The Influence of an Applied Heat Flux on the Violence of Reaction of an Explosive Device

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XSEDE 13'

Purpose of Research

- Analyze the effects of the heat flux and heating geometry on the cook-off response of an explosive device

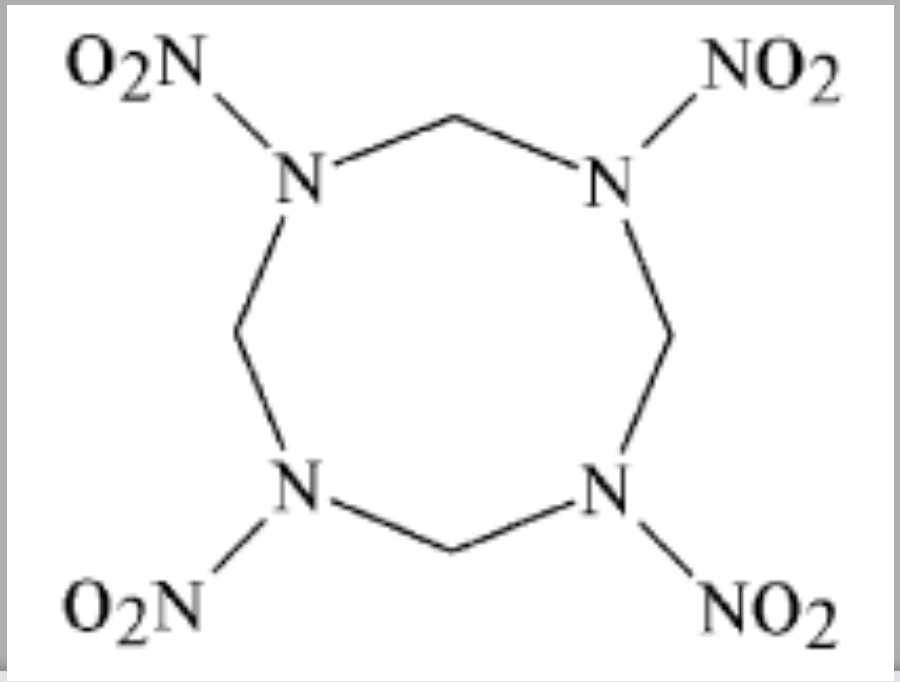
- Understand the underlying mechanism(s) of a Deflagration to Detonation Transition

Overview

- Background on Energetic Materials
- Uintah Computational Framework
- Cook-Off Results
- Future Research

Energetic Materials

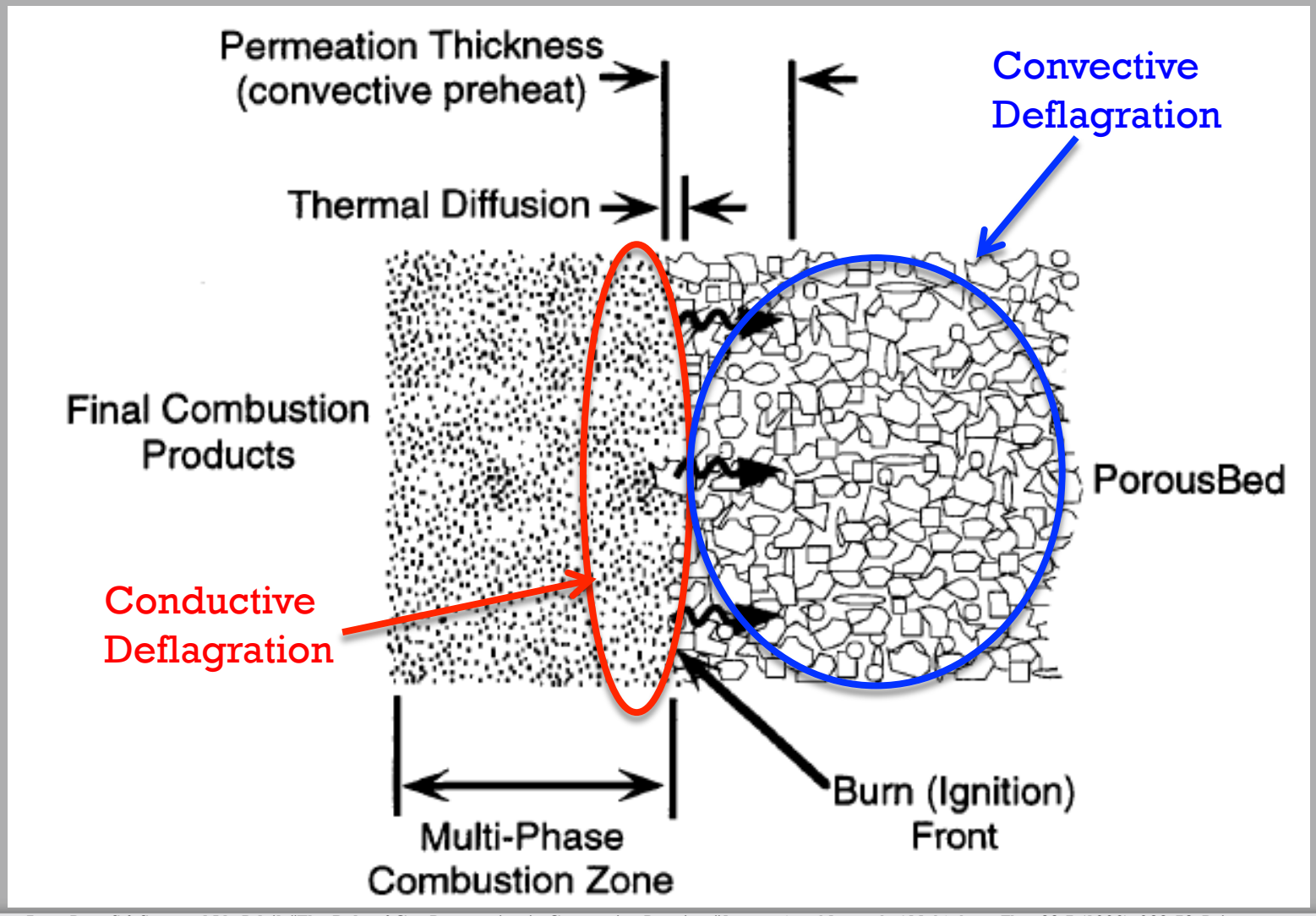
- Octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine (HMX)
- PBX9501 (Plastic Bonded Explosive)



