Modeling Explosive Detonations (A Calculus Application)

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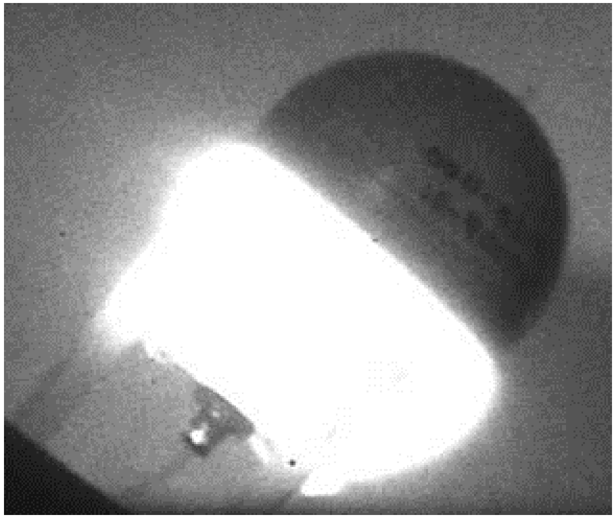

Faster than the Blink of an Eye

- Explosive detonation –
  A glimpse into an event that is much shorter in time than our senses can perceive
- Use diagnostic and analysis techniques to gain insight
- A basic principle from physics forms the foundation of numerical (computer) analysis tools
- Calculus is the mathematical tool under-pinning the physical laws and analysis approaches
  Relate rate of change of variables to response
- Distinguish between "reality", cartoons, and action sequences in movies (*i.e.*, leaps timed to escape from explosion consequences)

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Background

- Explosives are similar to solid rocket propellants and gun powders in that the "fuel" and "oxidizer" are on the same molecule
- When ignited, these materials have self-sustaining reactions
- Generate gas at controlled rates to do work
- Rocket propellants, gun powders are "slower-burning" relative to high explosives
  - Accelerate bullet out of a gun barrel (*e.g.*, 0-1200 mph in 2-3 ms)
  - Accelerate rocket (Shuttle) to escape velocities (~25,000 mph)
  - Nozzle designed to maintain constant pressure inside motor – otherwise can lead to explosion
- Explosives accelerate metals to high velocities in short time periods (microseconds)

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Explosive Applications

- Mining – Rock fracture, rubblization in quarrying, hard-rock ore excavation (drill / blast)
- Oil well stimulation – Shaped charge jets pierce rock like needles to create flow paths after well has been bored
- Geological exploration – Set multiple charges on surface with array of acoustic sensors to map underground geology (oil-bearing strata)
- Stage separation – rocket stages “unzipped” by explosive devices
- Road-building – Cuts
- Demolition – Drop tall buildings into base footprint in a few seconds
- Military – Extensive use in munitions (bombs, shaped charges, mines, torpedoes)

Two Sequences of Exploding Sphere

Explosive detonation of ½ lb sphere of explosive –

High-Speed Video (500 fps)

Framing Camera (1 million fps)

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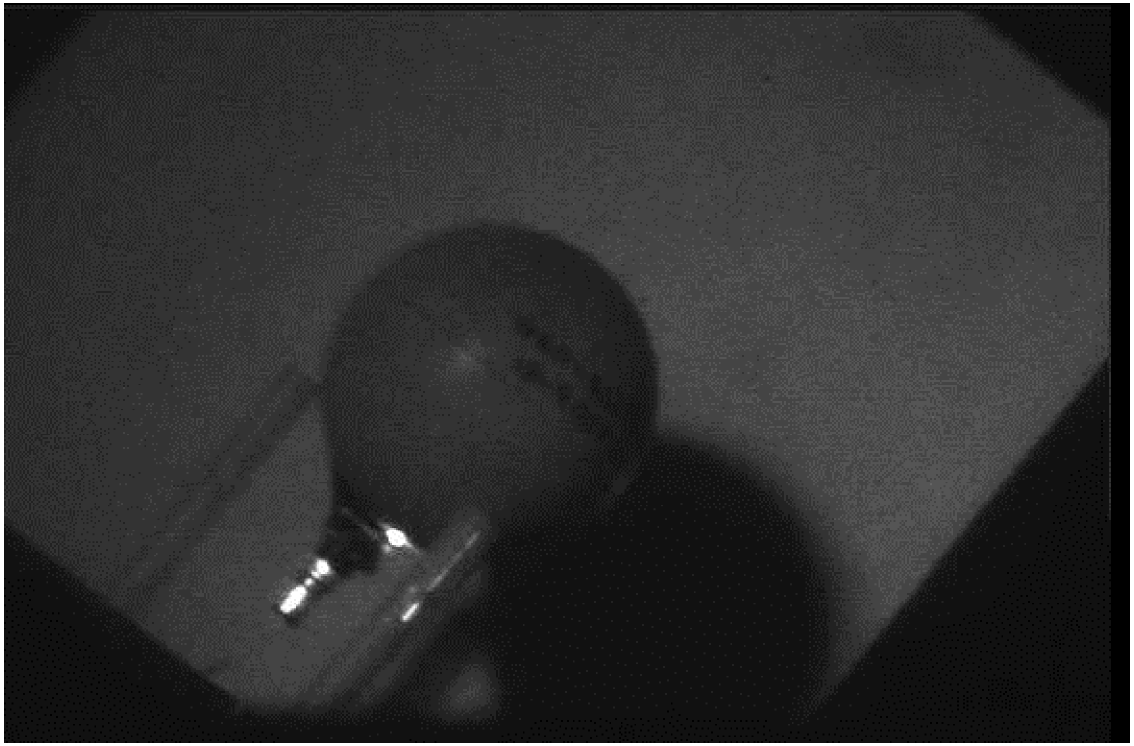
HMX Sphere Test

