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Atomistic Simulation of Initiation in Hexanitrostilbene (HNS)

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U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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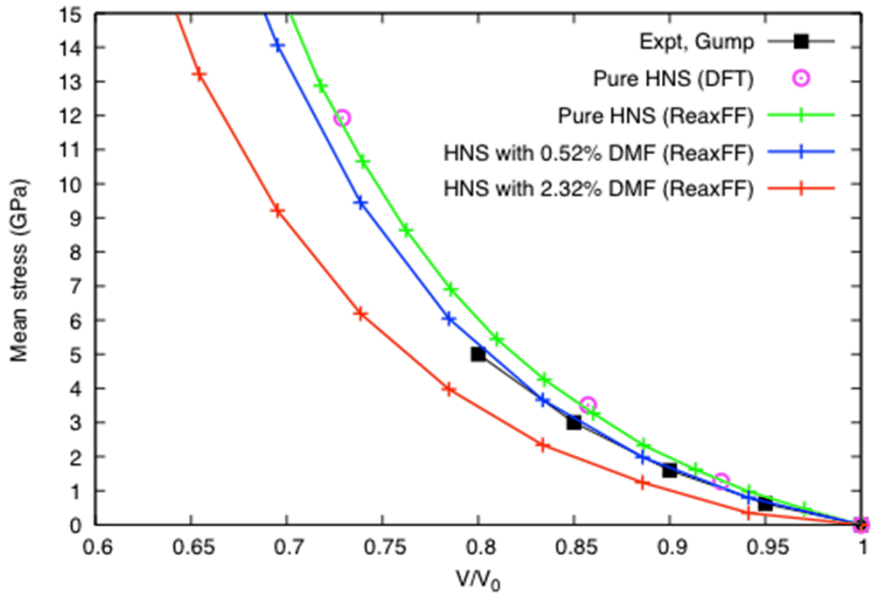
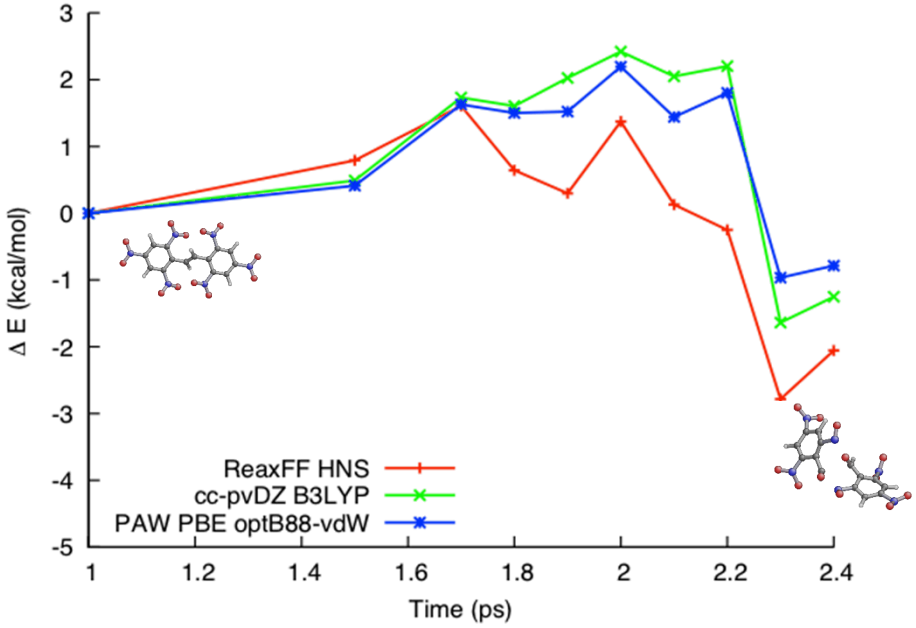
Introduction

- ReaxFF force field for HNS based on CHO combustion and CHNO nitramine force fields [a-d]
  - Provides good structural properties, isotherm, and primary dissociation pathway for HNS

Isotherm



Dissociation

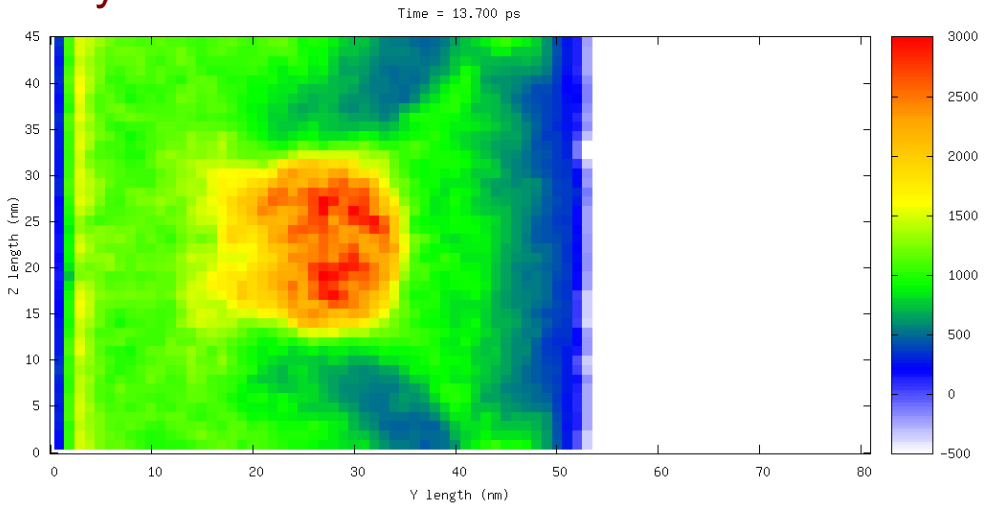


T.-R. Shan, R. R. Wixom, A. P. Thompson, Proc. 15th International Detonation Symposium, *in press*
SAND2014-15638 PE