Combustion

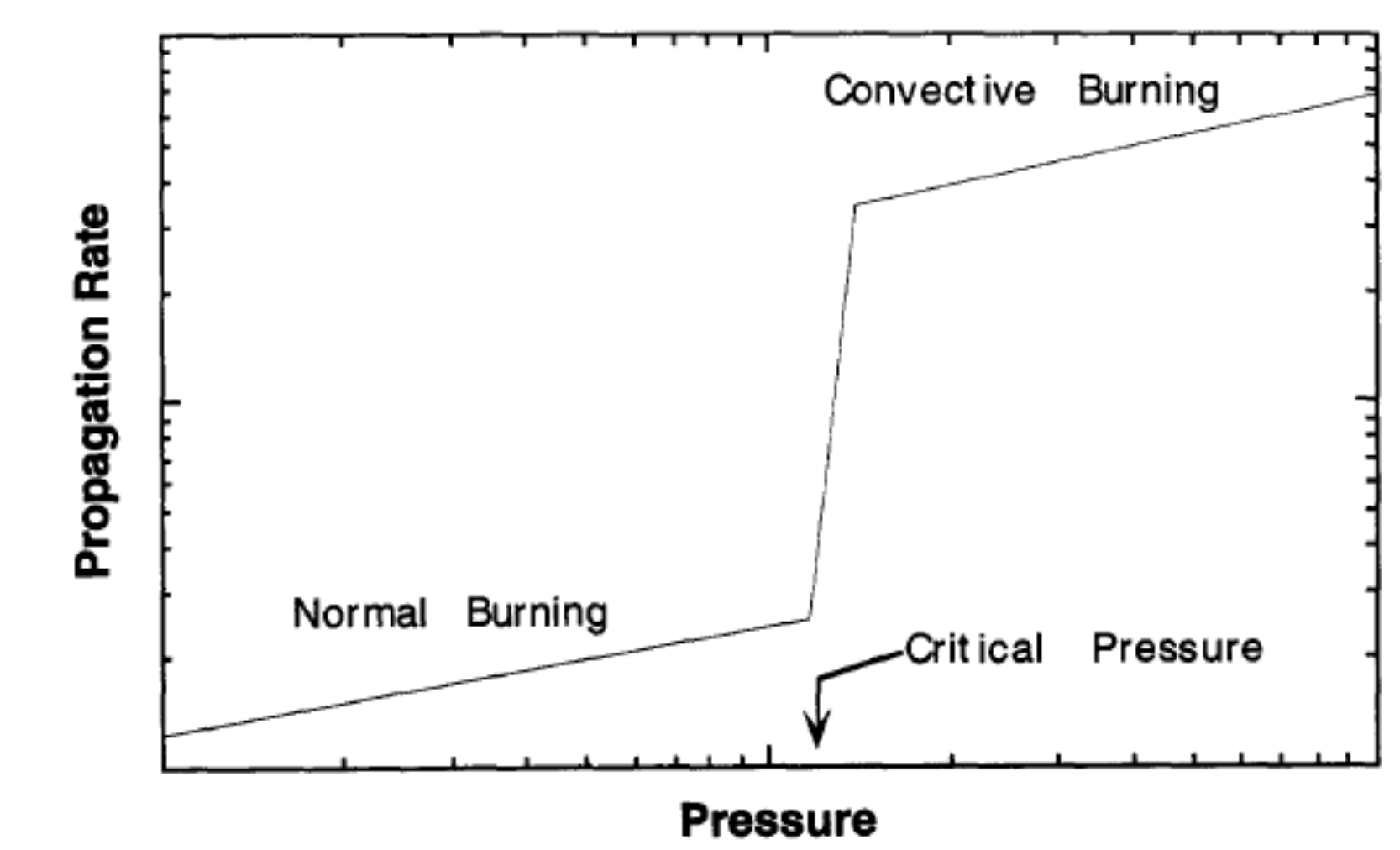
- Deflagration
  - Convective and Conductive Deflagration

Combustion: Deflagration



Asay, B.w., S.f. Son, and J.b. Bdzil. "The Role of Gas Permeation in Convective Burning."*International Journal of Multiphase Flow* 22.5 (1996): 923-52. Print.

Combustion: Deflagration



Asay, B.w., S.f. Son, and J.b. Bdzil. "The Role of Gas Permeation in Convective Burning."*International Journal of Multiphase Flow* 22.5 (1996): 923-52. Print.

Combustion: Detonation

- Deflagration
  - Convective and Conductive Deflagration
- Detonation

http://www.chamorrobible.org/gpw/gpw-20050304-English.htm

Combustion

- Deflagration
  - Convective and Conductive Deflagration
- Detonation
- Deflagration to Detonation Transition (DDT)
- Shock to Detonation Transition (SDT)

Uintah Computational Framework

- Material Point Method (MPM)
  - Lagrangian
  - Condensed phase models
- Multi-material CFD formulation (ICE)
  - Finite volume-Eulerian
  - Gas phase models
- MPM-ICE
  - Lagrangian/Eulerian
  - Solves fluid-structure interactions

- J. Guilkey, T. Harman, and B. Banerjee. An Eulerian-Lagrangian approach for simulating explosions of energetic devices. Computers and Structures, 85:660-674, 2007.

Uintah Computational Framework

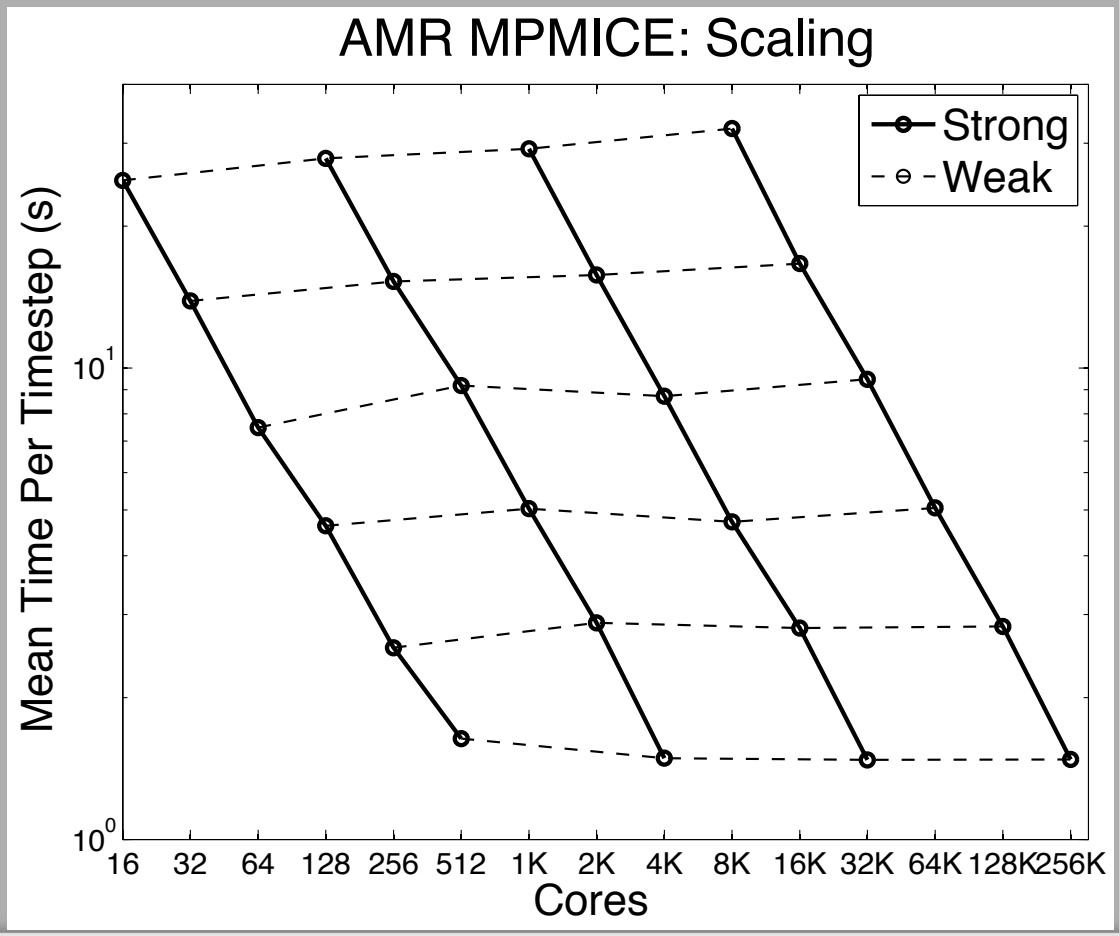
- Global Kinetics Model
  - represents the physics and chemistry of macroscopic energetic material combustion
- Breaks energetic material combustion into two parts
  - Condensed phase
  - Gas phase

Uintah Computational Framework

- Ward Son Brewster (WSB) Model
  - Burn model
- ViscoScram
  - Isotropic damage model
  - Stress depended cracking
- JWL ++
  - Detonation model
- Validation
  - J. Peterson and C. Wight. An Eulerian-Lagrangian computational model for deflagration and detonation of high explosives. *Combustion and Flame*, page in press, 2012.