- Static View

HMX Sphere Test



HMX Sphere Test

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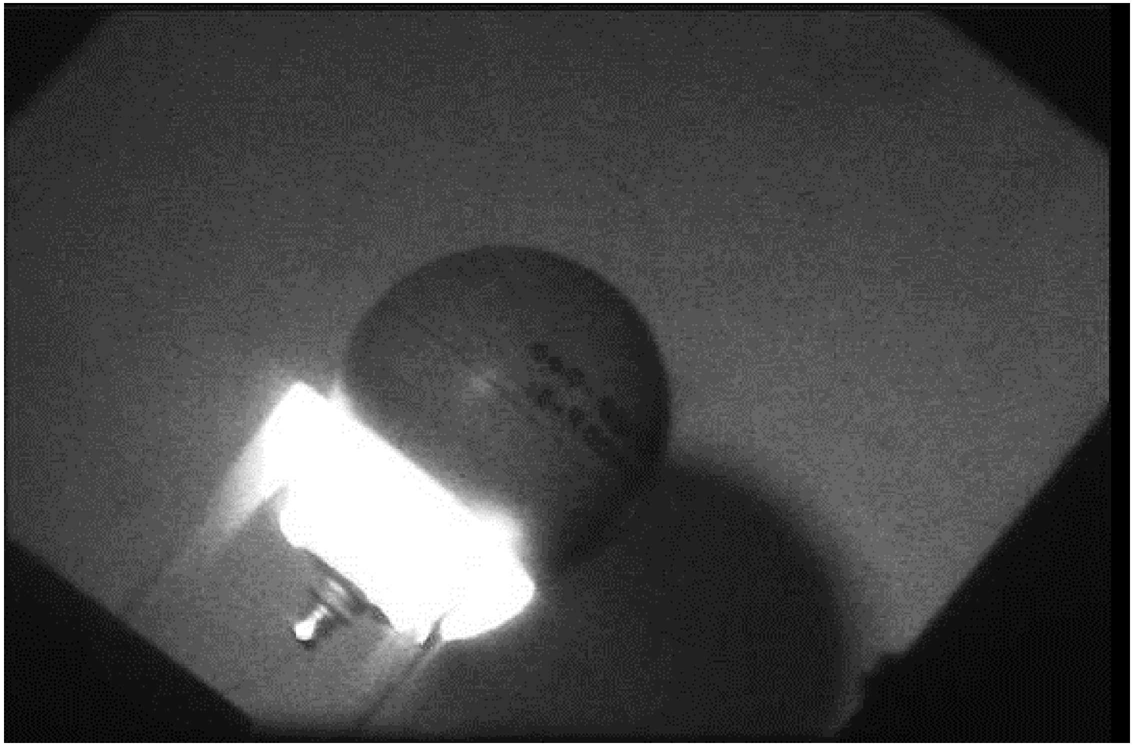
HMX Sphere Test



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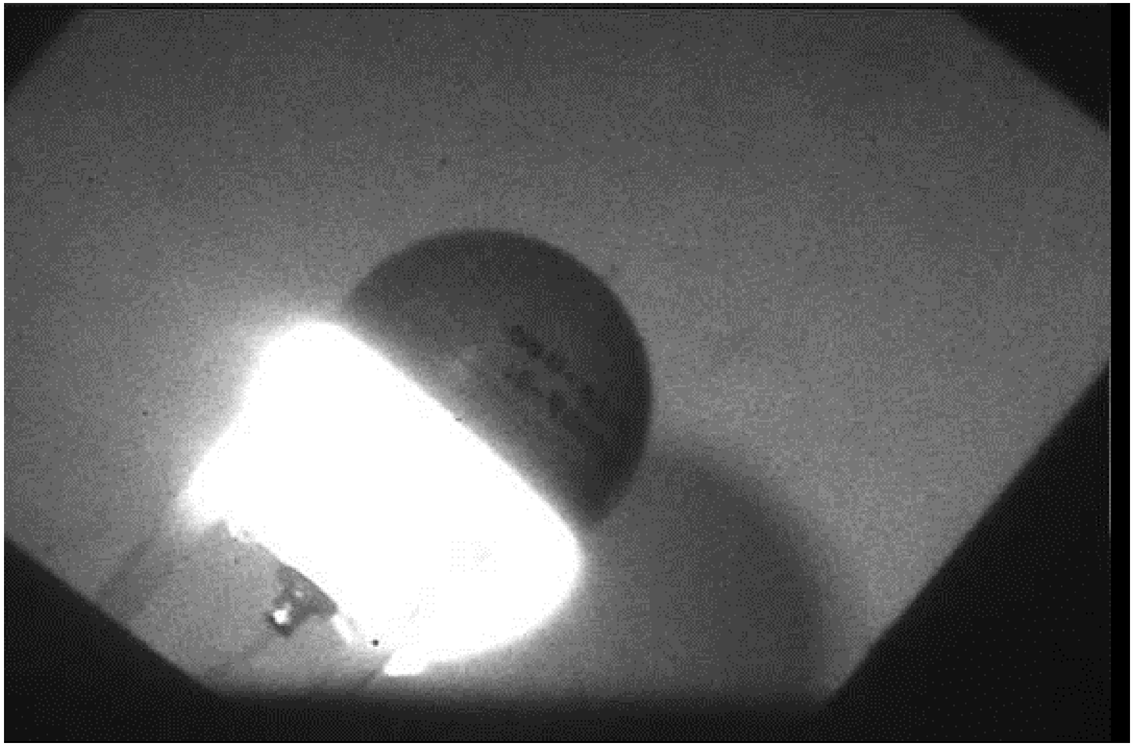

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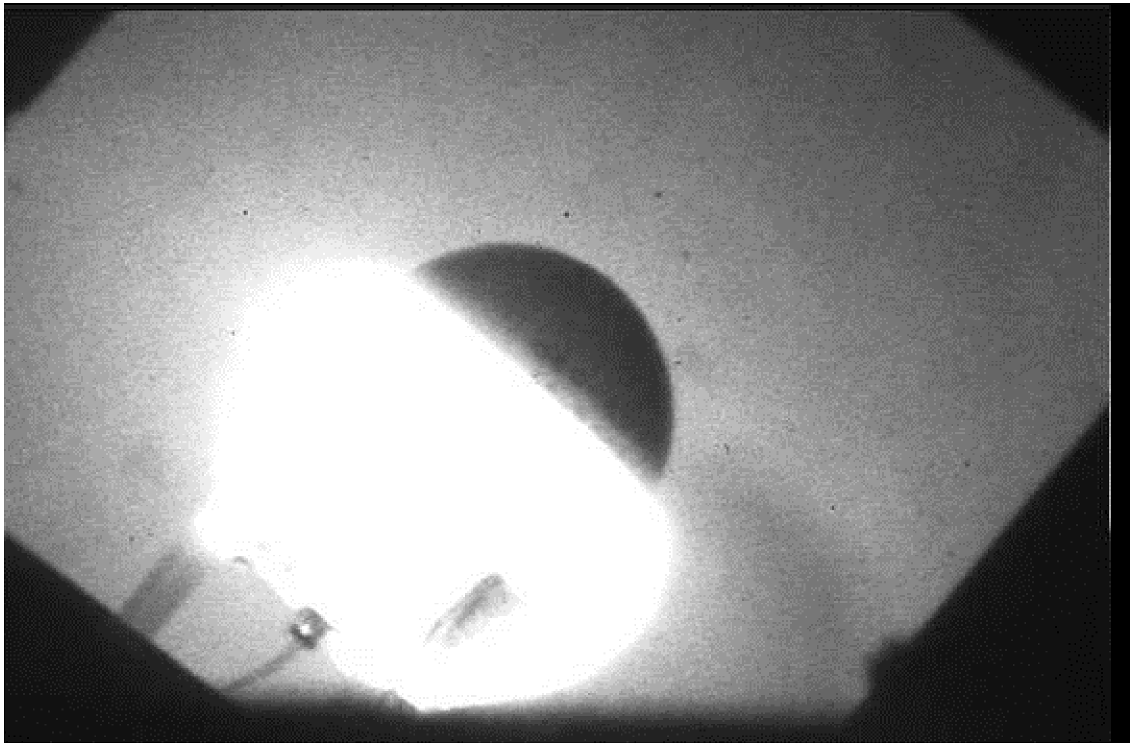