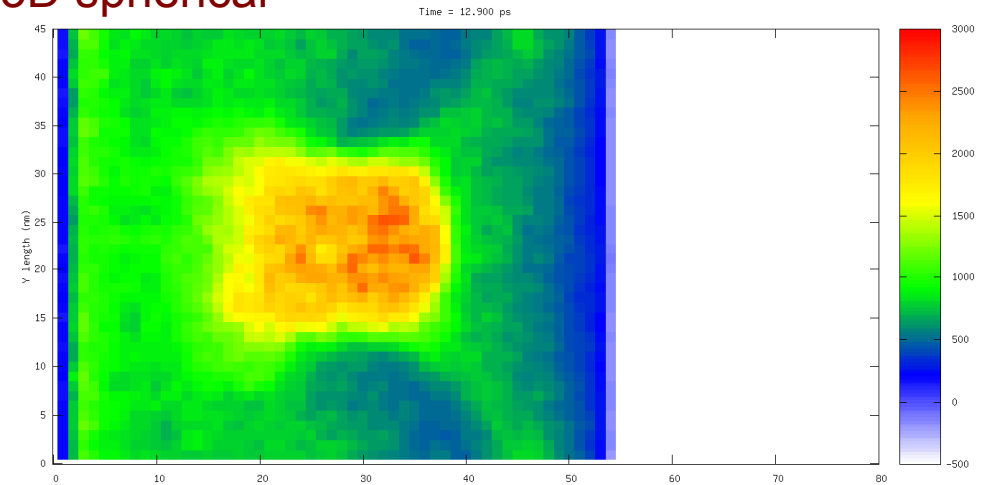
Introduction

- Comparison of spherical/cylindrical void
  - 20 nm diameter void
  - Impact velocity 2.25 km/s
  - 3D spherical void yields a hotter/larger hot spot
  - Very similar behaviors in void collapse, jetting of fragments, hot spot formation mechanism
- Reasonable to approximate void collapse with 2D cylindrical configurations
  - Main advantage: saves computational expense

2D cylindrical



3D spherical



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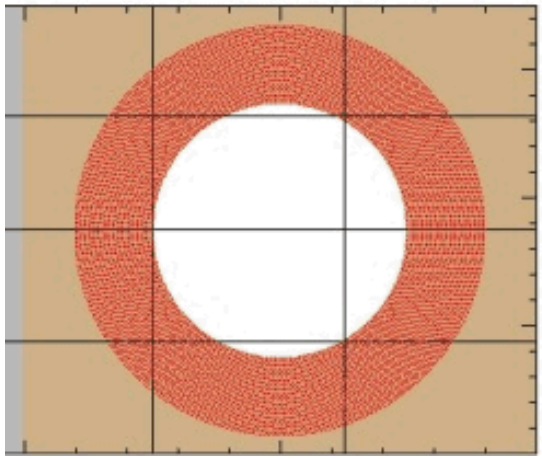
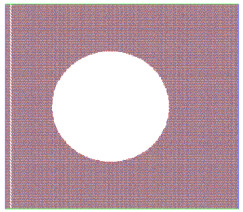
Introduction

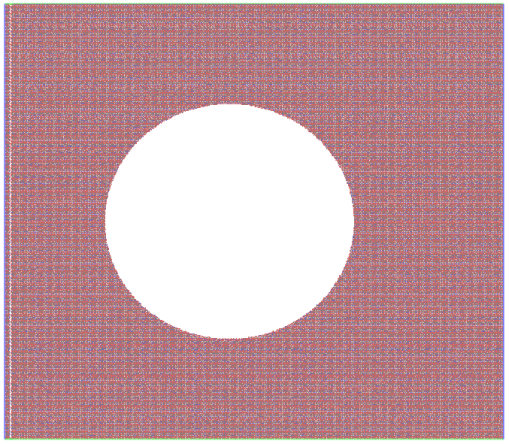
20 nm

Comparison to hydrodynamics
- 100 nm void

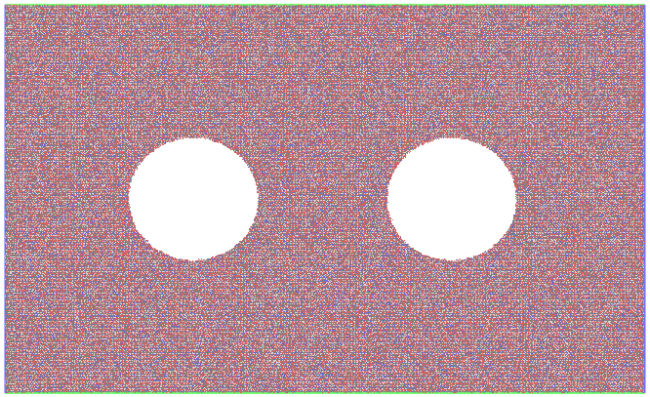


Effect of void size
- 50 & 100 nm void



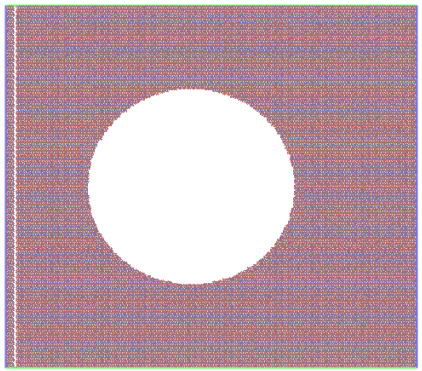


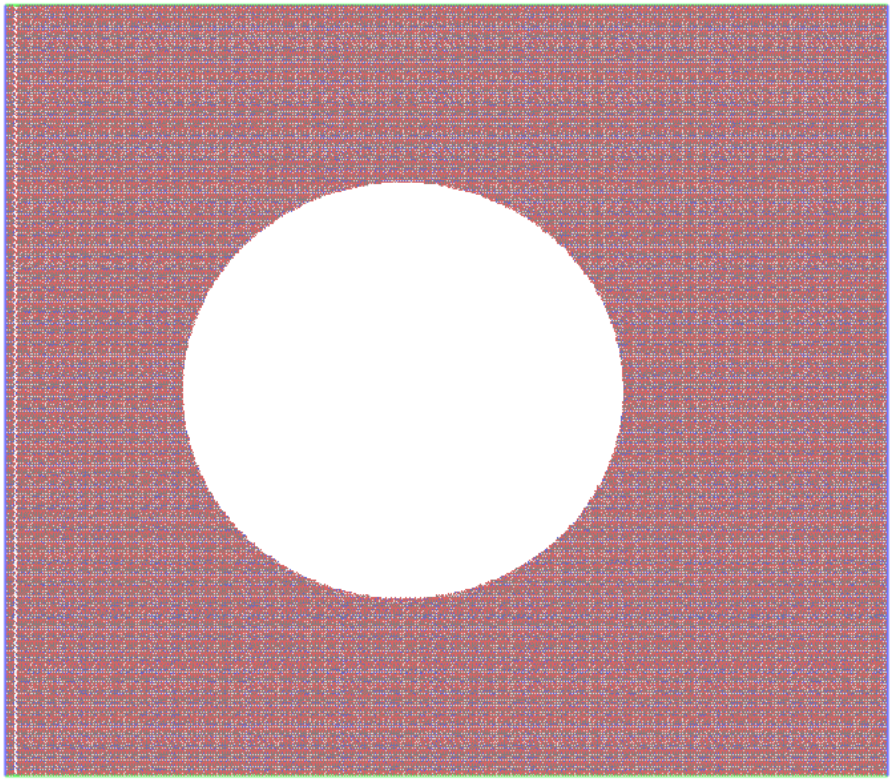
Effect of void interactions
- Two 50 nm voids