Scaling

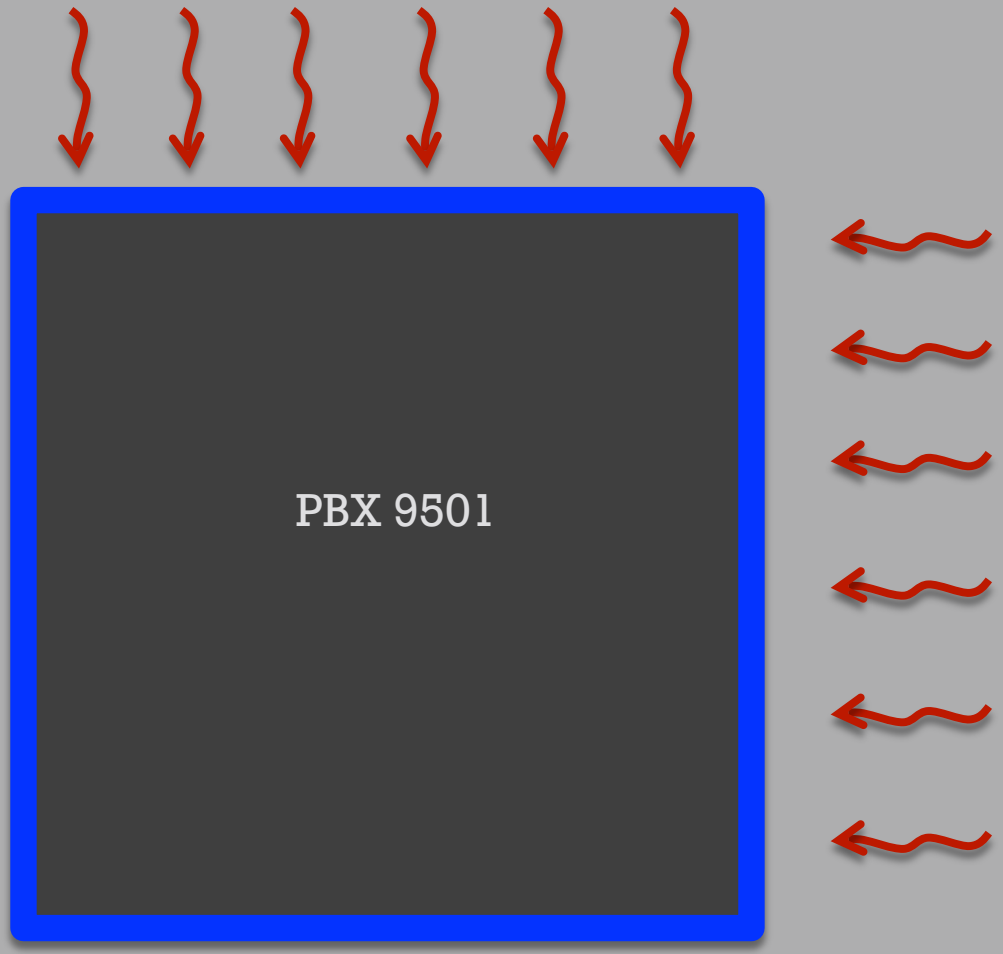
- MPM-ICE Scalable up to 256K Cores



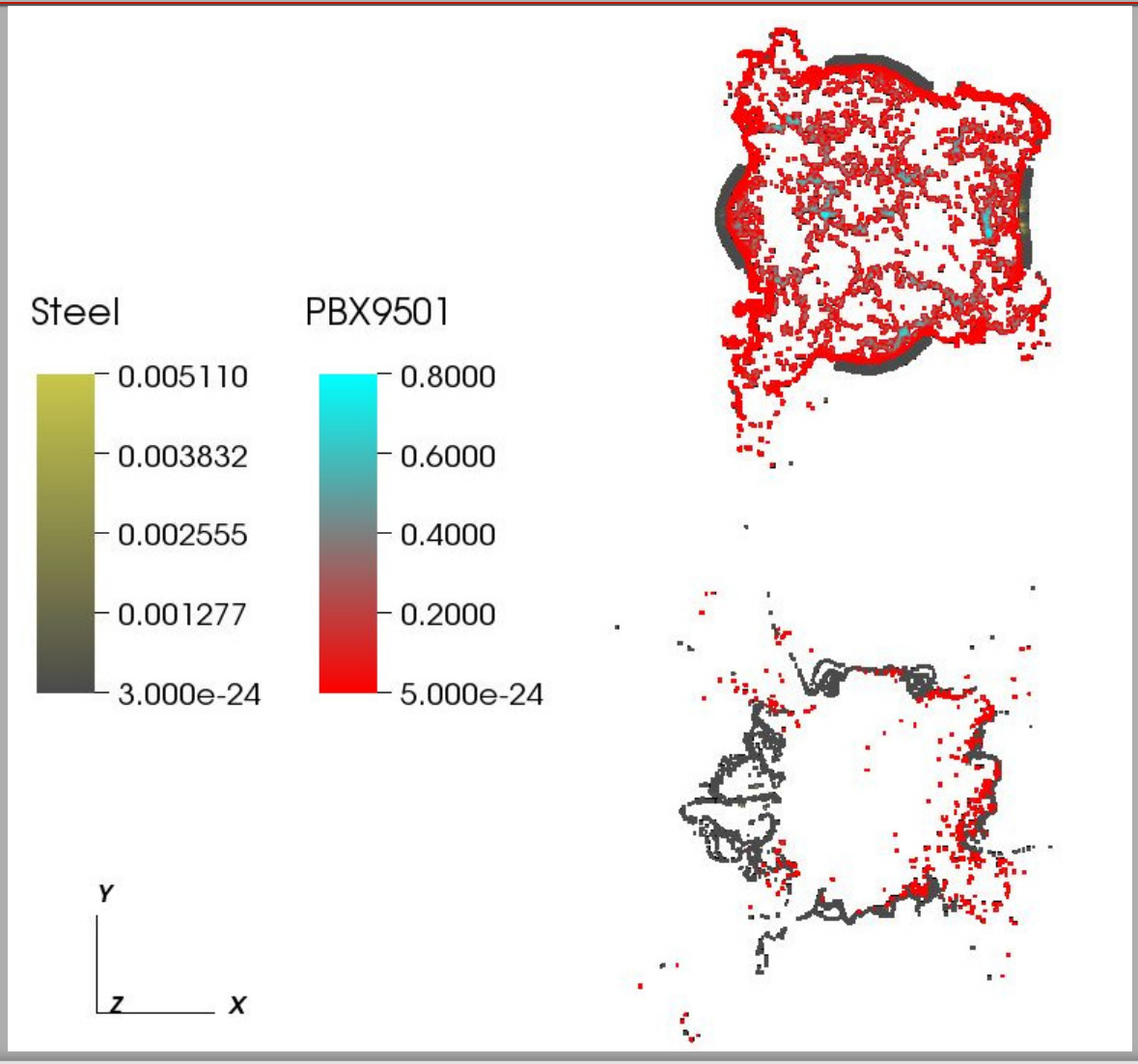
Current Work

- Heat flux and heating geometry effects on a cook-off response
- Deflagration to Detonation Transition mechanism