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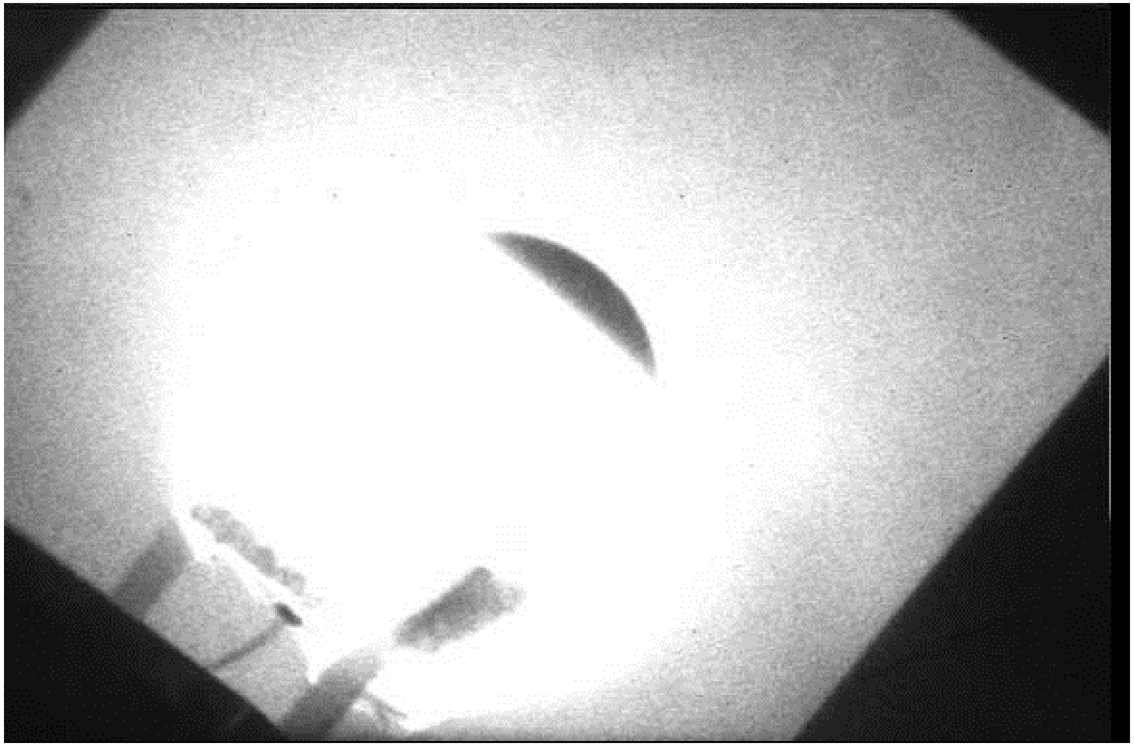

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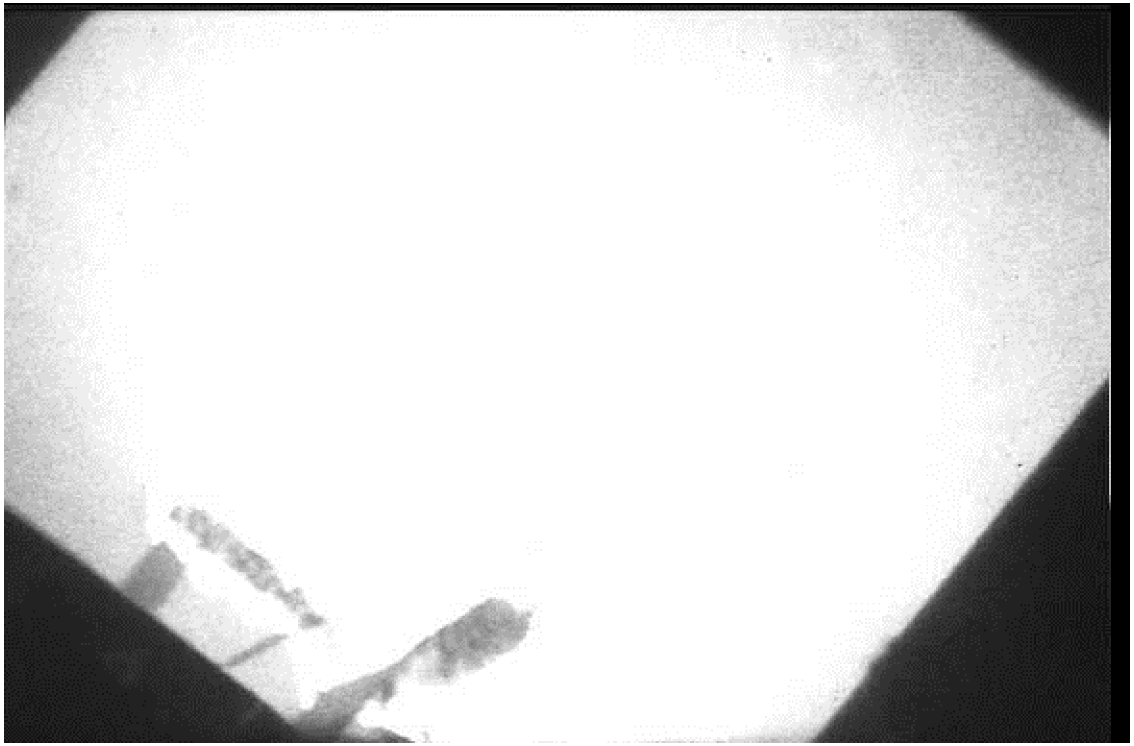

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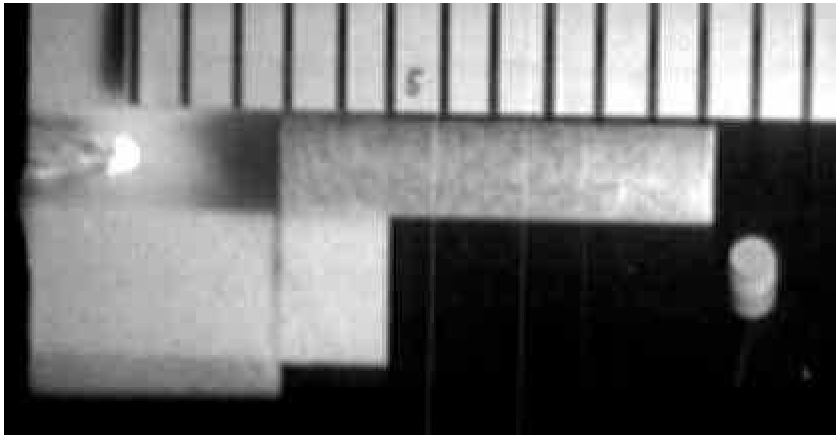
Detonation of TNT Cylinder

- TNT cylinder (bare) initiated by high-speed jet (approaching from left side of image)



