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All-Atom Simulation of 3D Hot Spot Formation in Shocked TATB Explosive

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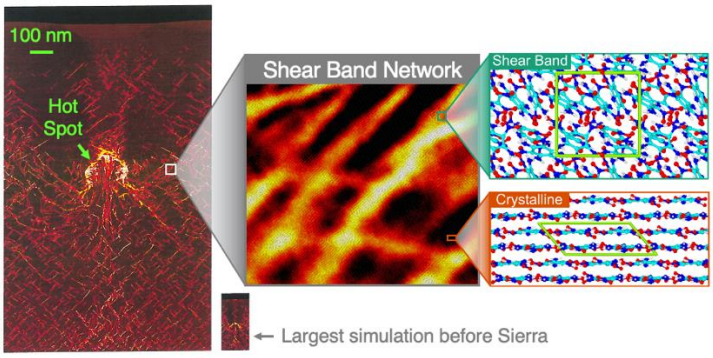
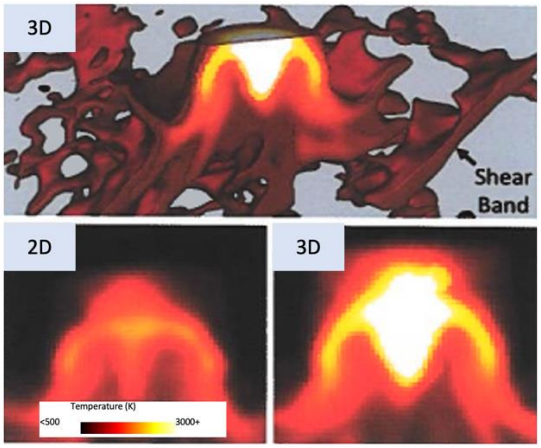
TATB is an insensitive high explosive (IHE) critical to the stockpile that is challenging to model at the continuum scale. Advanced detonation models in the Cheetah high explosive chemistry code require validation though subscale simulations. High explosive initiation is determined by micron-scale physics of hot spots formed a shock-collapsed pores. Pore sizes between 100 nm and 1 μm are believed to be the most important for determining the shock sensitivity of TATB. This range of pore sizes is difficult to access at the atomic scale through all-atom molecular dynamics (MD) simulations, even with Sierra-class computers. Quasi-2D simulations are widely used and allow much larger pore sizes (up to 400 nm) to be studied, but the applicability of 2D simulations to the actual 3D pore response is not understood. Resolving these uncertainties through "full physics" MD modeling is key for generalizing, parameterizing, and validating the kinds of continuum models used to inform design, safety, and performance.

This work was a continuation of FY20 efforts pushing simulations to full 3D with the largest-ever all-atom simulations of an explosive. These were the first all-atom full-3D simulations of large hot spots thought to govern explosive detonation and required over a billion atoms. Simulations were performed using LAMMPS, an open SNL science code. MD explosive models present unique challenges, even for established codes such as LAMMPS. Their model forms are more complex than typical models for metals, while simulating high temperature-pressure conditions is demanding and increases computational cost. Scaling problems in GPU-enabled MD algorithms initially limited simulations to <100 million atoms but were resolved through collaboration with SNL. An overall 24x speedup was obtained relative to CPU machines. Specialized analysis of these simulations required a bottom-up refactoring and algorithm parallelization of in-house codes and application of computer vision algorithms to extract meaningful information.



Sierra enabled the first all-atom simulations of large hot spots thought to govern shock initiation of high explosives. The material strength response is complex, leading to a network of highly reactive shear bands that explain the unusual detonation properties of insensitive high explosives.

Hot spots formed at 3D spherical pores were found to be much hotter than those at 2D cylindrical pores, which leads to substantially different predictions for hot spot chemistry as reaction kinetics depends exponentially on temperature. A plastic failure response producing highly reactive shear band networks was predicted in FY20 though quasi-2D simulations and was verified in the 3D simulations. Computer vision tools were developed to quantify the size and connectedness of the shear band network as a function of shock strength. Including this subscale physics in Cheetah models holds promise to yield a broadly applicable model for IHE detonation.



3D spherical pores lead to greater focusing and hotter hot spots than predicted for quasi-2D cylindrical cases. These hot spots are surrounded by a 3D shear band network.

This project is complete as of FY21-Q2. It demonstrated scaling of LAMMPS for organic materials out to the billion-atom scale and opens new application areas including polymers and other explosives. A transferable analysis suite was developed for billion-atom scale simulations of organic materials. Strong scaling limits the duration and size of billion-atom scale calculations (>30,000 atoms/GPU) on Sierra. The experience gained and tools developed have drastically increased the size for “routine” simulations of explosives to involve 10s to 100s of millions of atoms when performed on smaller machines of similar architecture to Sierra. The MD model used for the present simulations was non-reactive. A fully realized all-atom explosive modeling framework would extend substantially more expensive reactive MD models out to similar scales.

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