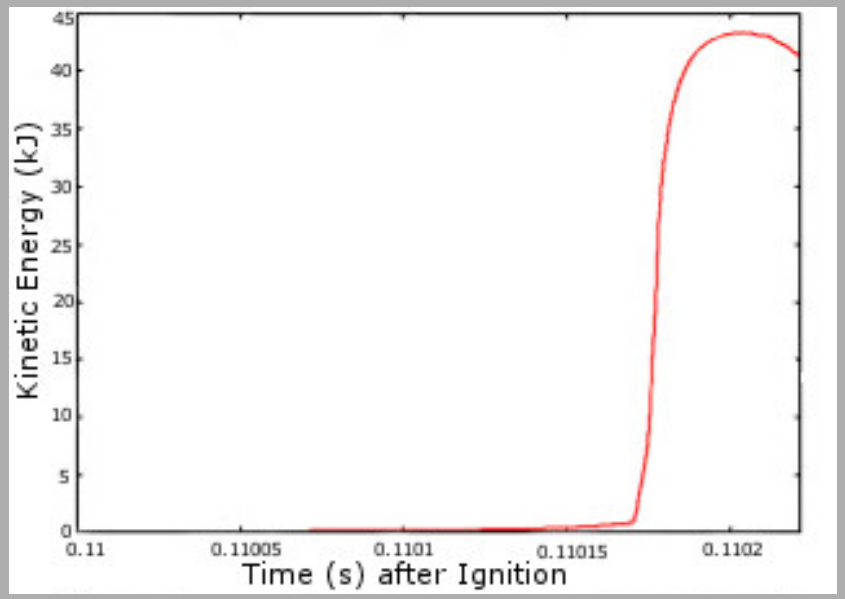
Simulation Set Up



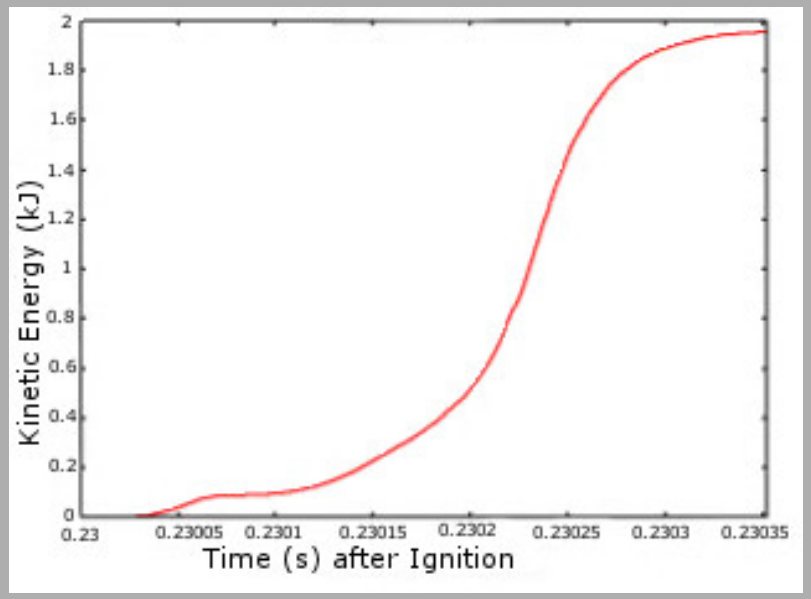
Violence of Reaction



Violence of Reaction

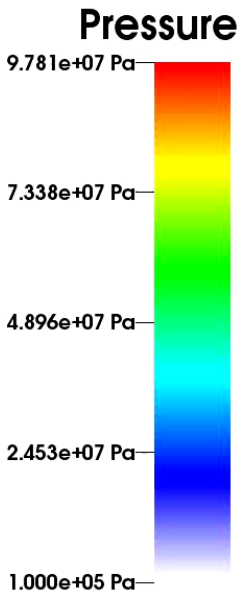


Detonation

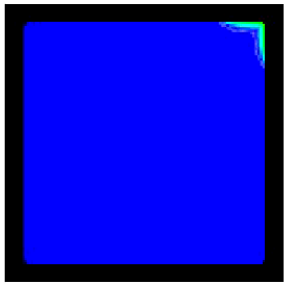


Case Burst

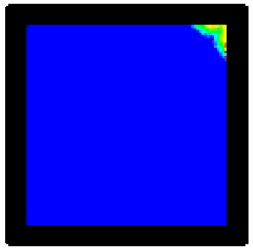
Violence of Reaction

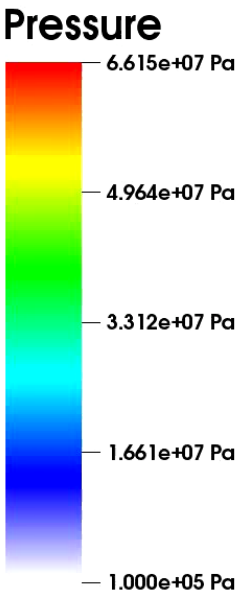


Case Burst

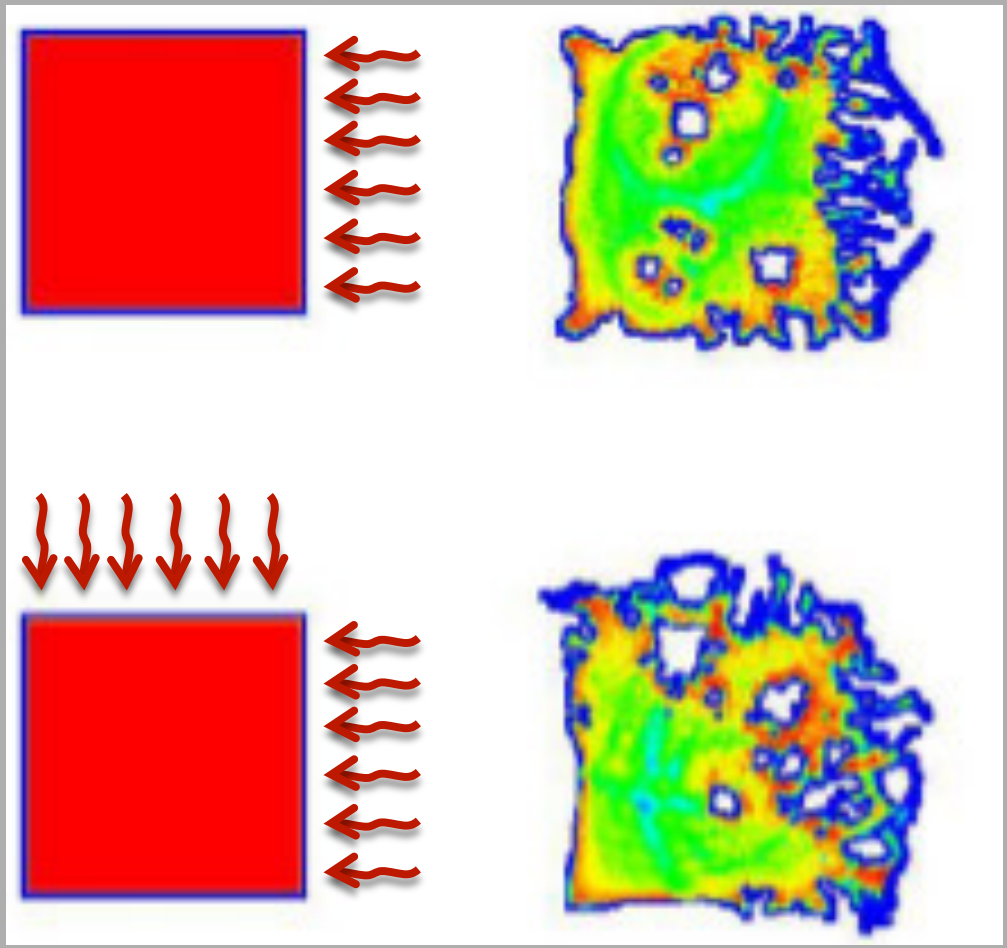