- Note the steady velocity of the detonation front in the TNT

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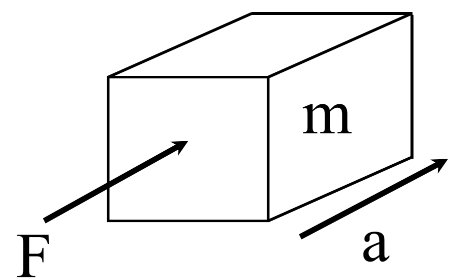
Modeling

- How do we model these events/devices with numerical simulations?
  - Models need to obey physical laws
  - Rate laws typically characterize material behavior (*e.g.*, burn rates)
- Why not just do experiments?
  - Combination of modeling / experiments leads to improved physical understanding, better experiments
  - Modeling reveals details of behavior in regions that cannot be instrumented
- A fundamental law relating local acceleration to the force –
  force = mass x acceleration

$$F = ma = m\frac{dv}{dt}$$

$$v = \frac{ds}{dt}$$



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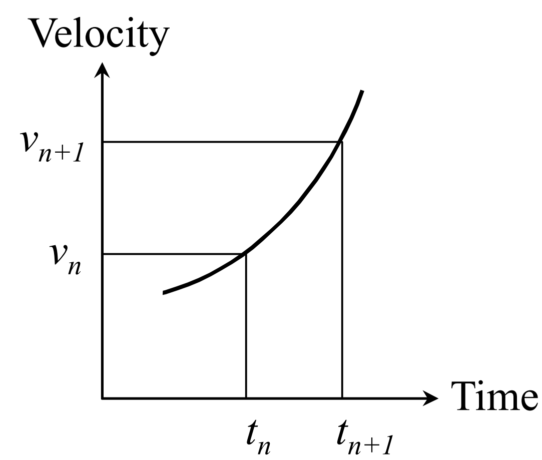
Discretizing the Derivatives

Rewrite the derivative as a difference:

$$F = ma = m\frac{dv}{dt} = m\frac{\Delta v}{\Delta t} = m\frac{v_{n+1} - v_n}{t_{n+1} - t_n}$$



Rearrange to determine new velocity from old velocity:

$$v_{n+1} = v_n + \frac{F}{m}\left(t_{n+1} - t_n\right)$$

Same procedure relating position, *s,* to velocity:

$$v = \frac{ds}{dt} = \frac{\Delta s}{\Delta t} = \frac{s_{n+1} - s_n}{t_{n+1} - t_n}$$

$$s_{n+1} = s_n + v_n\left(t_{n+1} - t_n\right)$$

Solving an Example – Free-Fall in Air

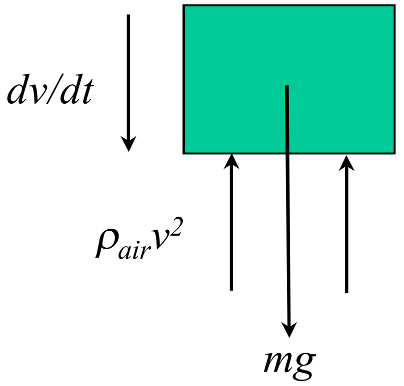
- Free-fall with air resistance: $F = ma$

  Sum forces on body, including weight (mg), and air pressure from the velocity (*air density x velocity*^{2}):

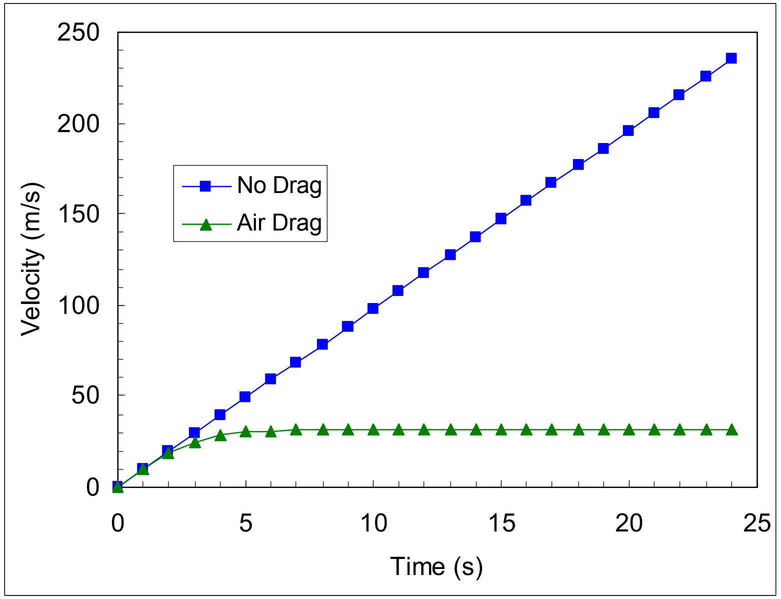
$$ma = mg - Area \cdot \rho_{air} v^2$$

$$m \frac{v_{n+1} - v_n}{t_{n+1} - t_n} = mg - A\rho_{air} v_n^2$$

$$v_{n+1} = v_n + \left[g - \frac{A\rho_{air}}{m} v_n^2 \right] (t_{n+1} - t_n)$$



- Apply initial conditions: $v=0$ at $t=0$; Increment over time to obtain solution



(Note: A=0.5m^2, m=50kg, ρ_{air}=1kg/m^3)

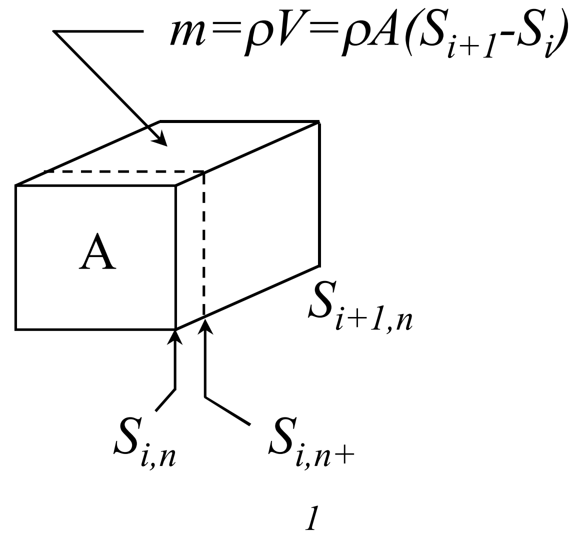
Add Some Material Behavior

- Pressure, P, in a volume of air is determined by its density, ρ, and energy, ε, (or temperature), e.g.,

$$P = (\gamma - 1)\rho\varepsilon$$

- Force is the area times the pressure:

