Granular Explosives
and Initiation Sensitivity

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Outline

- Explosives
  - Homogeneous (premixed gas)
    - Thermal explosion theory
  - Heterogeneous (Plastic Bonded Explosive)
    - Temperature fluctuations
    - Temperature sensitive reaction rate

- Shock initiation
  - Experimental phenomena

- Homogenized reactive models
  - Fluctuations not resolved
  - Phenomenological burn models
    - Account for sub-grid physics
    - Assumptions limit domain of applicability

- Granular explosives
  - Model for damaged explosives
  - More sensitive
    - Exacerbates effect of hot spots (Bowden-Yoffe)

▶ Meso-Mechanics Simulations
  - Compaction Waves in Granular bed
  - Subgrain fluctuations
  - Temperature distribution

▶ Improved Sub-grid Burn Models
  - Physics issues

Shock-to-Detonation Transition

Homogeneous explosive
(Campbell, Davis & Travis)

1. Thermal runaway at piston leads to detonation.
2. Detonation wave overtakes lead shock.
3. Detonation speed slows until CJ wave is formed.

Heterogeneous explosive
(Campbell, Davis, Ramsay & Travis)

1. The lead wave is a reactive shock.
2. Abrupt transition to detonation ahead of piston.
3. No overshoot in detonation speed
   Explosive next to piston only partially burned.

