + 2N_2O + 2HCN + NO_2 + NO + H_2O$$

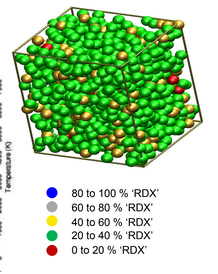
Step 2: CH_2O/NO_2 Combustion: exothermic

$$CH_2O + 2NO_2 \rightarrow \frac{3}{2}HONO + \frac{1}{2}CO_2 + \frac{1}{2}NO + \frac{1}{2}H + \frac{1}{2}CO$$

https://youtu.be/6cR6AfxgHmQ



slab of particles heated at time=0



Brennan, Lisal, Moore, Izvekov, Schweigert, Larentzos, J. Phys. Chem. Lett. (2014).

Constant Energy Dissipative Particle Dynamics (DPD-E)

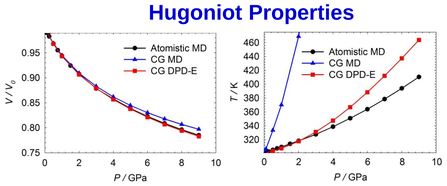
DPD-E provides a means to *recapture* the lost degrees of freedom due to coarse-graining by adding additional forces to account for momentum dissipation. A mesoparticle equation of state is coupled to the dynamics which accounts for internal degrees of freedom (i.e., chemical bonding) which were lost during coarse-graining. CG-MD gives poor Hugoniot properties since it is missing the meso-EOS.

$$m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{f}_i(t) = \sum_{i \neq j} \left(\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R \right)$$

$$\frac{du_i}{dt} = \frac{du_i^{mech}}{dt} + \frac{du_i^{cond}}{dt}$$

particles exchange ***momentum*** and ***heat***

Hugoniot Properties



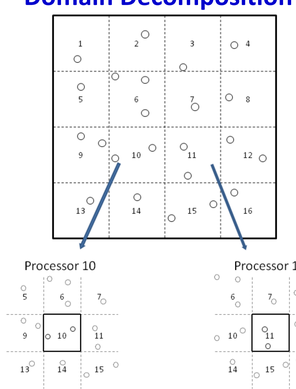
Recover Atomistic Physics through DPD-E Formulation

M. Lísal, J.K. Brennan, and J. Bonet Avalos, *J. Chem. Phys.*, **135**, 204105 (2011).

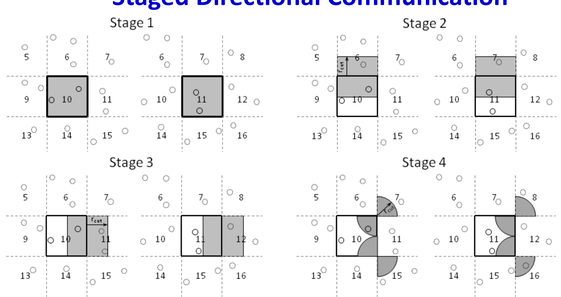
Brennan, Lisal, Moore, Izvekov, Schweigert, Larentzos, J. Phys. Chem. Lett. (2014).

Parallelization of SSA in LAMMPS

Domain Decomposition



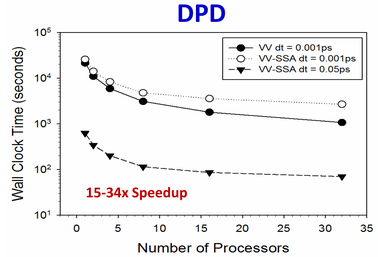
Staged Directional Communication



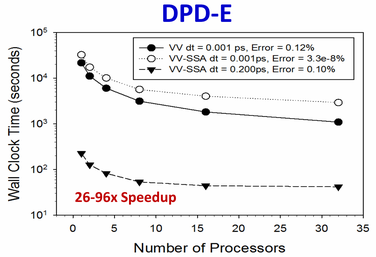
Highly-scalable constant-energy DPD simulations now possible, which allows micro- and mesoscale phenomena to be studied.

Larentzos, Brennan, Moore, Lísal and Mattson, *Comp. Phys. Commun.* (2014).

DPD



DPD-E

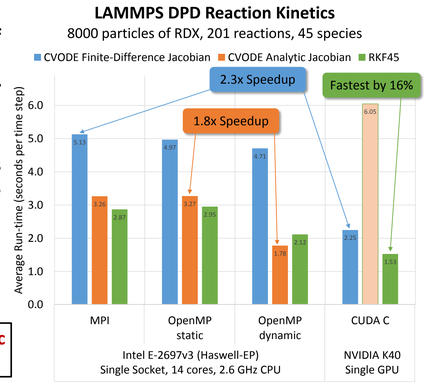


DPD Optimization and Acceleration

Chemical reaction equations within each DPD mesoreactor can be numerically stiff and costly to solve. The kinetics of each mesoreactor are independent of other particles and can be solved in parallel: an ideal candidate for many-core computing. Thus we accelerated the ODE solver tasks for each mesoreactor on a many-core processor using OpenMP or CUDA C.

$$\frac{dy_k}{dt} = V_{DPD}\, \dot{\omega}_k$$

Reaction Kinetics: 1.8x speedup using dynamic vs. static scheduling on a 14 core CPU.



ODE Algorithm + Programming Model + Compute Hardware → Performance

While the performance gains for complex reaction scenarios shown above are promising, the SSA consumes the vast majority of the runtime for non-reactive DPD scenarios (and for some simpler reactive scenarios). Thus, we are also improving the parallel efficiency of the SSA by restructuring/refactoring the MPI communications and the neighbor list construction for DPD. In addition, we are now using the Kokkos† C++ library (recently included in LAMMPS) to portably accelerate the intra-node performance of the SSA as well as the reaction DPD kernels for a diverse set of modern architectures, from GPUs to multi- and many-core CPUs.

†Edwards, Trott, "Kokkos: Enabling Performance Portability Across Manycore Architectures", *Extreme Scaling Workshop,* 2013

Acknowledgements

This effort is supported by the Institute for Multiscale Reactive Modeling of Insensitive Munitions (MSRM), which is a multi-team effort led by the U.S. Army Research Laboratory and the U.S. Army Armament Research, Development, and Engineering Center The authors also would like to acknowledge the computational resources and PETTT software support from the DoD High Performance Computing Modernization office under Contract No. GS04T09DBC0017.

* Corresponding author: timothy.mattox@engilitycorp.com