$$F = AP = ma = m\frac{dv}{dt} = m\frac{v_{n+1} - v_n}{t_{n+1} - t_n}$$



$$v_{n+1} = v_n + \frac{AP_n}{m}(t_{n+1} - t_n)$$

$$s_{n+1} = s_n + \frac{(v_{n+1} + v_n)}{2}(t_{n+1} - t_n)$$

$$\rho_{n+1} = m/\left[A\left(S_{i+1,n} - S_{i,n+1}\right)\right]$$

$$P_{n+1} = (\gamma - 1)\,\rho_{n+1}\varepsilon$$

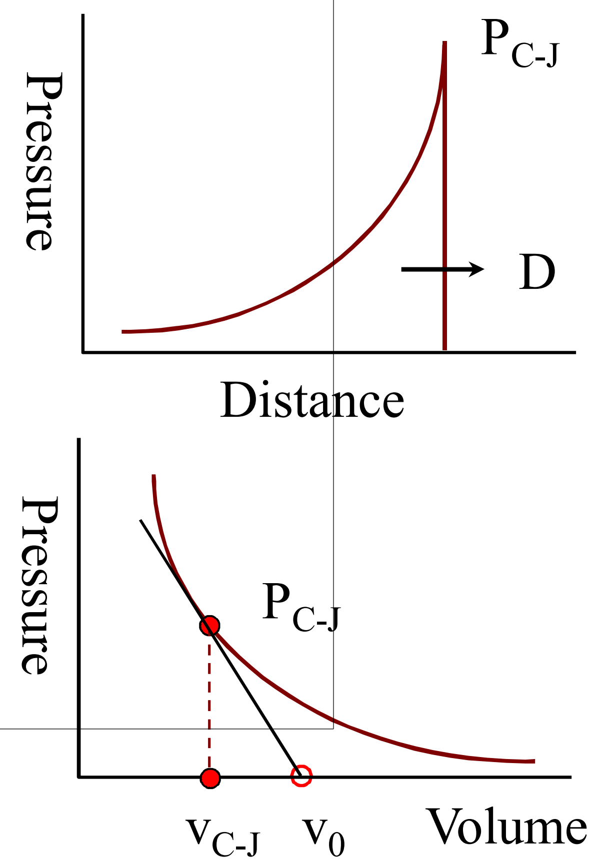
Continue to loop through space and advance in time to obtain a solution

Detonation Waves

- Pressure, *P*, of explosive products can be represented by the ideal gas equation of state, as a function of its density, *ρ*, and energy, *ε*, (or temperature)

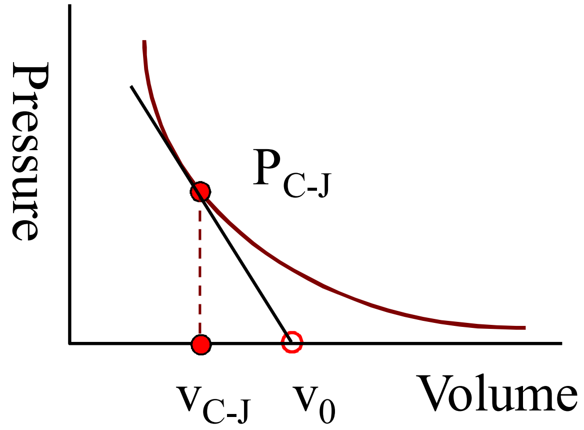
$$P = (\gamma - 1)\rho\varepsilon$$

- The detonation wave can be viewed as a self-sustaining shock front propagating at a constant velocity into unreacted explosive
- The shock activates the chemical energy in the explosive, converting the solid (or liquid) to hot, high density and pressure gas
- The gas expands, doing work as it pushes against the air or some object



Detonation Energy

- The available chemical energy in the explosive can be defined as the integral of the pressure from the C-J state over the volume expanded (the area under the curve), minus the energy to the shocked state,



$$Q = \int_{V_{C-J}}^{\infty} P_S(V)dV - \frac{1}{2}P_S(V_O - V_{C-J})$$

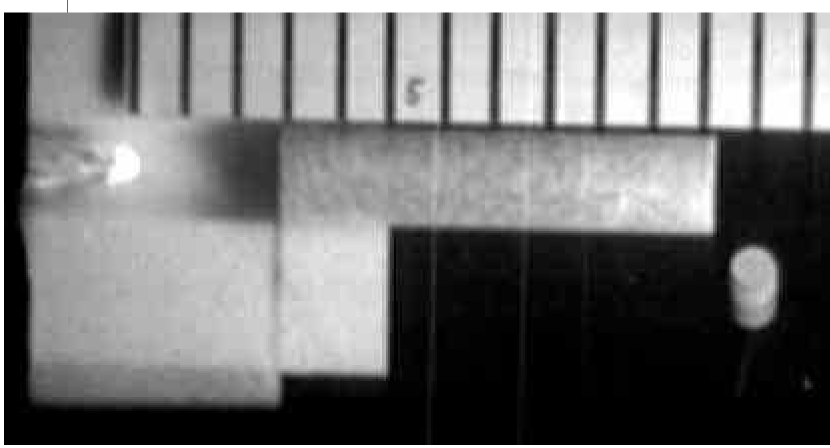
- For this example,

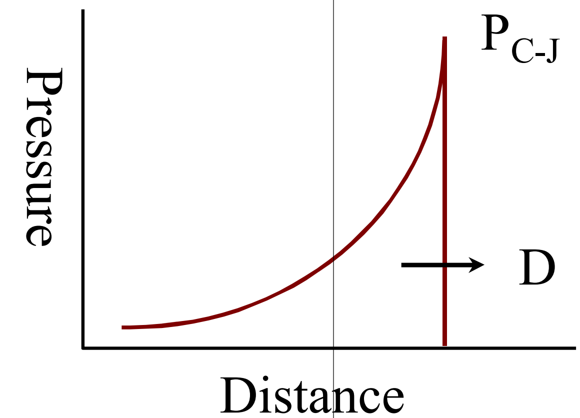
$$Q = \frac{D^2}{2(\gamma^2 - 1)}$$

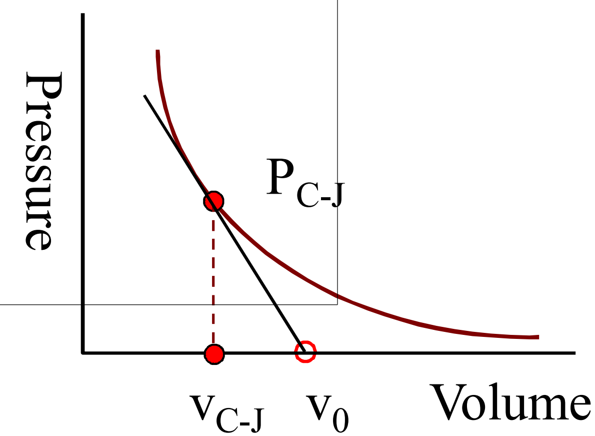
- Energy in 10 lb sphere, about 20 Mega joules
- (A lightning bolt is estimated to have about 300,000 Mega joules of energy)

Detonation Waves

- Experiments required to measure detonation velocity, D, and infer P_{C-J} , V_{C-J} , and γ
- Another look at the detonating cylinder of TNT
- The detonation front is moving at about 7 km/s (23,000 ft/s)







Basic Detonation Model

- Require reactant and product equations of state

$$P_R = \frac{\rho_0 c_0 \eta^2}{(1 - s\eta)^2} + \rho_R \gamma_R \varepsilon_R$$