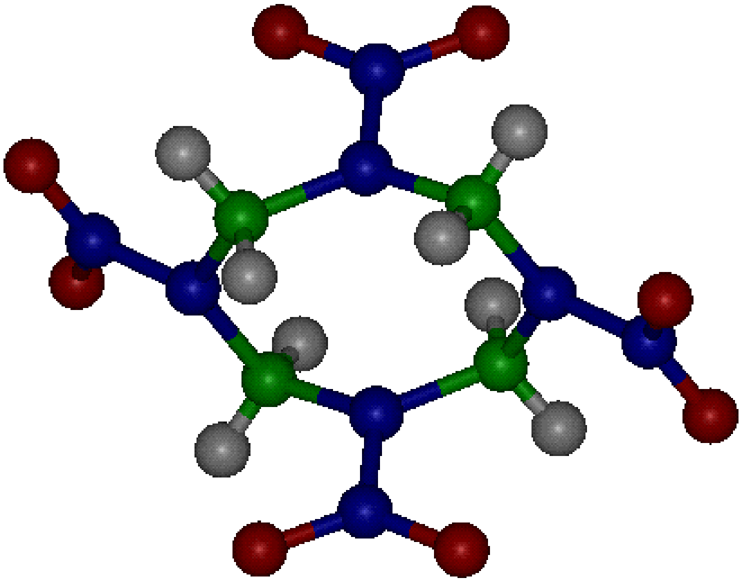
Qualitatively different behavior

Wedge experiments

1. Measure shock trajectory

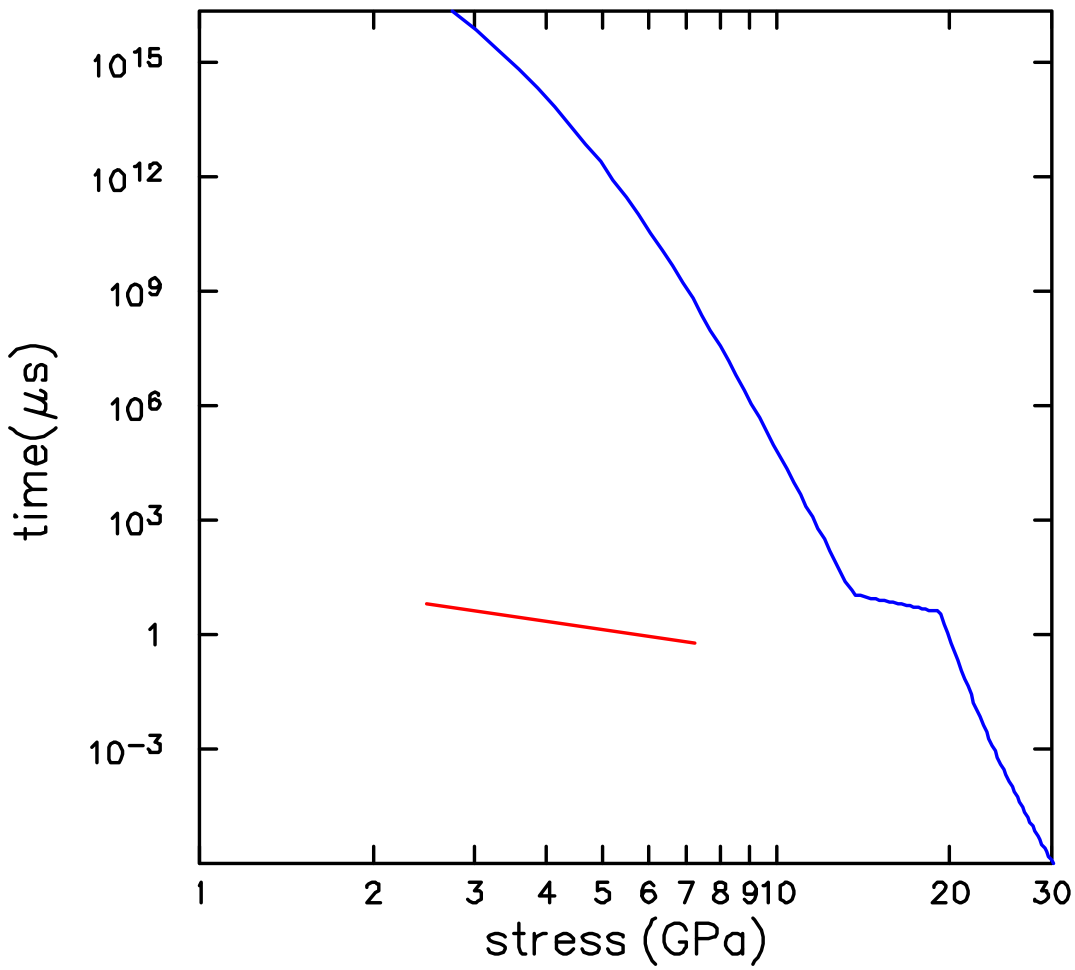
2. Pop-plot
   Distance of run vs. shock pressure
   Linear on log-log plot over range of experiments

Examples for HMX
(cyclo-tetramethylene-tetranitramine, $C_4H_8N_8O_8$)



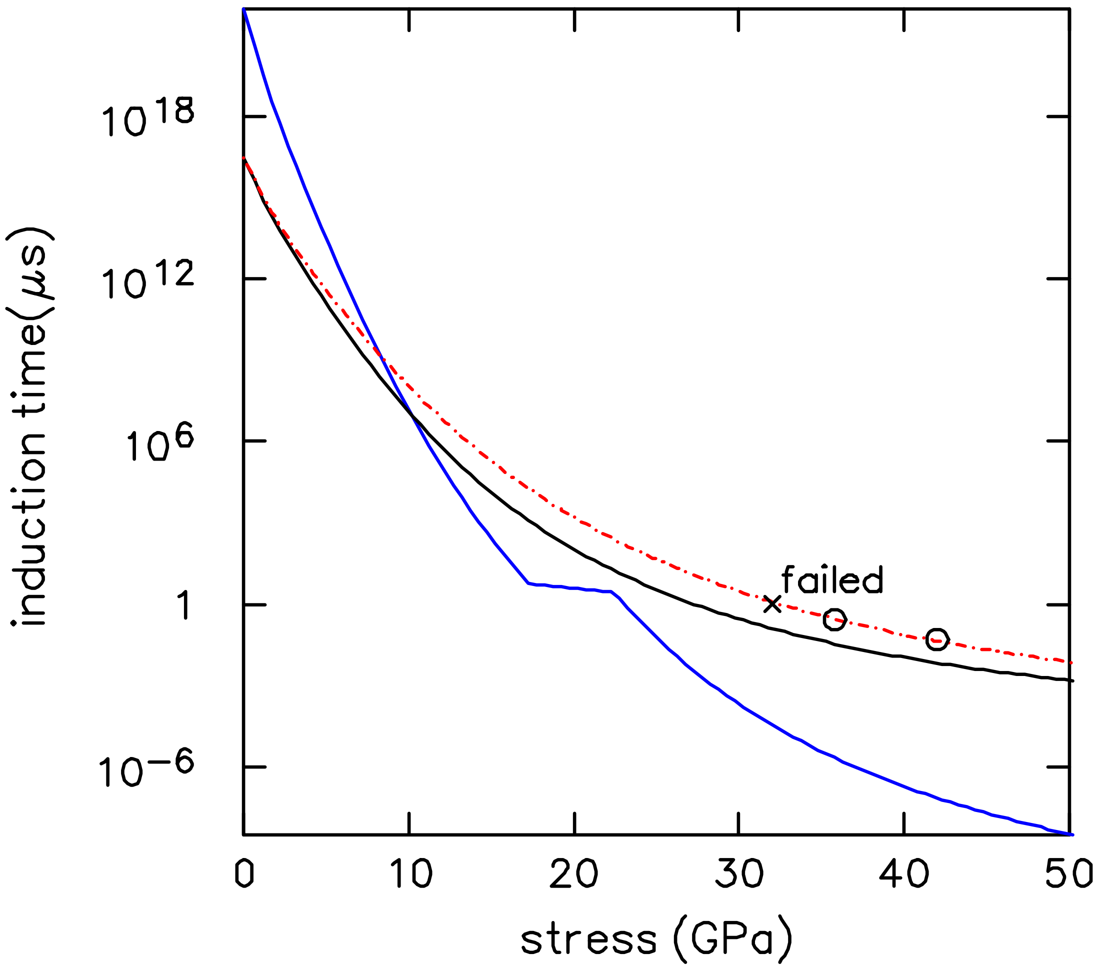
carbon in green, nitrogen in blue,
oxygen in red and hydrogen in grey