Detonation

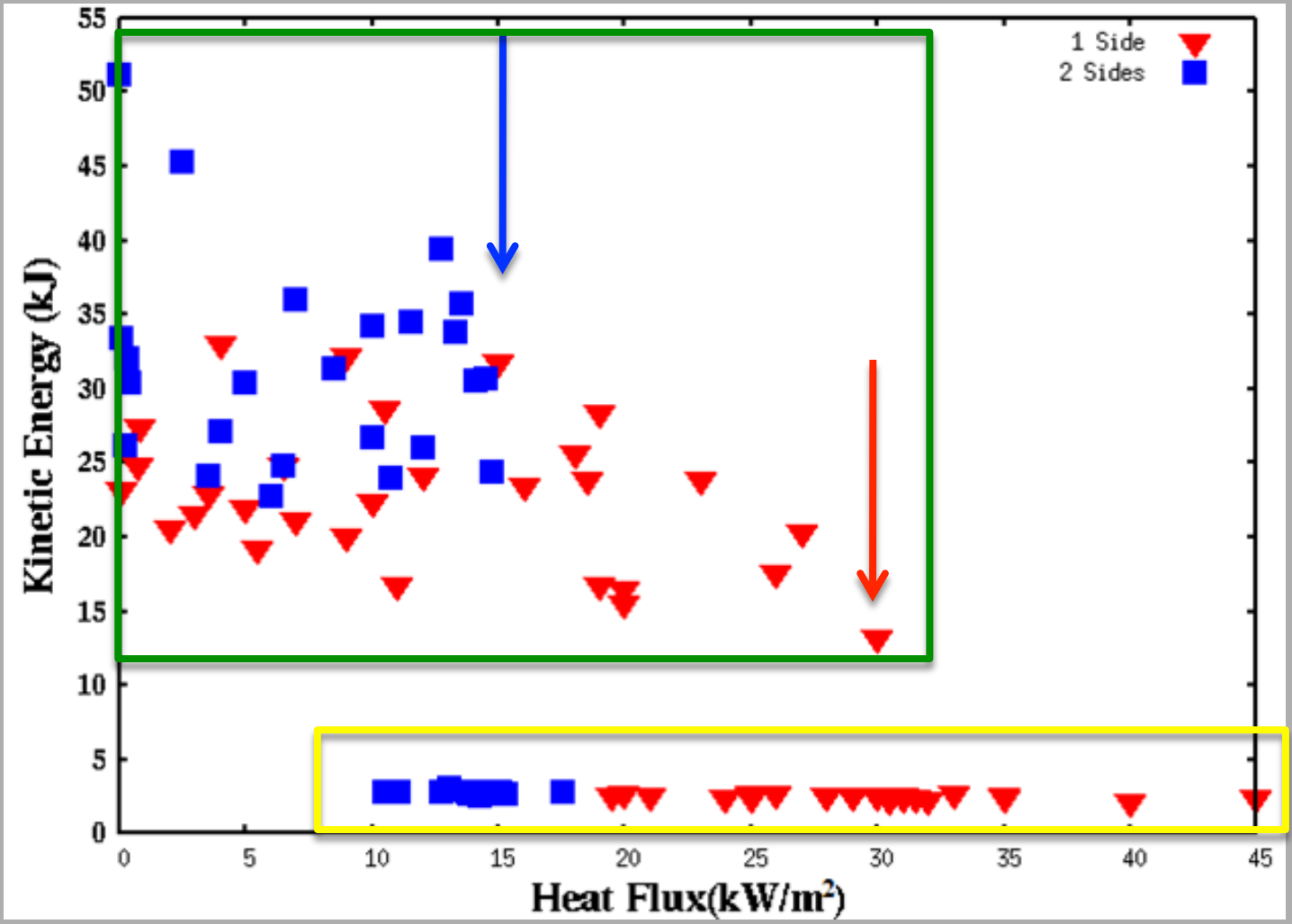




Heating Geometries



Heat Flux and Heating Geometry Effect

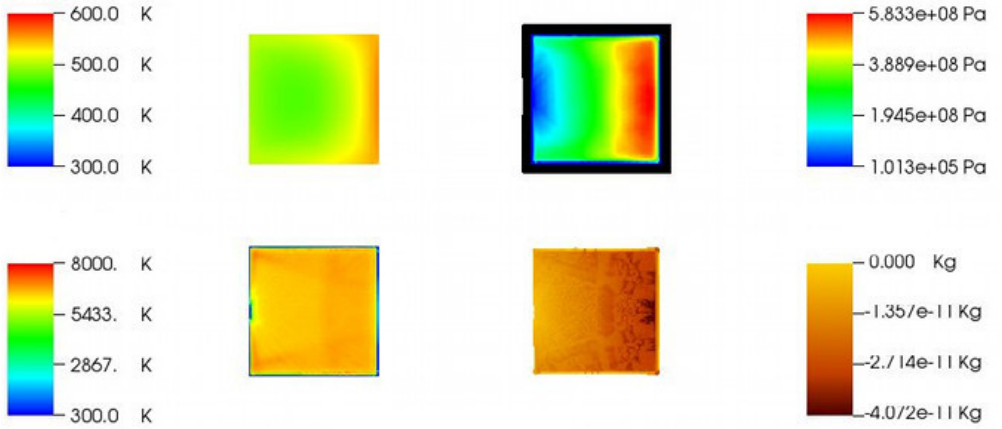


Deflagration to Detonation Transition

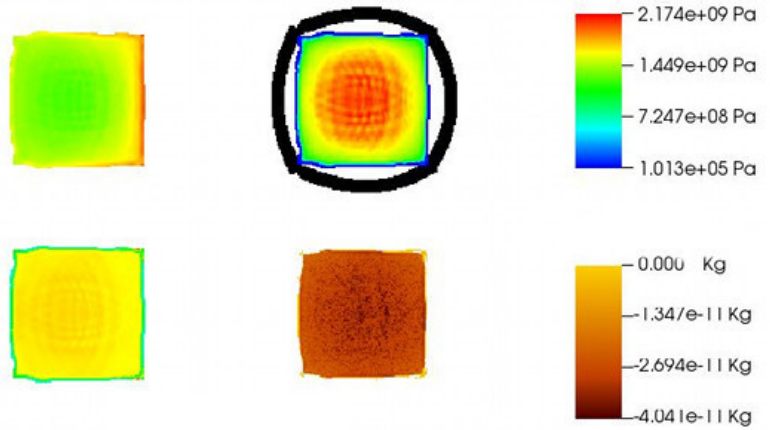
- Under adiabatic conditions deflagration of PBX9501 will reach ~2 GPa
- Detonation requires 5.3 GPa

Where did the other 3.3 GPa come from?

