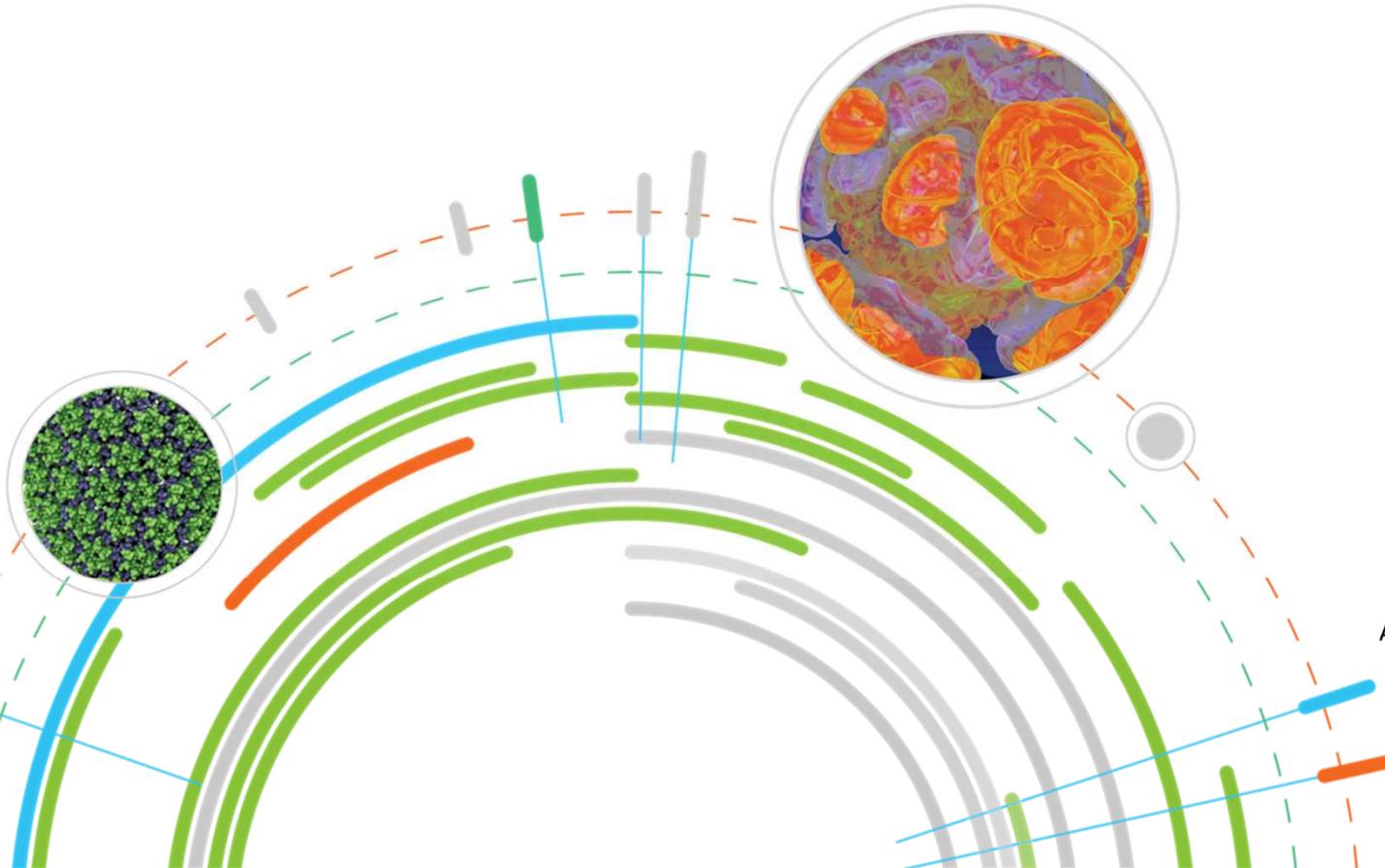


# Nanostructure-enhanced Chemical Reactivity and Detonation in Energetic Materials

SAND2015-7576R



Argonne Leadership  
Computing Facility

# Nanostructure-enhanced Chemical Reactivity and Detonation in Energetic Materials

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ALCC-2014

## Impact and Approach

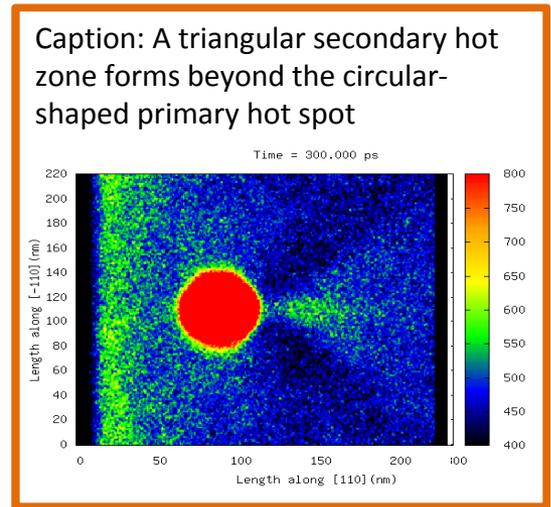
- Scientific impact: The project supports the investigation of energetic materials. This work is providing fundamental insight into initiation mechanisms in energetic materials.
- Computational approach: Molecular dynamics simulations using ReaxFF (Reactive force field) reactive interatomic potential as implemented in LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)
- ReaxFF MD simulations on the required scale of 10 million particles can only be done on capability-class machines like Mira

## Accomplishments

- Spherical and cylindrical voids have similar effects on hot spot formation and initiation in energetic materials under shock conditions, although averaged hot spot temperature is somewhat lower for cylindrical voids.
- We observed the formation of a secondary hot zone located beyond the primary hot spot. Its formation may be attributable to the secondary shock wave generated when upstream void fragments collide with the downstream void surface.

## ALCF Contributions

- Nichols Romero assisted in porting the Kokkos version of ReaxFF in LAMMPS to Mira



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