PBX-9501 Pop-plot and HMX induction time



Hot spots dominate ignition of PBX

Single crystal HMX initiation



Blue line: liquid Arrhenius reaction rate

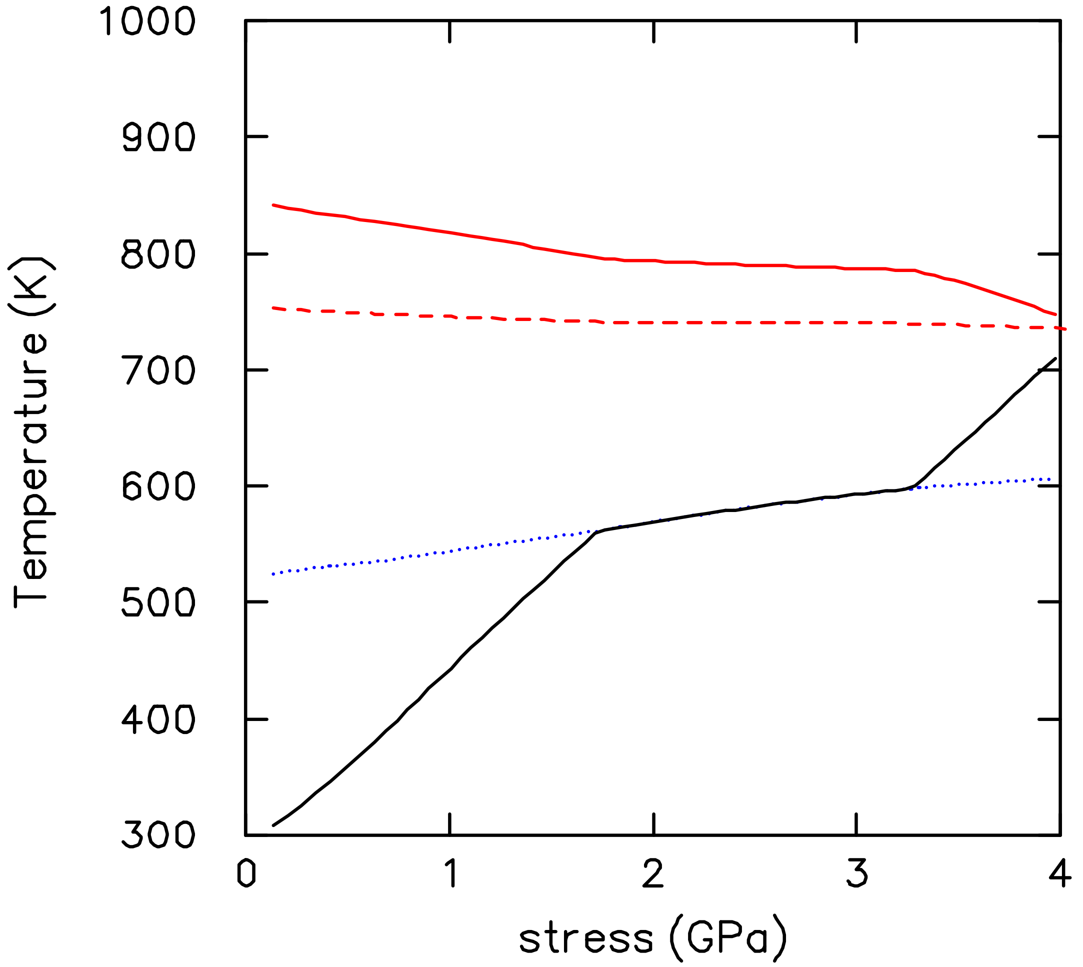
Red and black lines: Solid Arrhenius reaction rate sensitivity to specific heat