Effect of void size

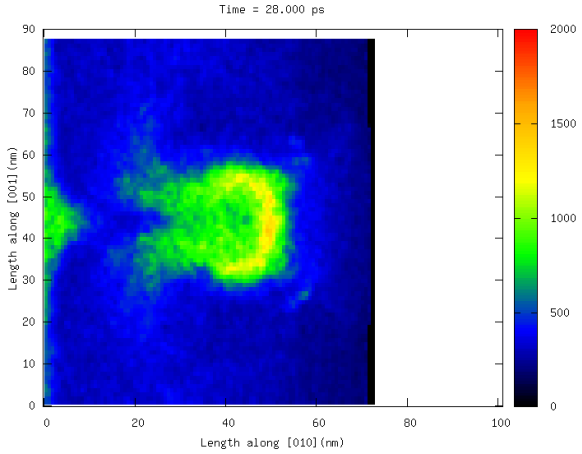
- Compare 50 and 100 nm
  - with U_S=4.0 km/s (U_P=1.25 km/s)
  - with U_S=6.0 km/s (U_P=2.25 km/s)

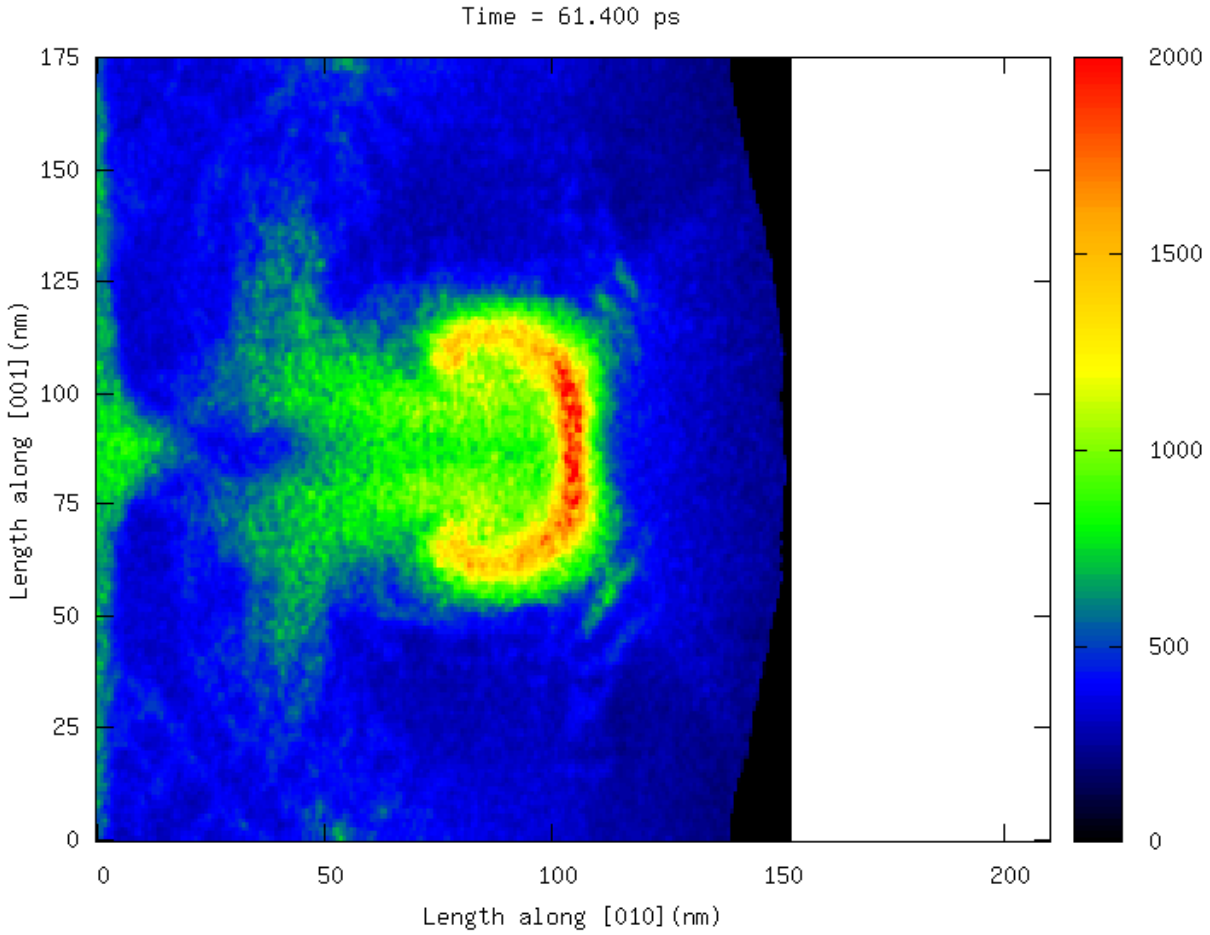




Effect of void size

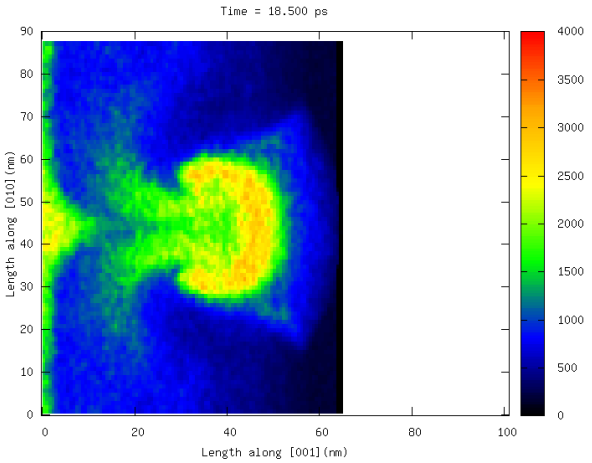
- Compare 50 and 100 nm with U_S=4.0 km/s (U_P=1.25 km/s)

