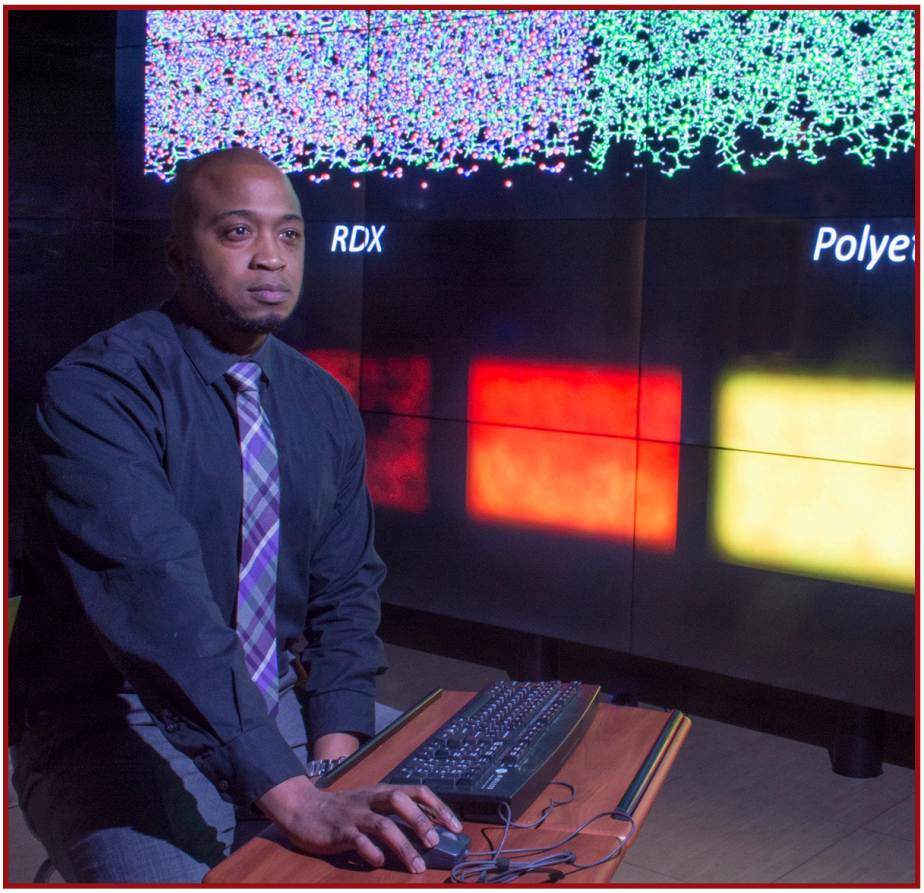
ATOMISTIC SIMULATION OF AN EXPLOSIVE FORMULATION (COMPOSITION A3 Type II)

Project Description

In order to enable a computational capability for design of next generation energetic materials (EMs), ARL has made a large investment in the development of a multi-scale modeling and simulation (MM&S) paradigm that incorporates all of the length scales (atomistic through continuum) that have to be addressed in order to computationally characterize an explosive. Although MM&S is not new, the novelty of the ARL approach is strict adherence to the principle that all models used in the MM&S hierarchy must be derivable purely from the physical and mathematical considerations underlying the problem of interest. This can be achieved by development of models at the atomistic level using accurate first principles quantum mechanical approaches with subsequent homogenization and "upscaling" of the first principles derived reference data into models that operate at the nanoscale, mesocale, and continuum level.



Currently, our target modeling material is the real formulation Composition A3 Type II which is a two-component formulation consisting of cyclotrimethylene trinitramine (RDX) energetic and polyethylene plasticizer (Figure 1). The overarching goal of this research effort is to demonstrate a completely coupled multi-scale simulation of this test system with experimental validation of all findings. However, before this can be accomplished, material models being applied in this study have to be developed and validated.