Symbols are experiments by Craig
32 GPa failed detonation after 6.6 mm run
CJ pressure is 36 GPa

Single crystal is very insensitive

Hot-Spot temperature for 1 μs induction time

Granular HMX, 35% porosity



Solid red line 1 μm hot spot
Dashed line 10 μm hot spot

Black line is shock temperature
Dotted blue line is liquid-solid coexistence curve

Hot spots above melting

$$\frac{\text{Latent heat}}{C_v} \approx 200\,\text{K}$$

Hot-Spot evolution

1. Temperature sensitive reaction rate
   Constant volume burn
   $P_{cv} = 15\,\mathrm{GPa}$ and $T_{cv} = 1800\,\mathrm{K}$

2. Shock in solid
   $P \sim 8\,\mathrm{GPa}$, $T \sim 490\,\mathrm{K}$ and $u = 0.8\,\mathrm{mm}/\mu\mathrm{s}$
   Negligible reaction

3. Expansion of reaction products in hot spot

$$\frac{T}{T_{cv}} = \left(\frac{\rho_{cv}}{\rho}\right)^{\Gamma} = (1 + ut/r_0)^{-3\Gamma}$$

   In time of $t = r_0/u$ temperature drops by factor 1/8
   either quenches reaction
   or leads to deflagration wave on hot spot surface.

Ref. Simulations by Mader

- Fast energy release
- Small hot spots quenched by rapid expansion
- Large hot spots grow by deflagration
- Ignition is collective phenomena of many hot spots

Phenomenological Burn models

- Forest Fire model (Chuck Forest)
  Single curve build up principle
  Reactive shock trajectory independent of P_0
  Rate(P) from Pop-plot + reactive Hugoniot
  analog of Chisnell-Whitham rule for shock in duct
  relates change in shock speed to change in area

- Ignition & Growth model (Lee & Tarver)

$$\text{Rate}(V,P,\lambda) = \underbrace{I \cdot (1-\lambda)^x (V_0/V - 1)^r}_{Ignition} + \underbrace{G \cdot (1-\lambda)^x \lambda^y P^z}_{Growth}$$

- JTF model (Johnson-Tang-Forest)
  Additional internal degrees of freedom
  Hot-spot mass fraction f and temperature T_s
  shock pressure P_s (based on artificial dissipation)

$$\frac{df}{dt} = Rate(T_s)$$

$$\frac{dT_s}{dt} = \frac{\Gamma T_s}{k}\frac{dP}{dt} - C_p^{-1}\frac{dq}{dt} \qquad \text{and} \qquad T_s(P_s) \text{ initially}$$

$$\frac{d\lambda}{dt} = \underbrace{\mu\frac{df}{dt}}_{Ignition} + \underbrace{\Big[1-\lambda-\mu(1-f)\Big]\left(\frac{f-f_0}{1-f_0}\right)_+ G(P,P_s)}_{Growth}$$

Limitations of Current Burn Models

Tacit assumption on hot-spot distribution
Same as experiment used to calibrate model
  One-dimensional for simplicity

Problems sensitive to hot-spot distribution

- Shock desensitization
  Few per cent voids in plastic bonded explosive
  Weak shock compress out voids
    Reduces heterogeneities
    Can extinguish propagating detonation wave
    Experiments by Campbell & Travis on PBX-9404

- Corner turning
  Rarefactions from side
    quenches growth of hot spots
    partially burnt regions or dead zones

- Failure diameter
  Also, curvature effect
  Hot spots affect propagation of detonation wave

- Structure of heterogeneous
  Grain size effects
    Specific surface area effects growth of hot spots
  Pressed vs. cast TNT
    Surface area and connectivity of pores
  Effect of damage and aging