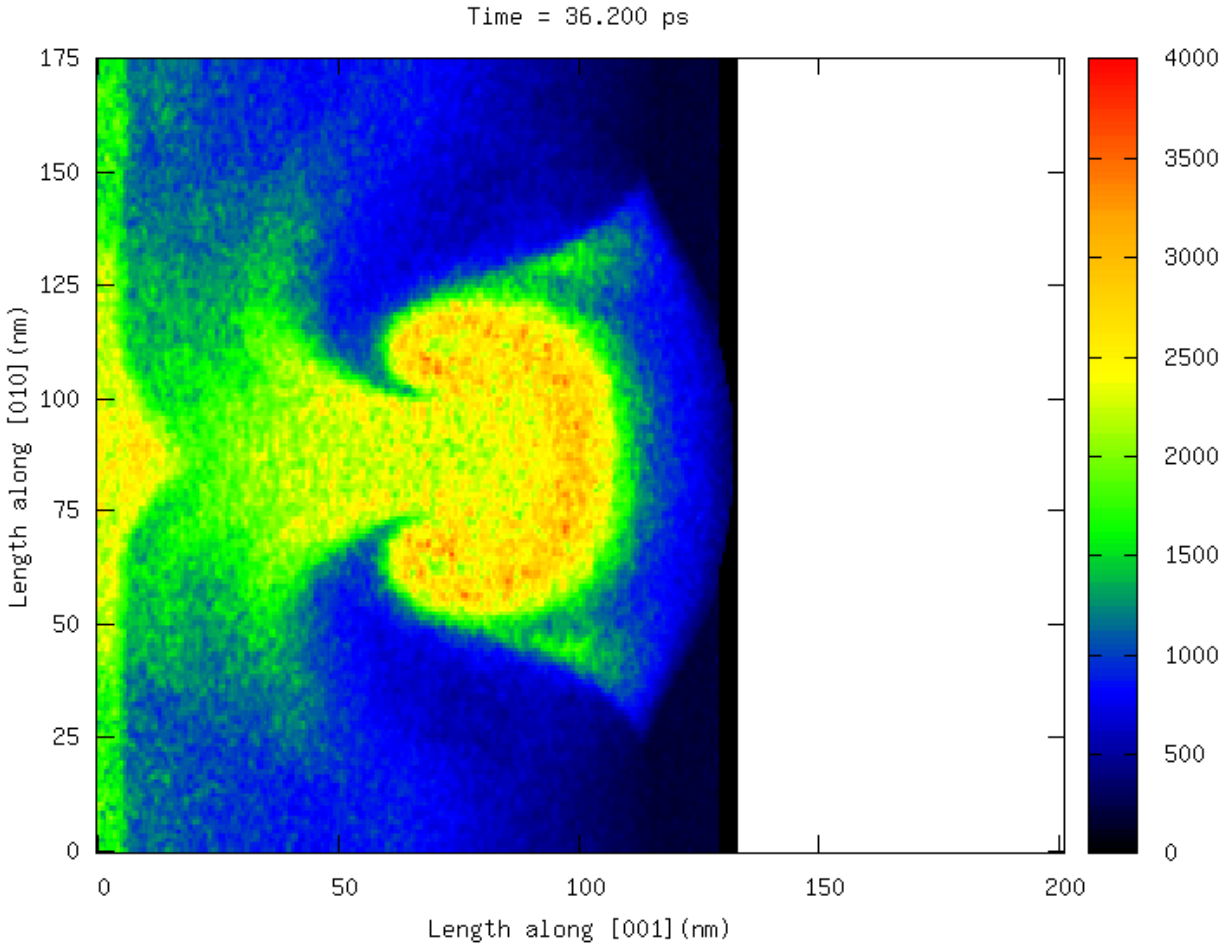




Effect of void size

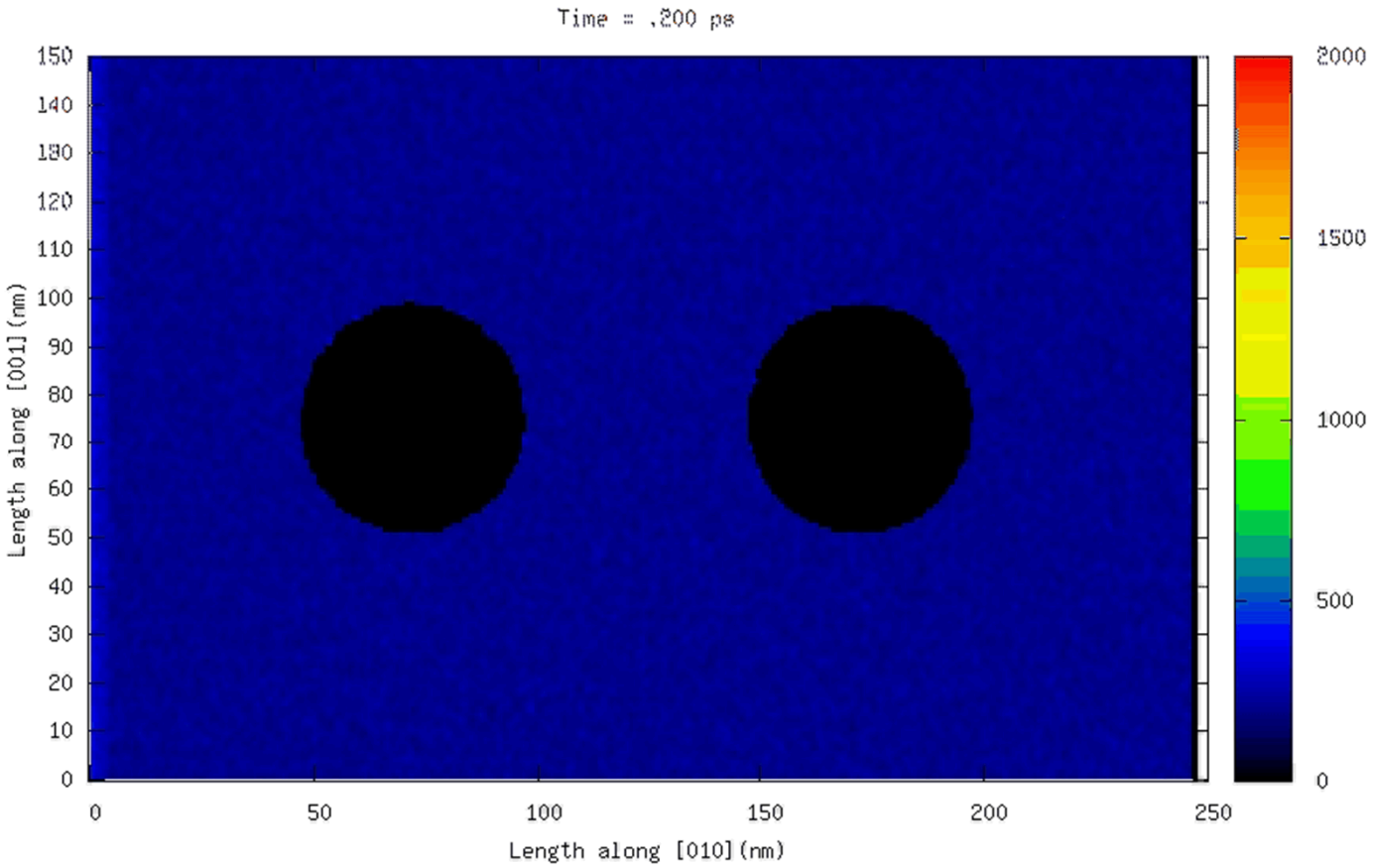
- Compare 50 and 100 nm with U_S=6.0 km/s (U_P=2.25 km/s)