Pressure Induced Detonation



20 μ sec



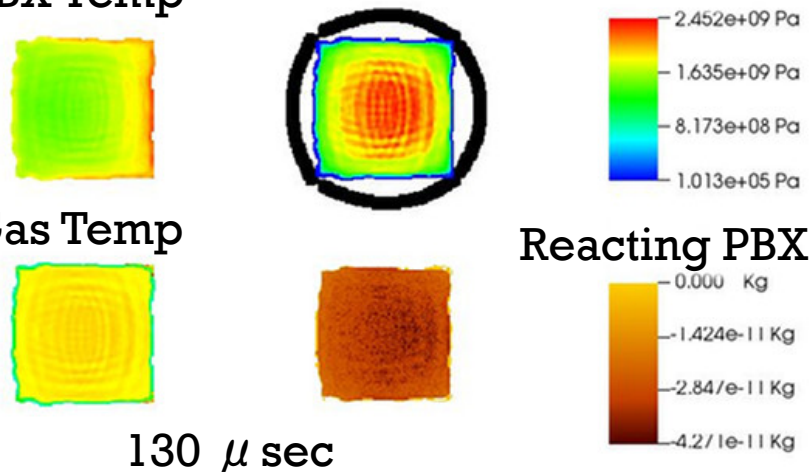
120 μ sec

PBX Temp

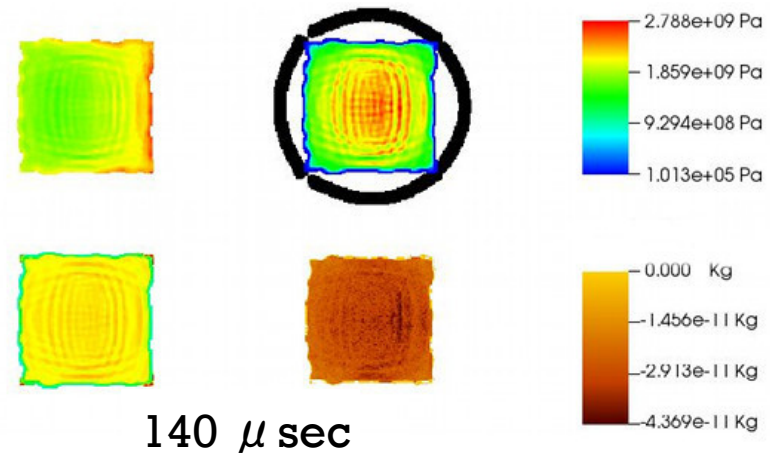
Gas Temp

Pressure

Reacting PBX

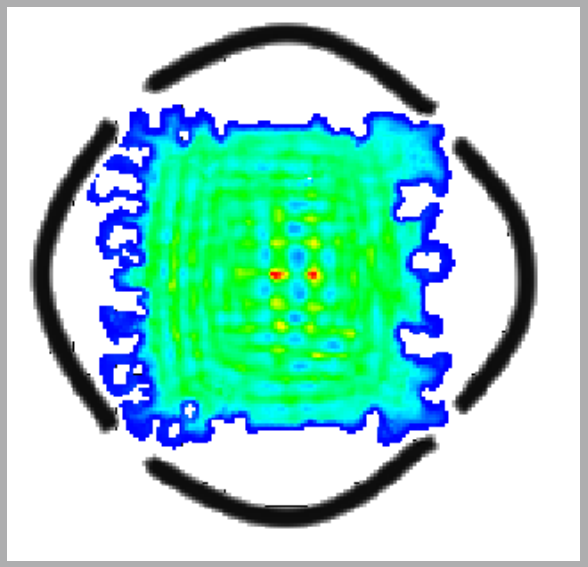


130 μ sec

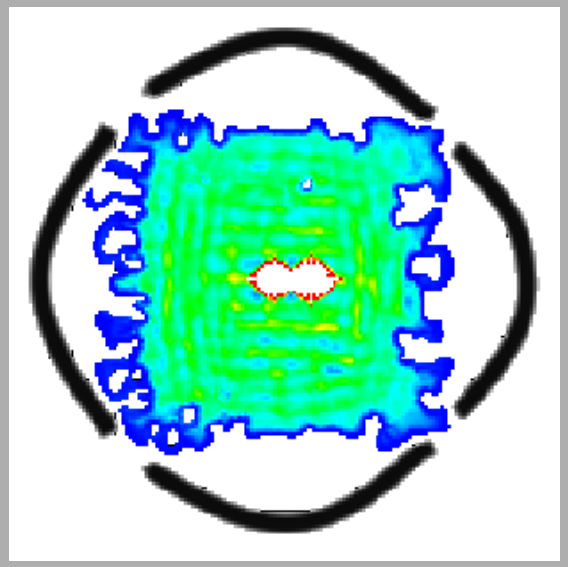


140 μ sec

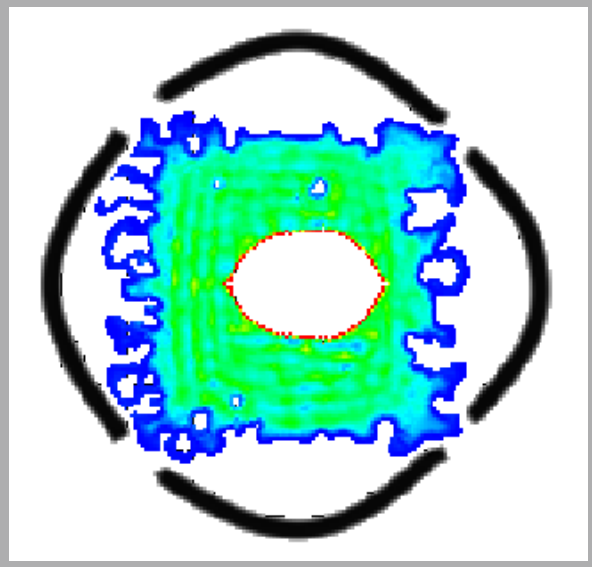
Pressure Induced Detonation



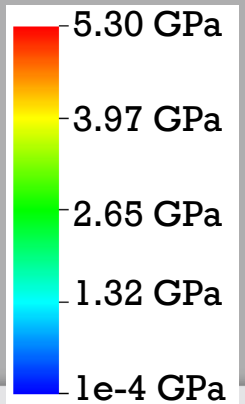
170 μ sec

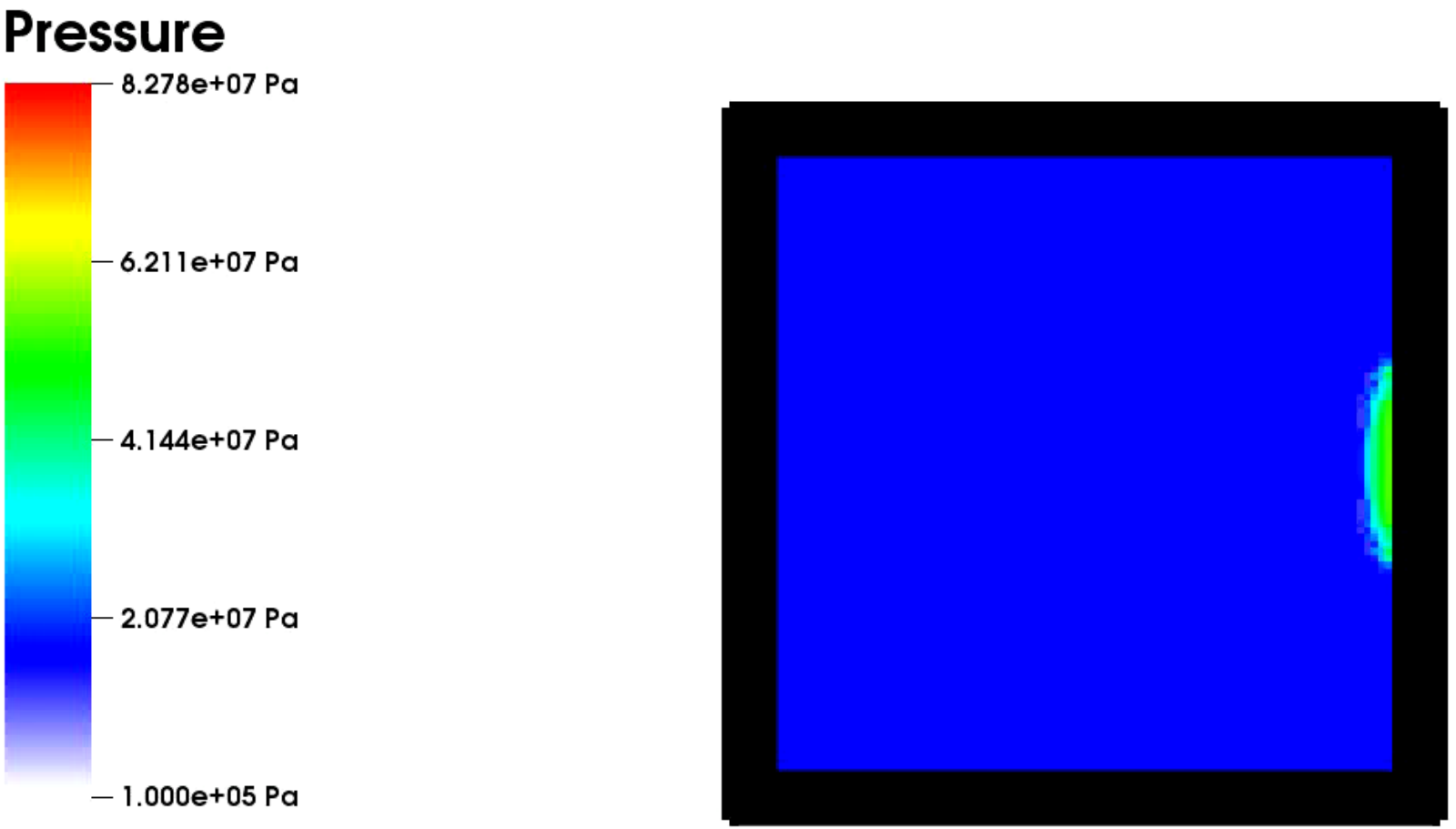


171 μ sec

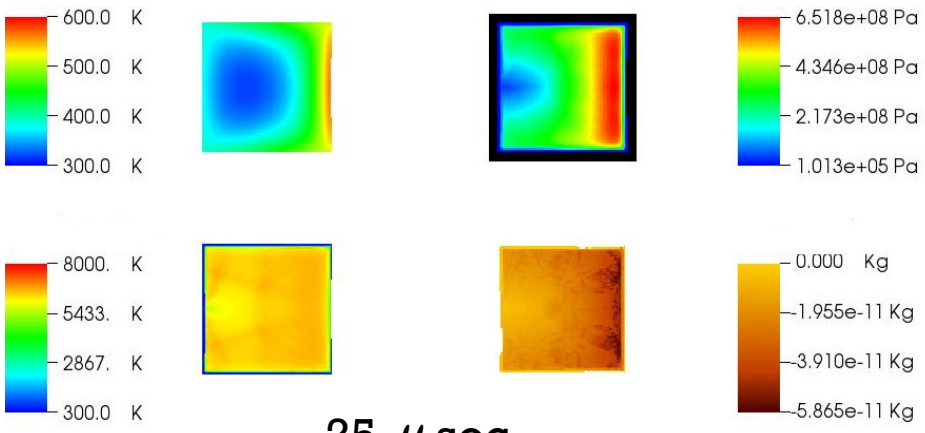


172 μ sec

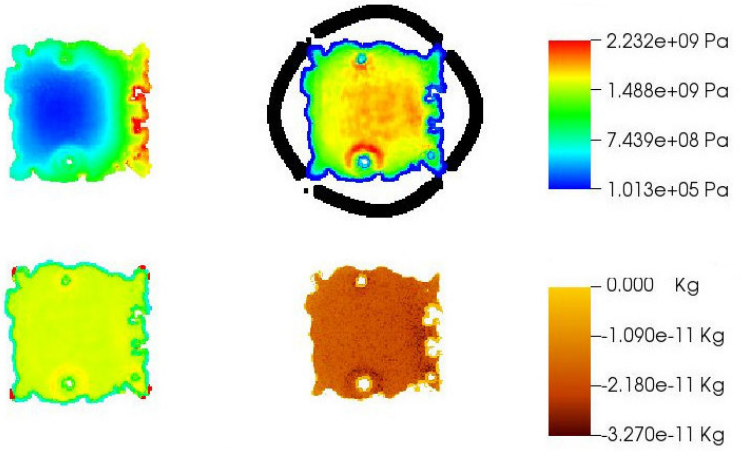



Pressure
8.278e+07 Pa
6.211e+07 Pa
4.144e+07 Pa
2.077e+07 Pa
1.000e+05 Pa