Granular Explosive

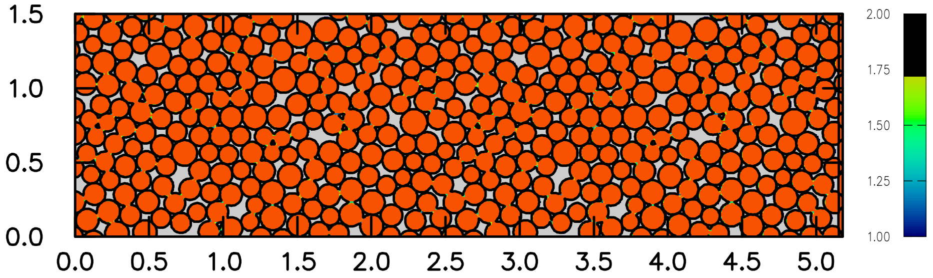
- Model for damaged explosives
  Degree of freedom from porosity

- More sensitive to ignition
  More heterogeneities than solid
    Exacerbates effect of hot spots
  Deflagration-to-Detonation Transition experiments
    Longer time scale than for shock initiation
    Multiple waves more important

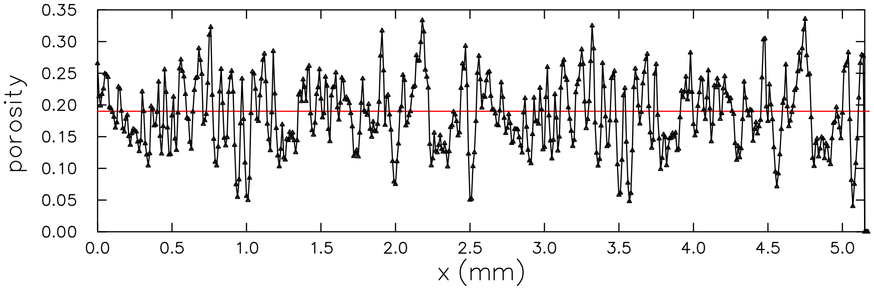
- Two-Phase models
  Coarse grained thermodynamic variables
    Homogenized theory with volume fraction
    Hot spots not resolved
  Require phenomenological burn model
    Reaction rate depends on fluctuations

Piston driven compaction waves

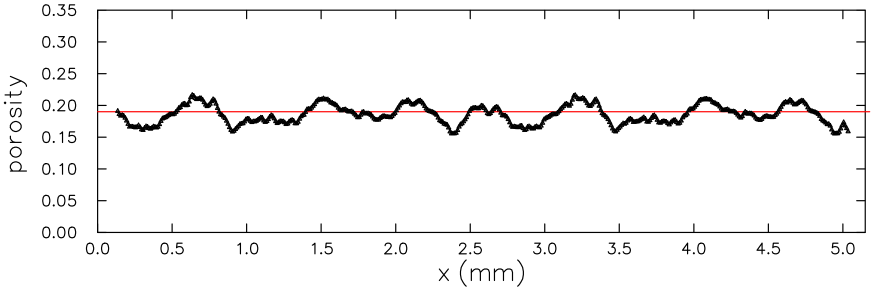
Density (pores are void and shown in gray)



Porosity profile



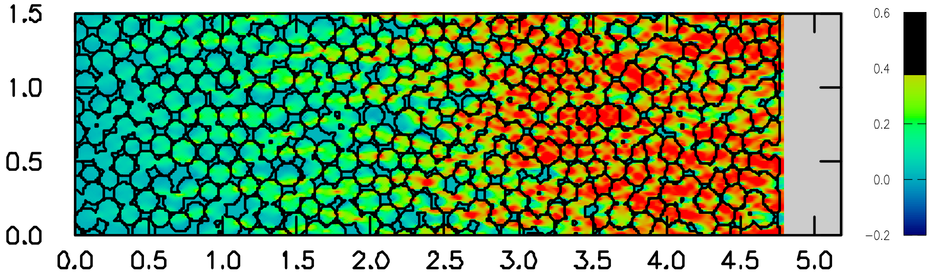
Porosity, smoothed over 2 grain diameters