Effect of void interactions

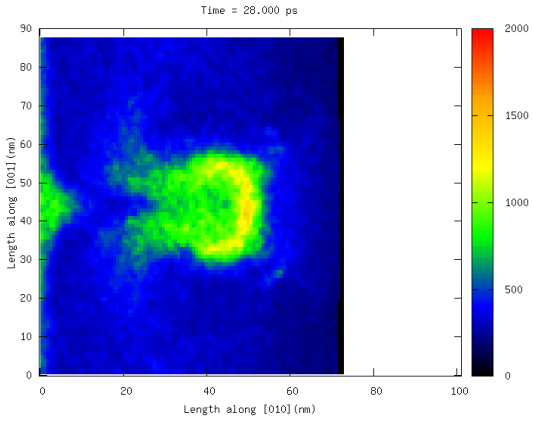
- Two 50 nm voids shocked at U_S=4.0 km/s (U_P=1.25 km/s)
  - Sequence of temperature maps showing two voids collapse



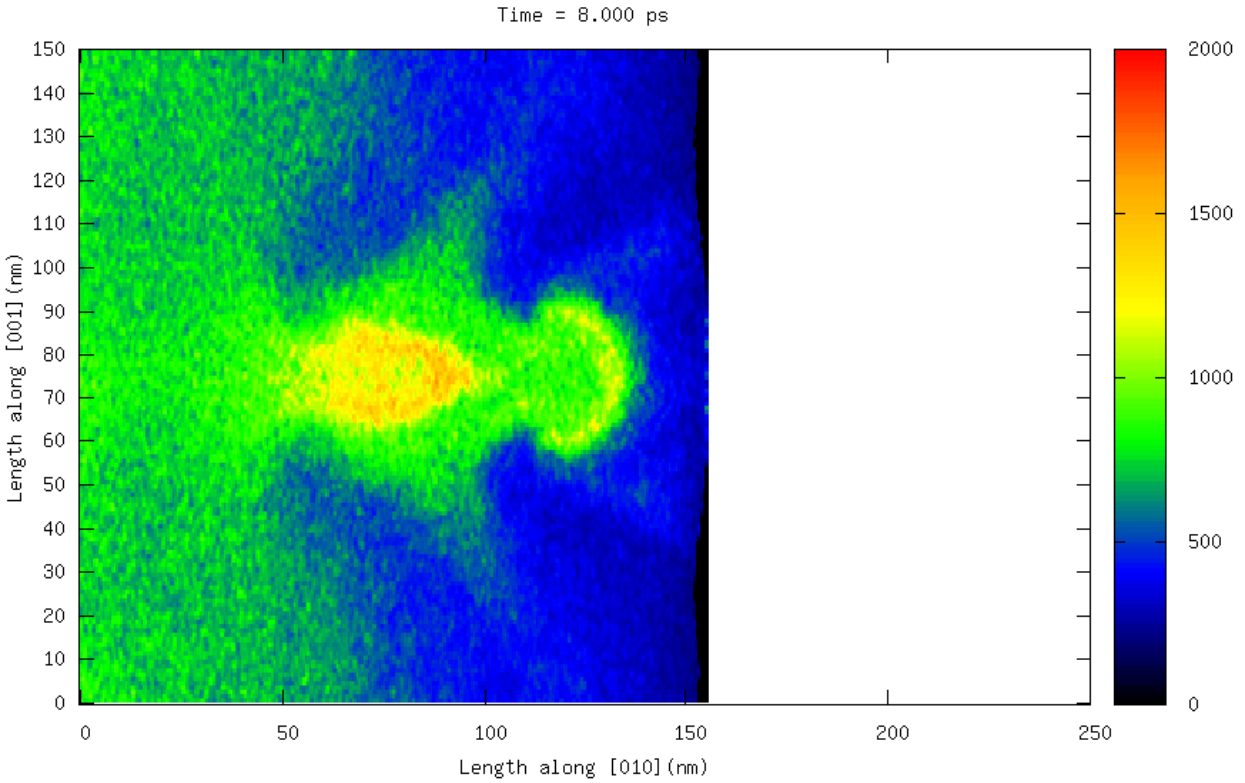
Effect of void interactions

- Formation of a hot spot with extended size due to void-void interactions

Single 50 nm void