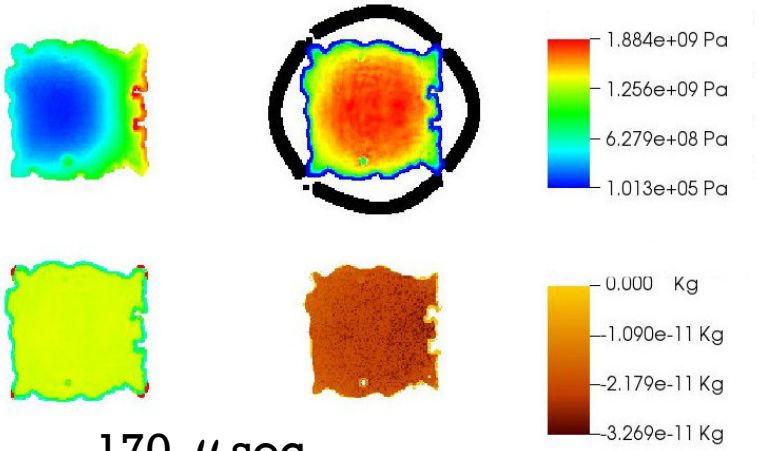
Ignition Site Detonation



25 μ sec



175 μ sec



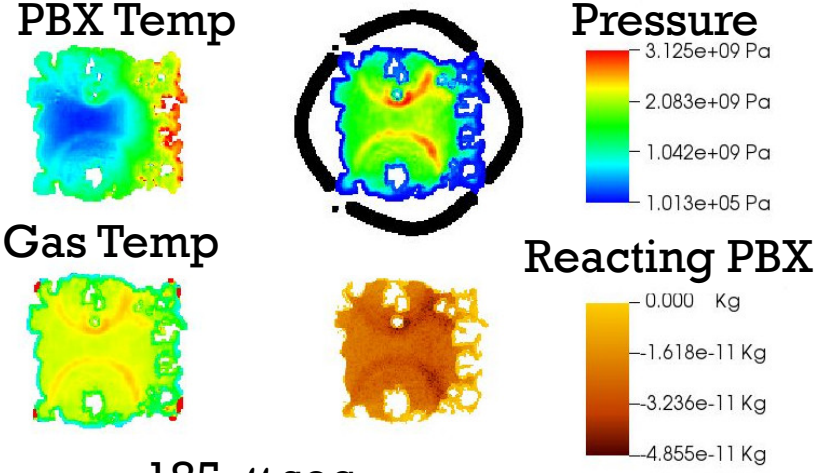
170 μ sec

PBX Temp

Pressure

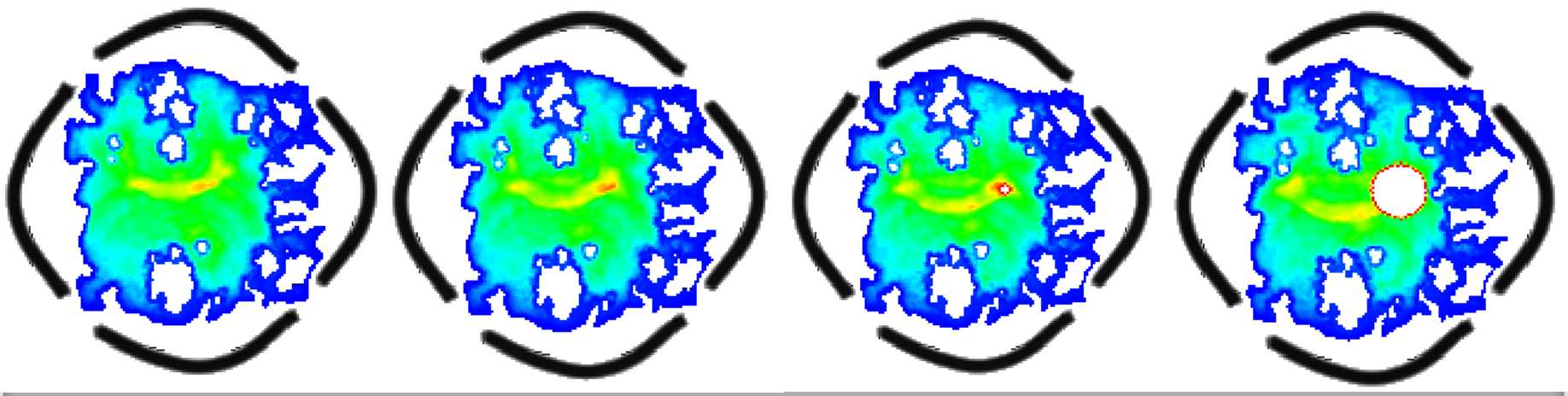
Gas Temp

Reacting PBX



185 μ sec

Ignition Site Detonation

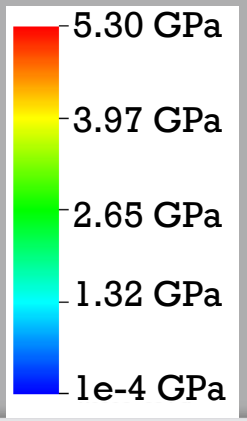


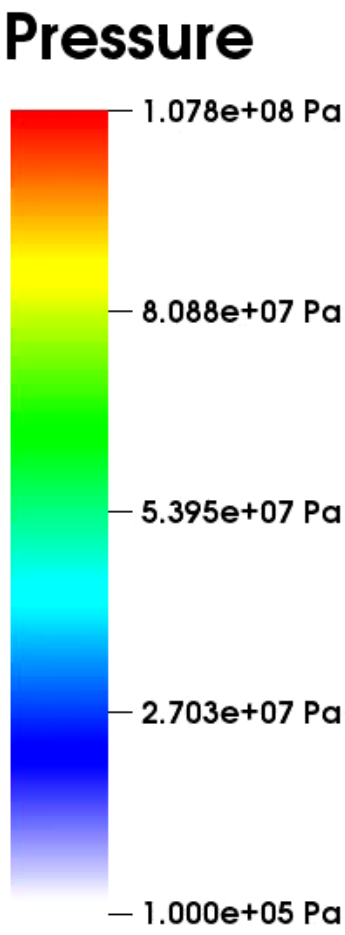
192 μ sec

193 μ sec

194 μ sec

195 μ sec




Pressure
1.078e+08 Pa
8.088e+07 Pa
5.395e+07 Pa
2.703e+07 Pa
1.000e+05 Pa

Conclusions

- Detonation occurs from two colliding pressure waves
- Lower heat flux is more likely to detonate
- One sided heating is more likely to detonate