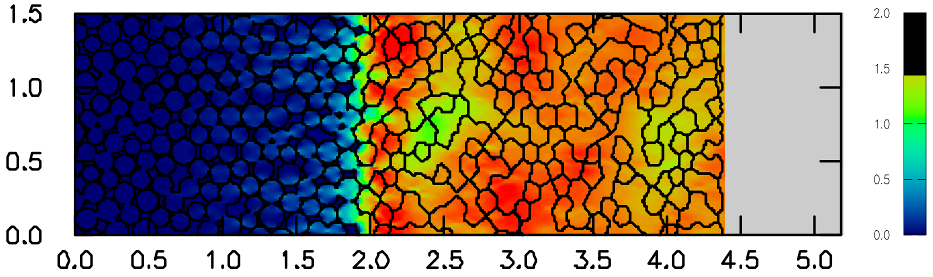
Tightly packed bed HMX grains, 19% porosity

Stress field

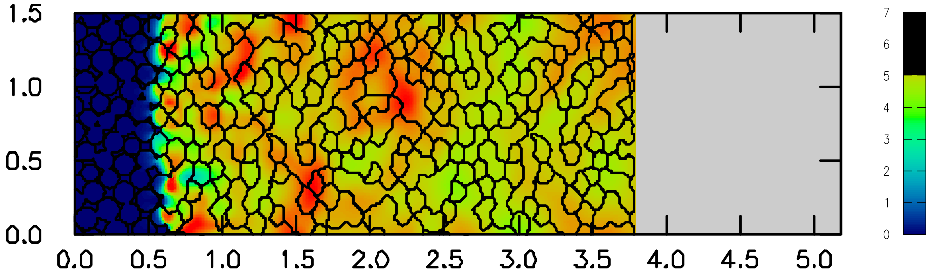
200 m/s piston at time = 2.0 μs



500 m/s piston at time = 1.6 μs



1000 m/s piston at time = 1.4 μs



Stress profile

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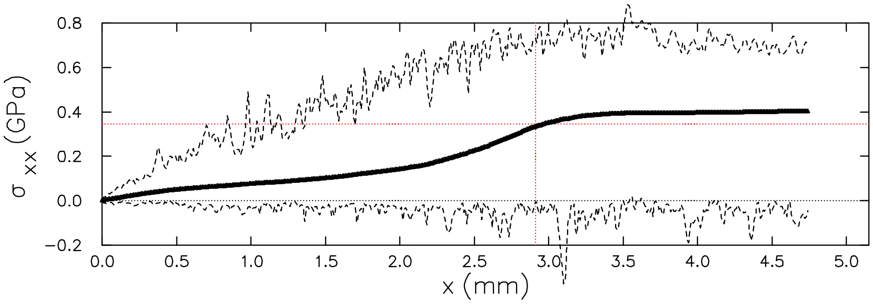

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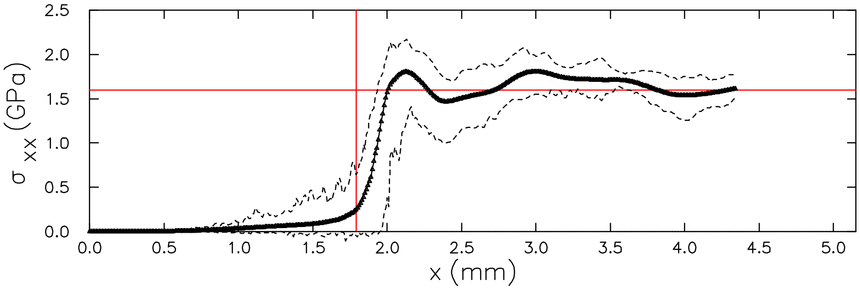

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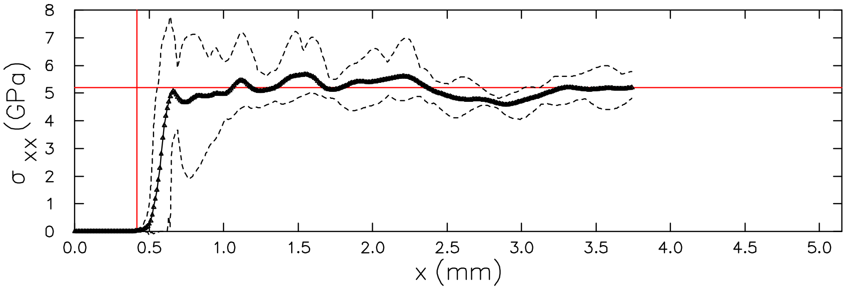