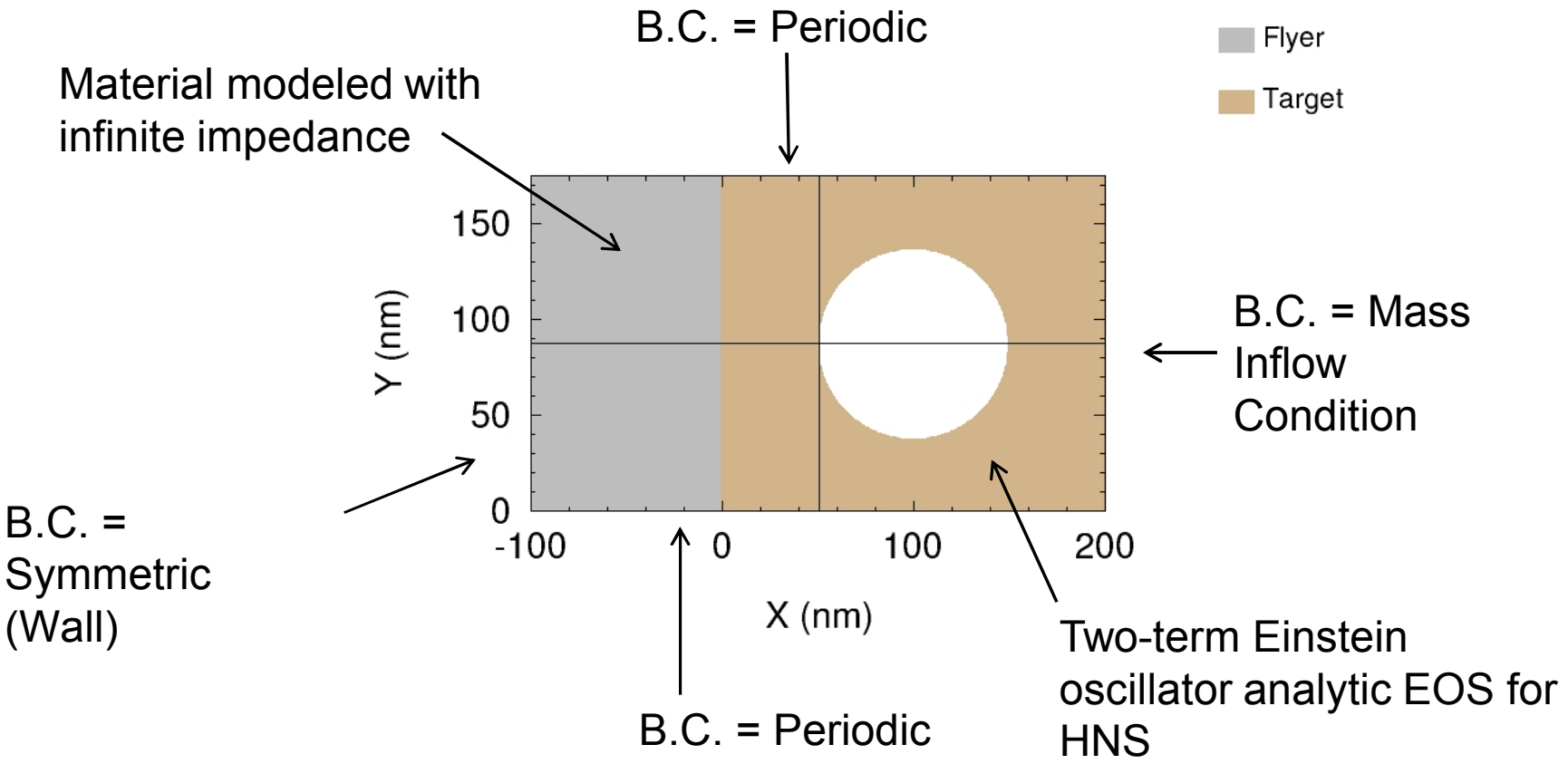


Two 50 nm voids



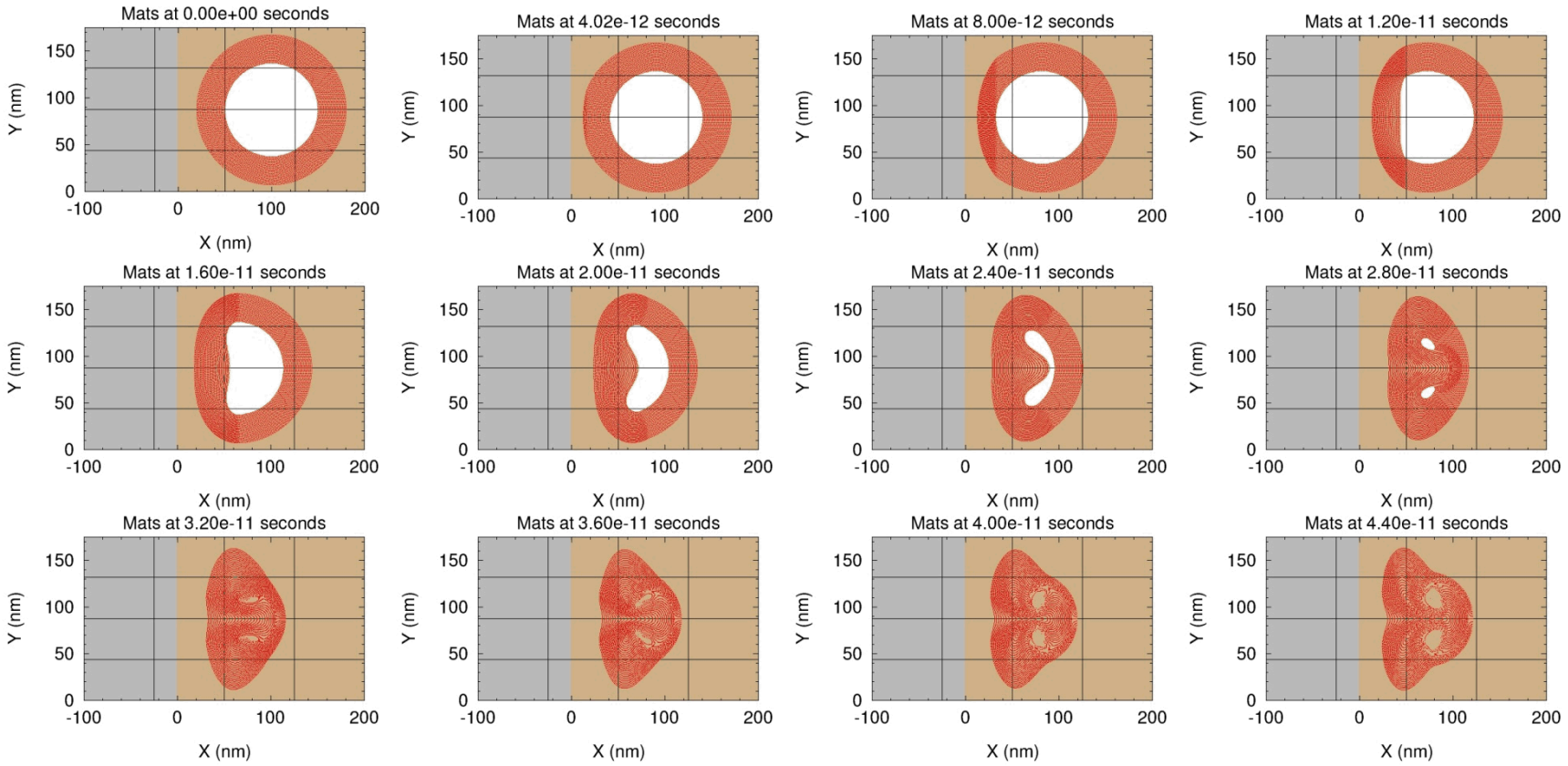
Comparison to hydrodynamics

- CTH software setup
  - Using 2.25 km/s flyer velocity as baseline case



Comparison to hydrodynamics

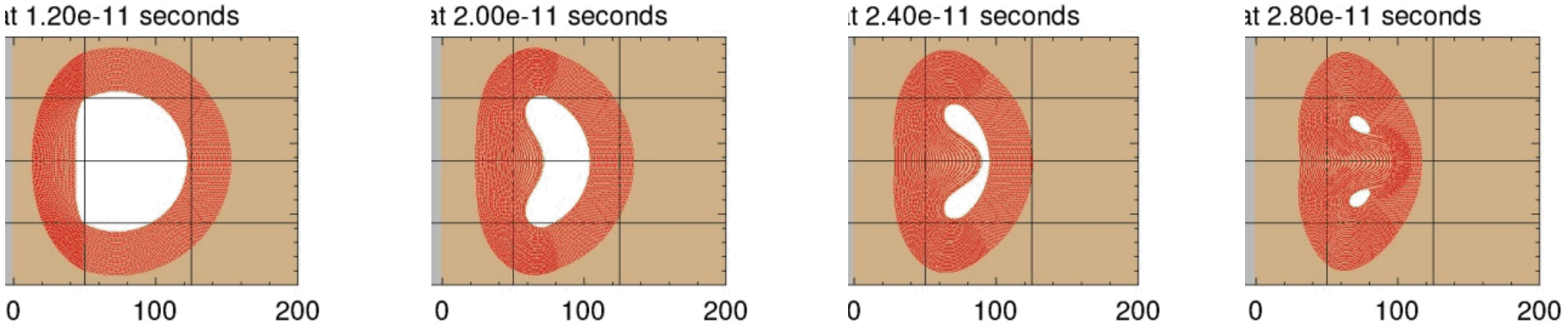
- Lagrangian Tracer Mesh
  - A 30 nm thick “shell” of Lagrangian tracers tracking void collapse process