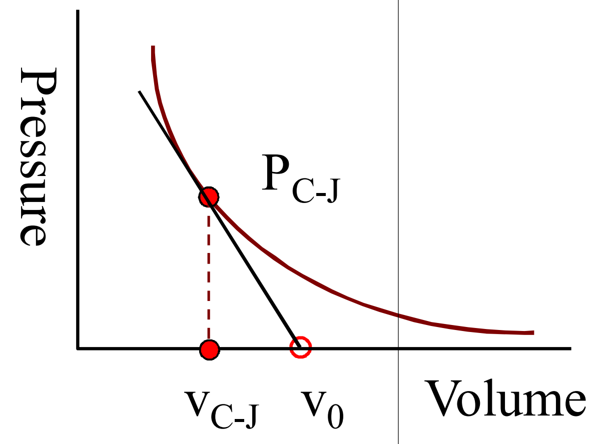
$$P_G = (\gamma_G - 1)\rho_G \varepsilon_G$$

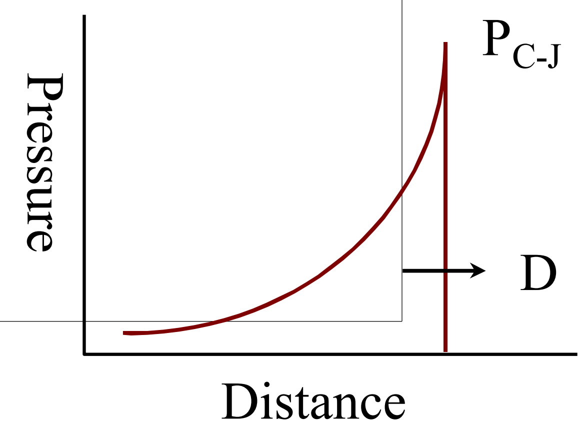
- Mixing assumption for partially reacted material

$$P_{Mix} = (1 - \lambda)P_R + \lambda P_G$$

- Reaction rate

$$\frac{d\lambda}{dt} = (1 - \lambda)P_G^n$$





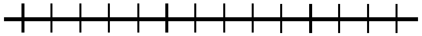
Analysis Code - CTH

- CTH – an Eulerian Shock Physics Wave Propagation Code
  - Multi-dimensional (1-D, 2-D, 3-D)
  - Developed, maintained at Sandia National Laboratories
  - Model dynamic events with large deformations (e.g., explosive detonation, high-velocity impact)
  - Materials convected through fixed spatial mesh (uniform, graded cell size)
  - Interactions of up to 20 materials
  - Geometric insert packages to construct complex device configurations
  - Material response - EOS for solids, melt, vaporization, explosives
Plasticity models for strength (deviatoric)
- Typically, large problems run on parallel computing platforms, with large memory and many processor resources

Discretizing Spatial Regions

- Discretize a region of space into finite volumes (cells)
- Each cell contains local information
  e.g., velocity, position, density, pressure, energy

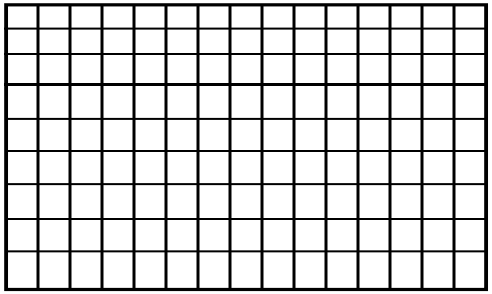
One-Dimensional



i=1,L

Two-Dimensional

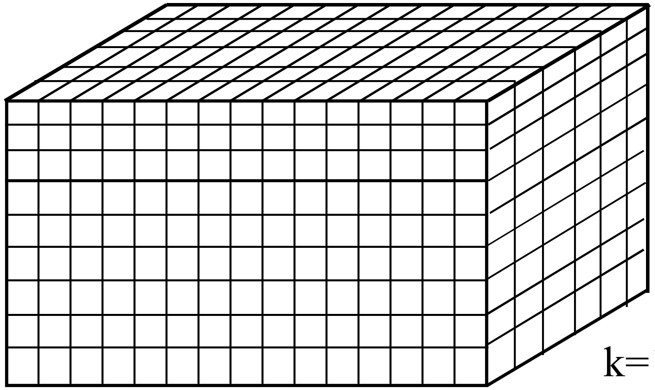
j=1,M



i=1,L

Three-Dimensional

j=1,M

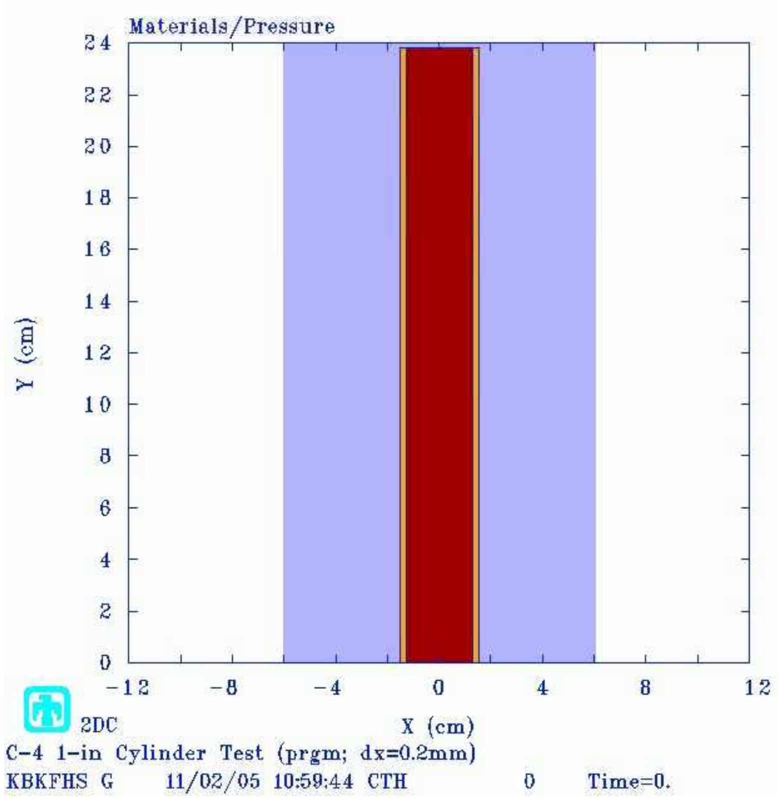


k=1,N

i=1,L

Explosive / Copper Cylinder Test

- How do we verify the accuracy of our model?
- Compare with cylinder test data for specific explosive
  - Copper tube filled with explosive
  - Monitor velocity and displacement of expanding copper surface with laser interferometer device