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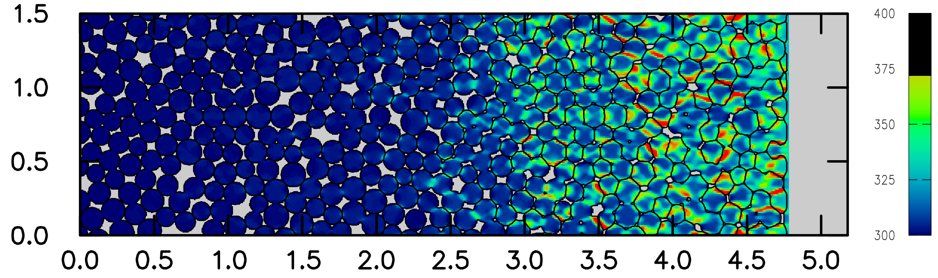
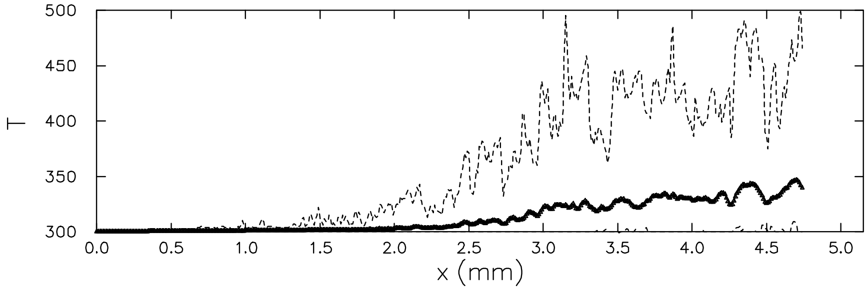
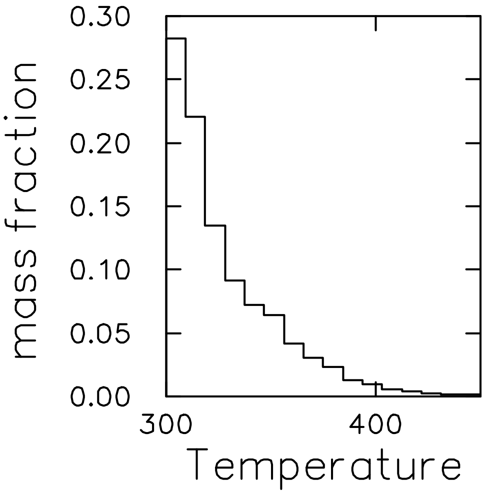
Temperature field



Temperature profile



Temperature distribution behind wave



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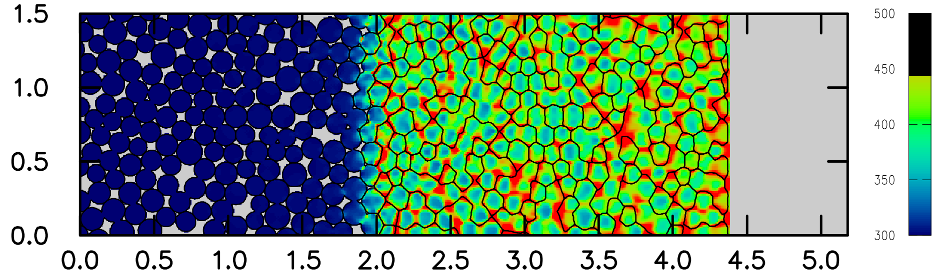
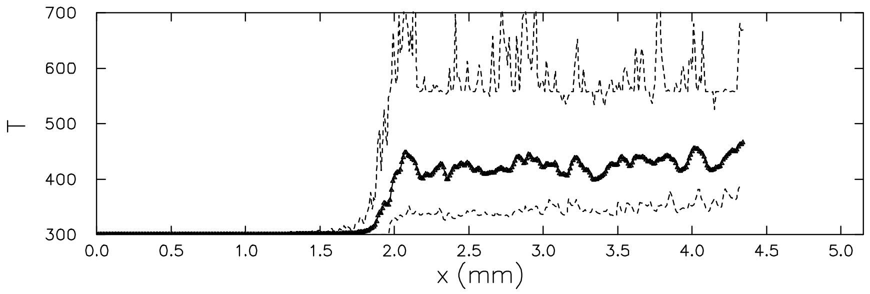