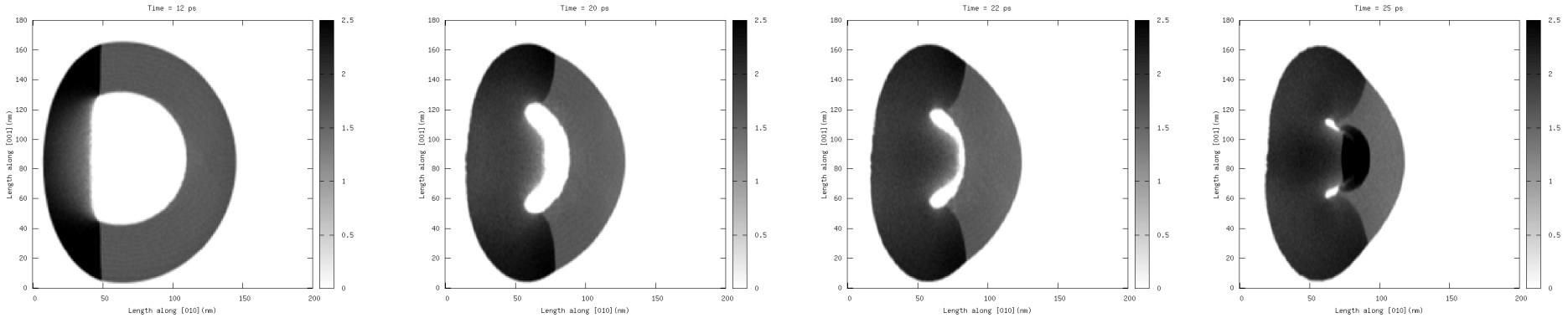
Comparison to hydrodynamics

- Void collapse behavior

CTH hydrodynamics



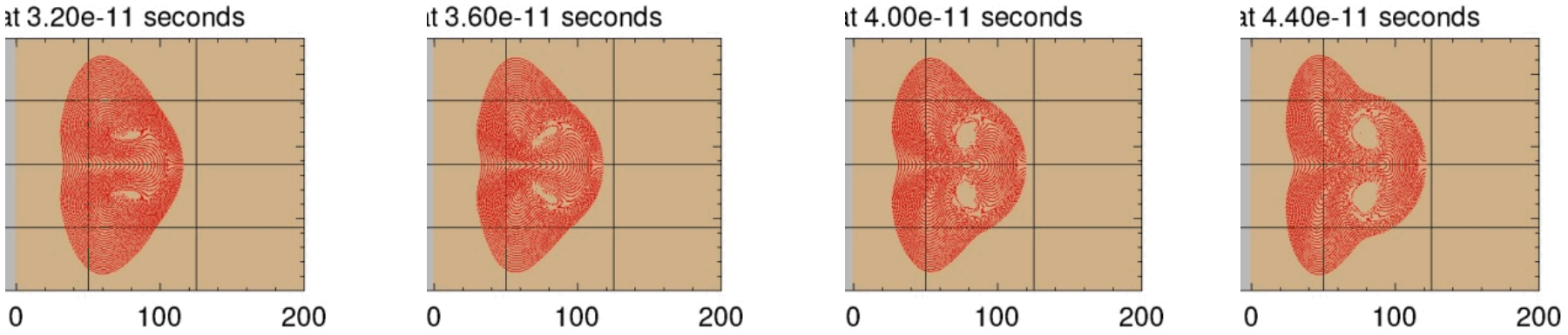
LAMMPS ReaxFF MD



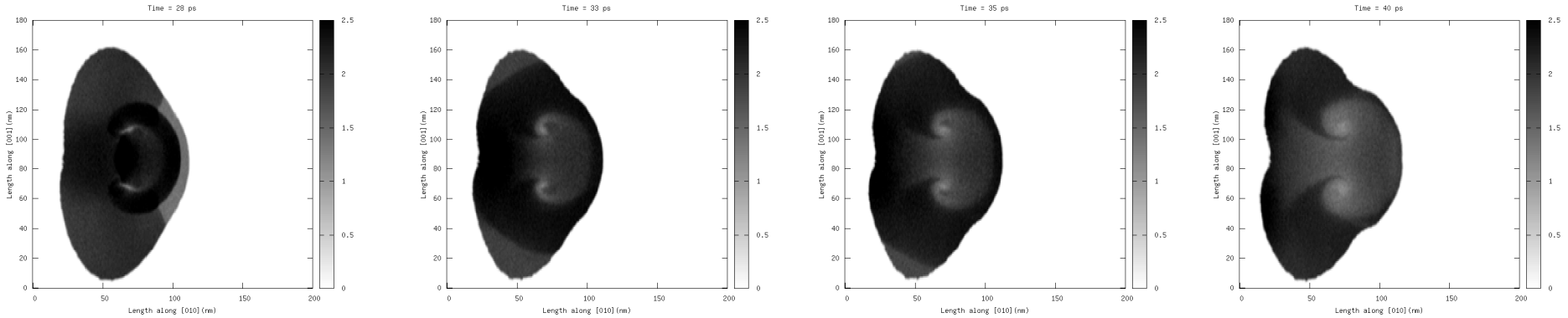
Comparison to hydrodynamics

- Void collapse behavior

CTH hydrodynamics



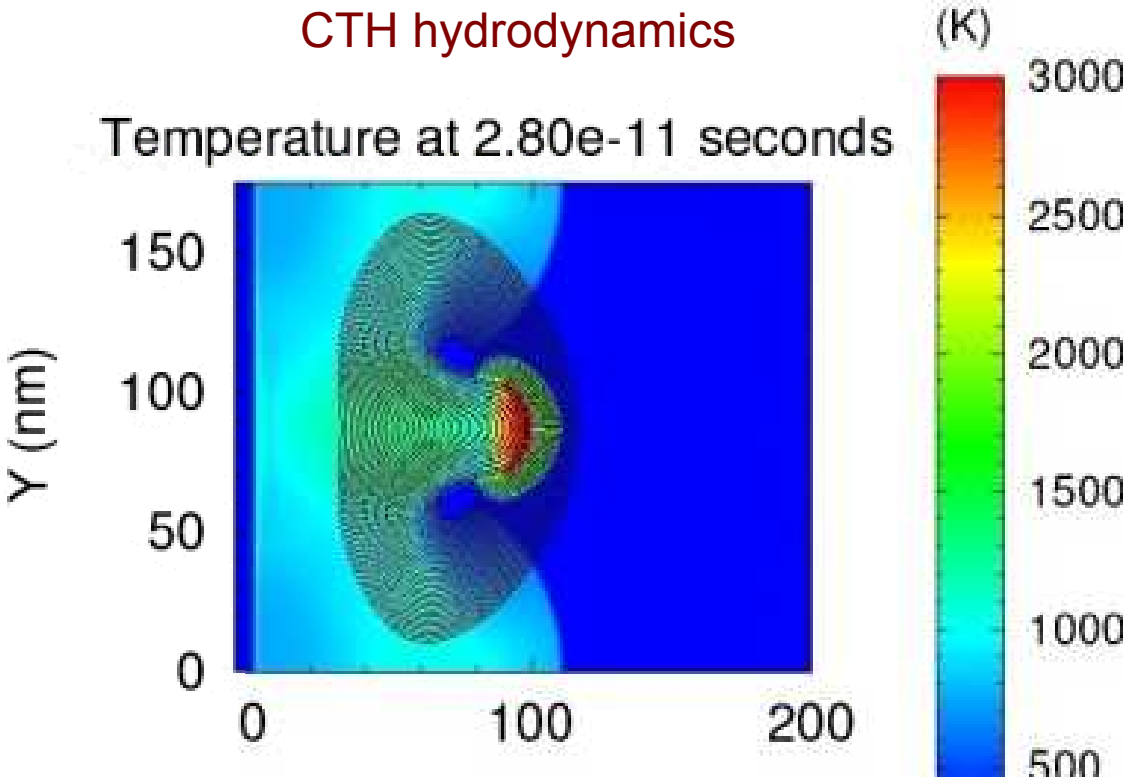
LAMMPS ReaxFF MD



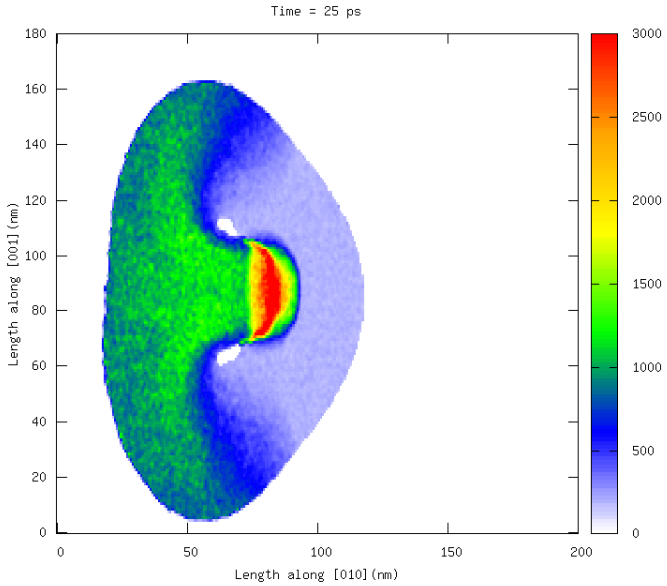
Comparison to hydrodynamics

- Temperature field

CTH hydrodynamics



LAMMPS ReaxFF MD



Conclusions

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- Large scale reactive molecular dynamics simulations with ReaxFF force field in LAMMPS
- Hot spot size and temperature increase with void size
- Formation of a hot spot with extended size due to void-void interactions
- Good qualitative agreement with hydrodynamics simulations using CTH