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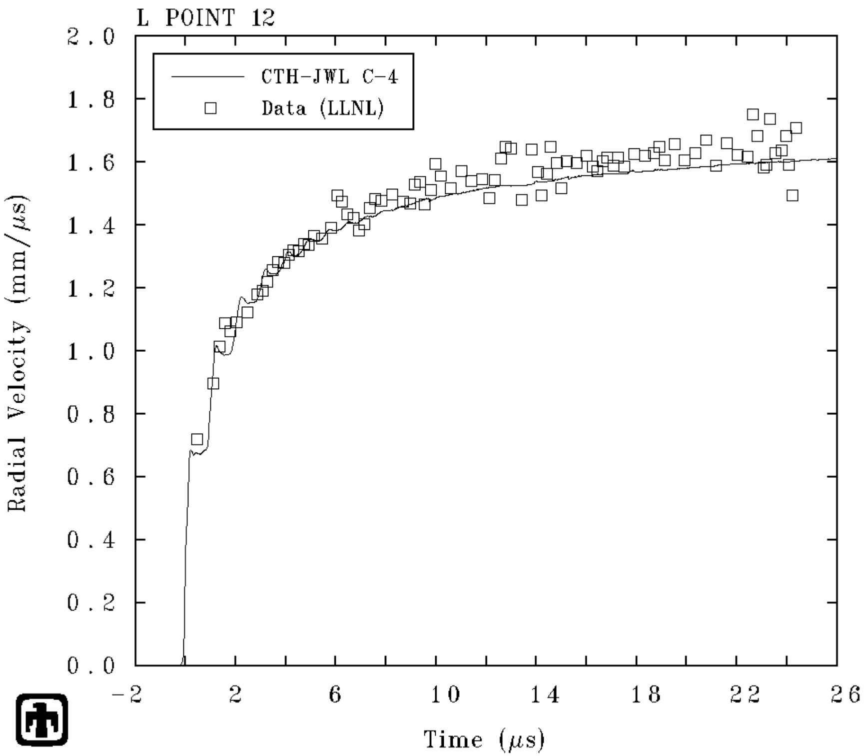
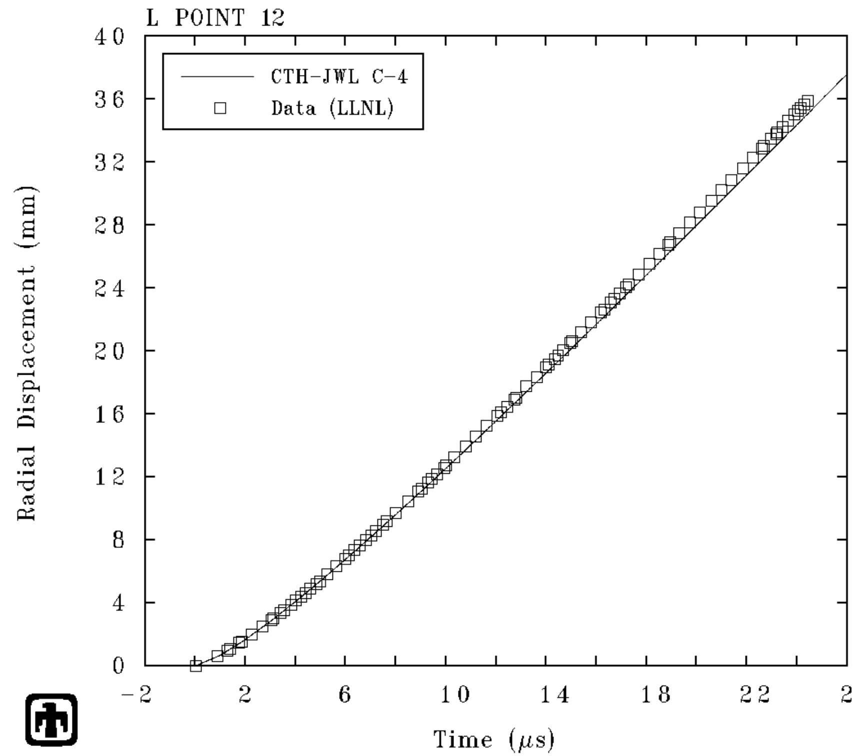
Explosive Models

- Compare calculation with velocity and displacement data for expanding copper surface





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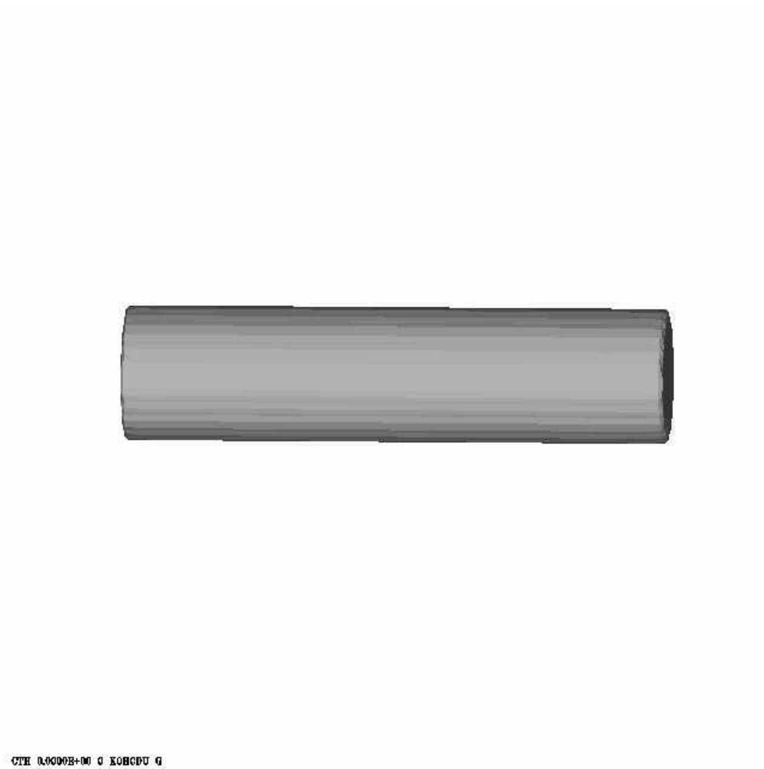
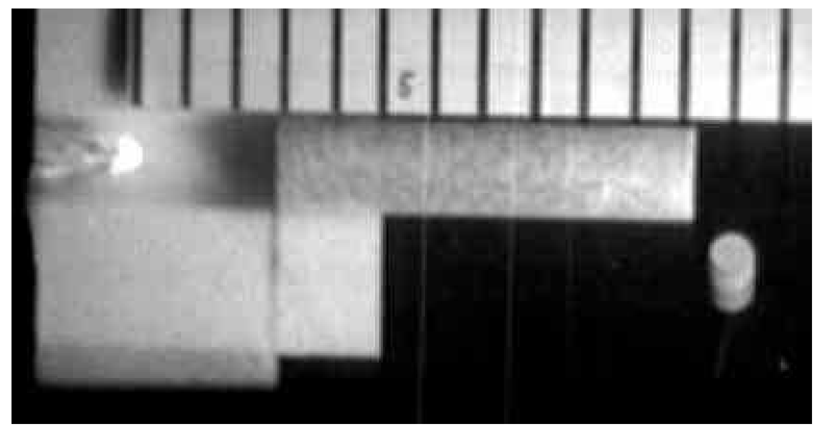
Bare TNT Cylinder Test