Relevance of Work to DOD

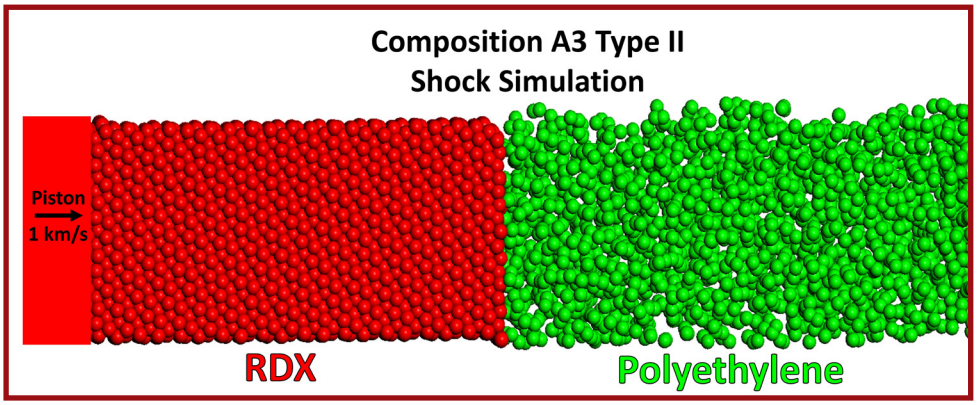
The goal of the Multiscale Response of Energetic Materials program, under which this work is being executed, is the development of advanced energetic materials with increased energy output and decreased sensitivity to initiation. Although advanced experimentation can be used to develop and characterize novel EMs, the experimental development cycle is a costly process that historically requires a minimum of twenty years from initial concept to fielding. However, the overall development time can be significantly reduced via application of advanced modeling and simulation techniques which enable virtual screening, virtual optimization and virtual exploration of novel materials thus expediting the design and development of new explosives for use by the Department of Defense.

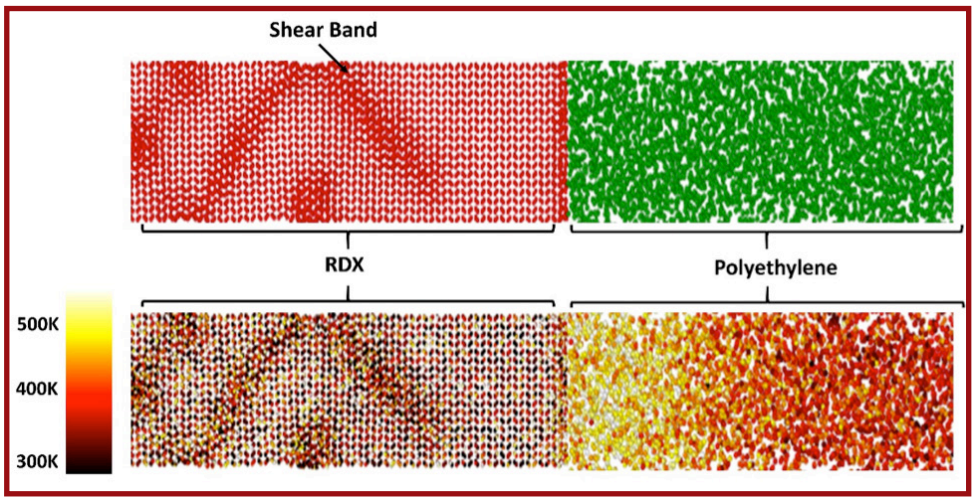
Computational Approach

Composition A3 Type II consists of RDX (91%) and polyethylene (PE) plasticizer. As such, atomistic modeling of this system requires not only a proper description of the intra-component (RDX-RDX and PE-PE) interactions, but also the inter-component (RDX-PE) interactions. The RDX-RDX and PE-PE interactions were treated using quantum mechanically

Figure 1: (top)
Simulator setup for Composition A3 Type II

Figure 2: (Bottom)
OpenFlow data structures for MPI integration





derived potentials available in the literature. The cross terms (RDX- PE) were developed at ARL by fitting a classical interaction potential of exponential-6 form to interaction energies of a polyethylene chain on an RDX surface. The resulting potential was validated via comparison to experimental interaction energies obtained using force-distance spectroscopy.

Following validation, the potential was used to perform large scale shock simulations of Comp A3 Type II in order to determine the effect of the polymer on the response of RDX to shock loading. All simulations were performed using the LAMMPS molecular dynamics software package on 3200 cores of a Cray XC40 (Excalibur) at the ARL DSRC. The simulation cells contained 2 million atoms and the shock was initiated by driving a piston, with a particle velocity of 1 km/s, into the RDX edge of the cell (Figure 1). The material was shocked along multiple orientations including the 100, 010, 001, and 210 directions

Results

A snapshot of shock compressed Comp A3 Type II, for a shock propagating along the 100 direction, is shown in Figure 2. In both panels, only the center of mass of each RDX molecule and PE oligomer is represented and the bottom panel is color coded by the internal temperature of each molecule. As shown, at the given compression rate, shear bands nucleate in the RDX layer, however RDX remains crystalline near the polymer interface. This results from stress relaxation that occurs in RDX due to the higher compressibility of the PE at the leading edge of the shock. It can also be observed that there is significant heating of the sample on the polymeric side of the interface.

Future

The models developed in this work, though derived using quantum mechanical methods, are non-reactive potentials. Given the significant heating that is evident in the shock compressed polymer, it can be expected that chemical reactions will occur. At present, the models we have developed cannot account for any degree of chemical transformation, beyond molecular conformation, therefore development of reactive models is currently underway.

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