Temperature profile



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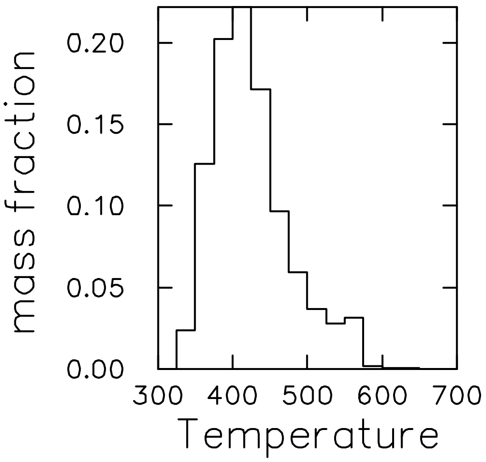
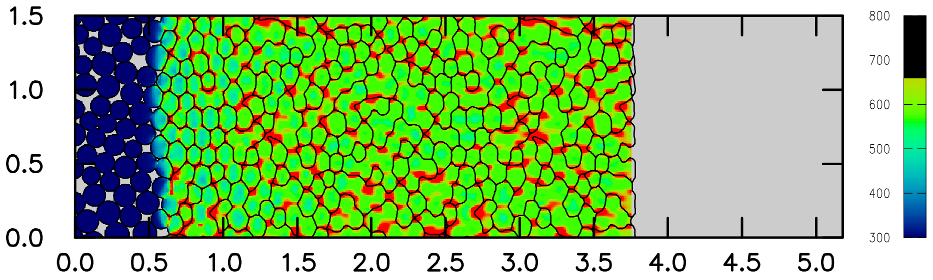


1000 m/s piston at time $= 1.4\,\mu s$

Temperature field



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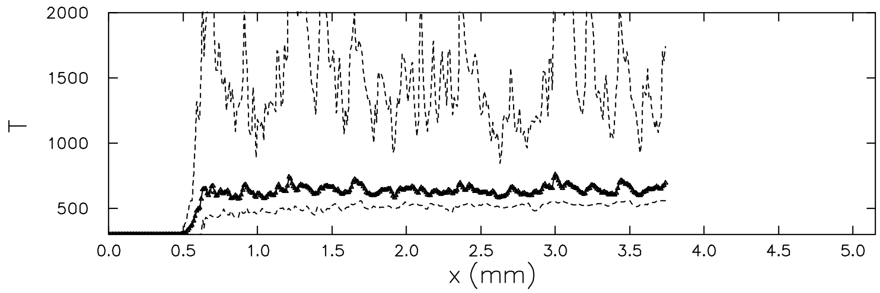

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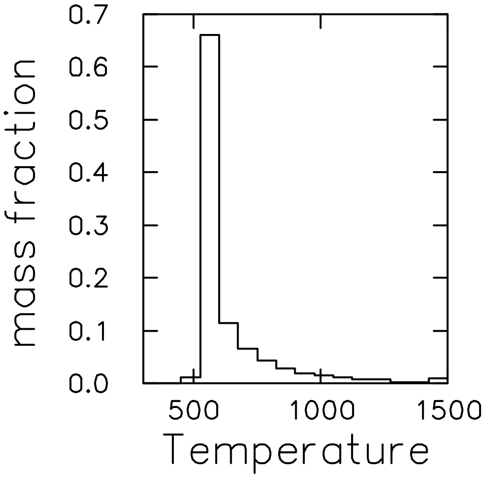

Improved burn models

Cover wider domain of application
▶ Effect of multiple waves

- Need to incorporate underlying physics
  Ignition and growth of hot spots
  ▶ Insight from meso-scale simulations
    Experimental diagnostics do not have resolution

- Ignition stage
  Hot spot distribution
    Nature of heterogeneities
    ▶ Internal degrees of freedom
      e.g. porosity
    Stimuli, strength of wave
    Dissipative mechanisms
      Plastic work, shear heating, void collapse, etc.
      Effect of melting
  ▶ Governing equations for dynamics

- Growth stage
  Hot spots trigger deflagration
  ▶ Regression rate depends on confinement
  ▶ Spreading over surface of grains
      Gas permeation on grain scale
      Connectivity depends on dimension

- Verify model
  Velocity profiles from gas gun experiments
  Data on average quantities