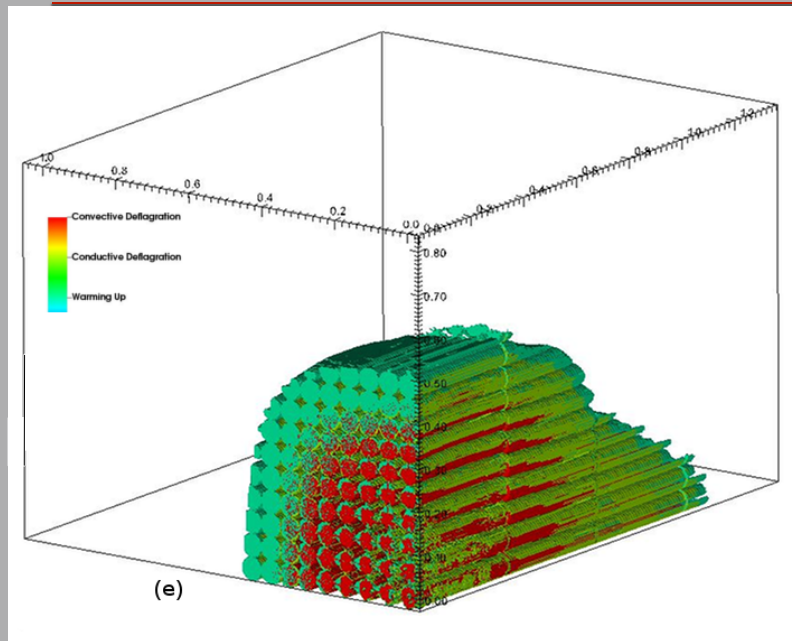
Future Work

- Pressure amplification as a function of mass burned
- Look at large scale simulations to determine a critical density for transporting explosives

Spanish Fork Canyon, Utah

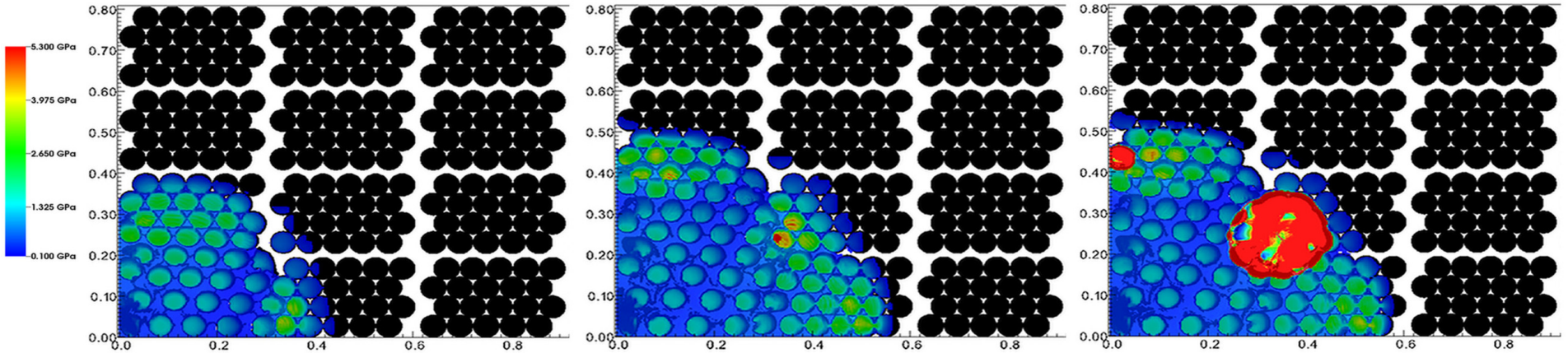
"Truck Explosion Leaves Huge Crater On Highway." *DREAMS OF THE GREAT EARTH CHANGES*. Web. 25 Feb. 2012. <http://www.greatdreams.com/homeland-security.htm>.

Large Scale Simulations



80,000 Processors on Titan
1m x 1m x 1m Domain

6,000 Processors on Stampede
1.2m x 0.8m x 0.2m Domain



Acknowledgements

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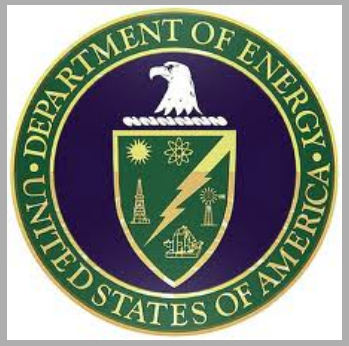
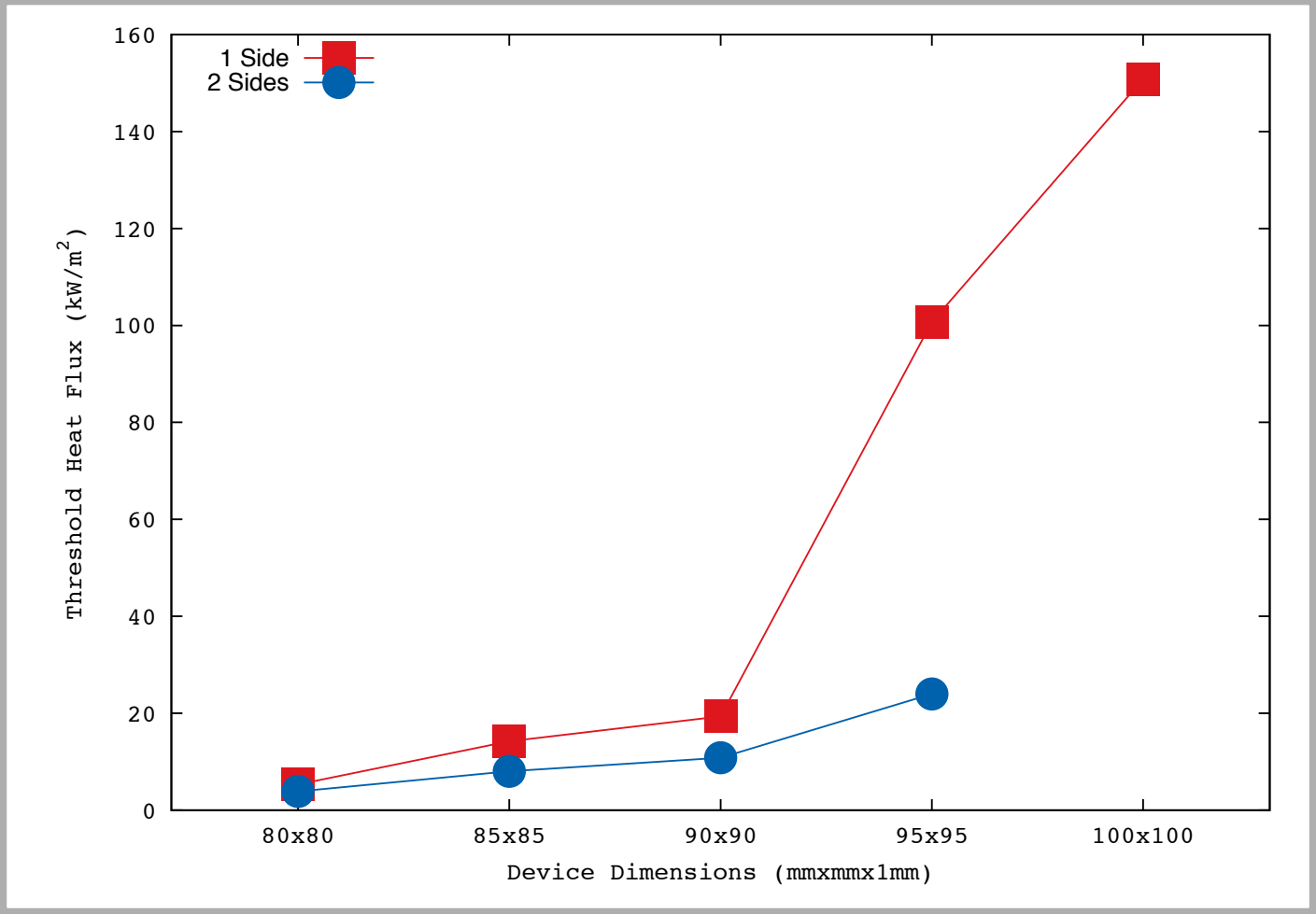
XSEDE

Extreme Science and Engineering Discovery Environment



Size Effect


1 Side
2 Sides
Threshold Heat Flux (kW/m^2)
160
140
120
100
80
60
40
20
0
80x80
85x85
90x90
95x95
100x100
Device Dimensions (mmxmmx1mm)

Temperature Dependence