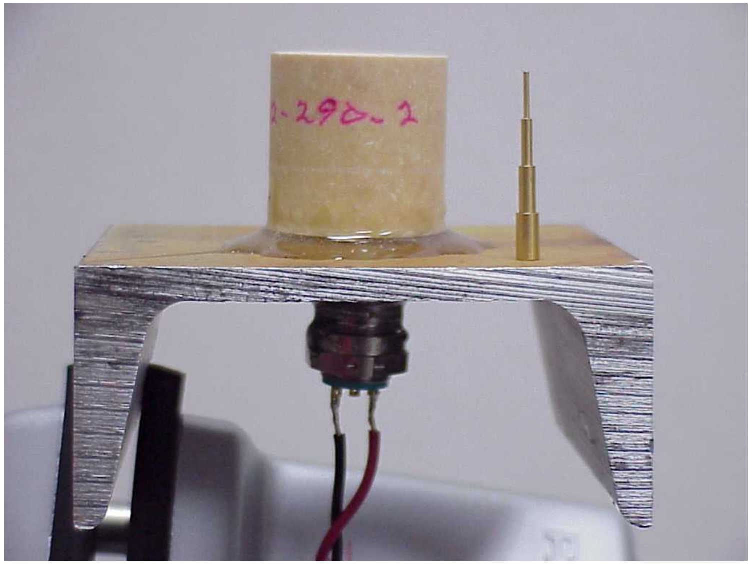
- Compare calculation of bare TNT cylinder test with framing camera record





Explosive Pellet Test

- 1 inch x 1 inch PBX-9404 (HMX) explosive pellet (24 g) (0.053 lb)



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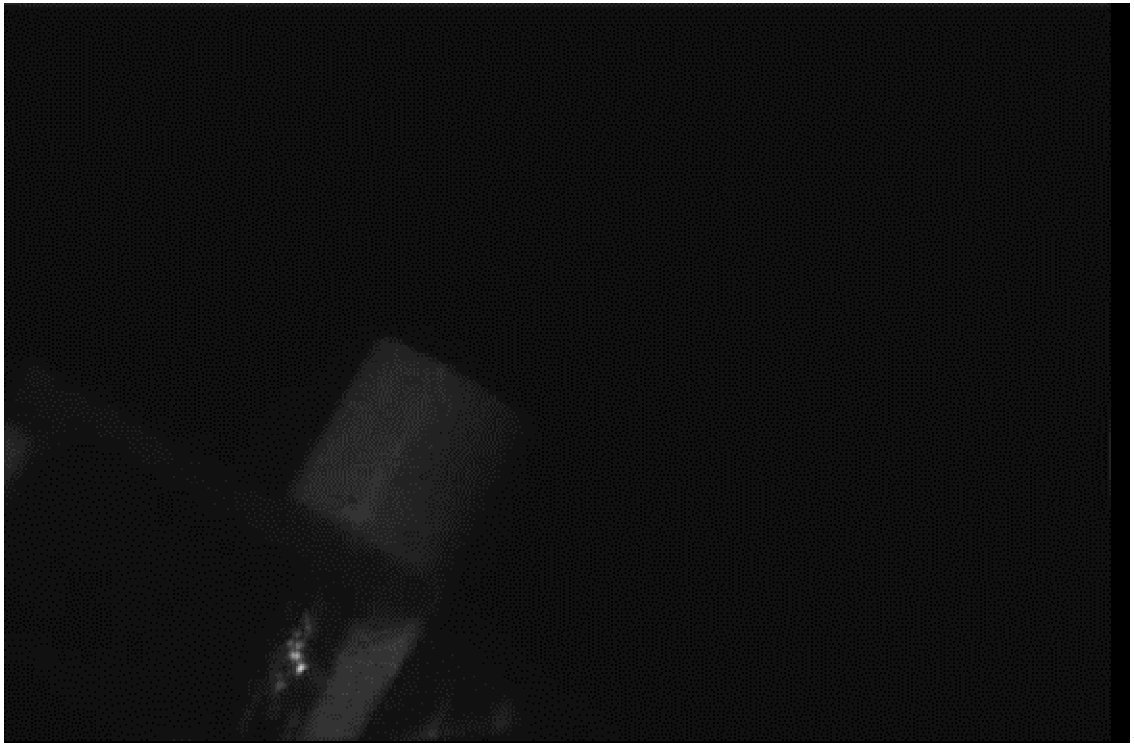
HMX Pellet Test

- Static View



HMX Pellet Test

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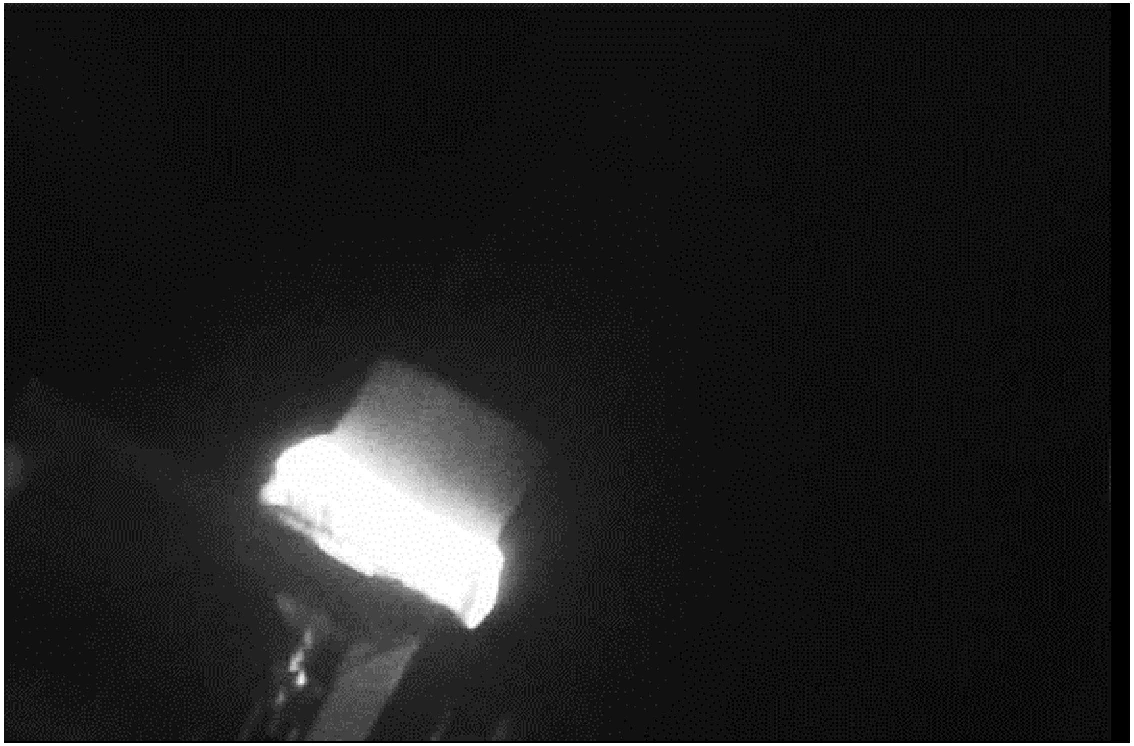
HMX Pellet Test



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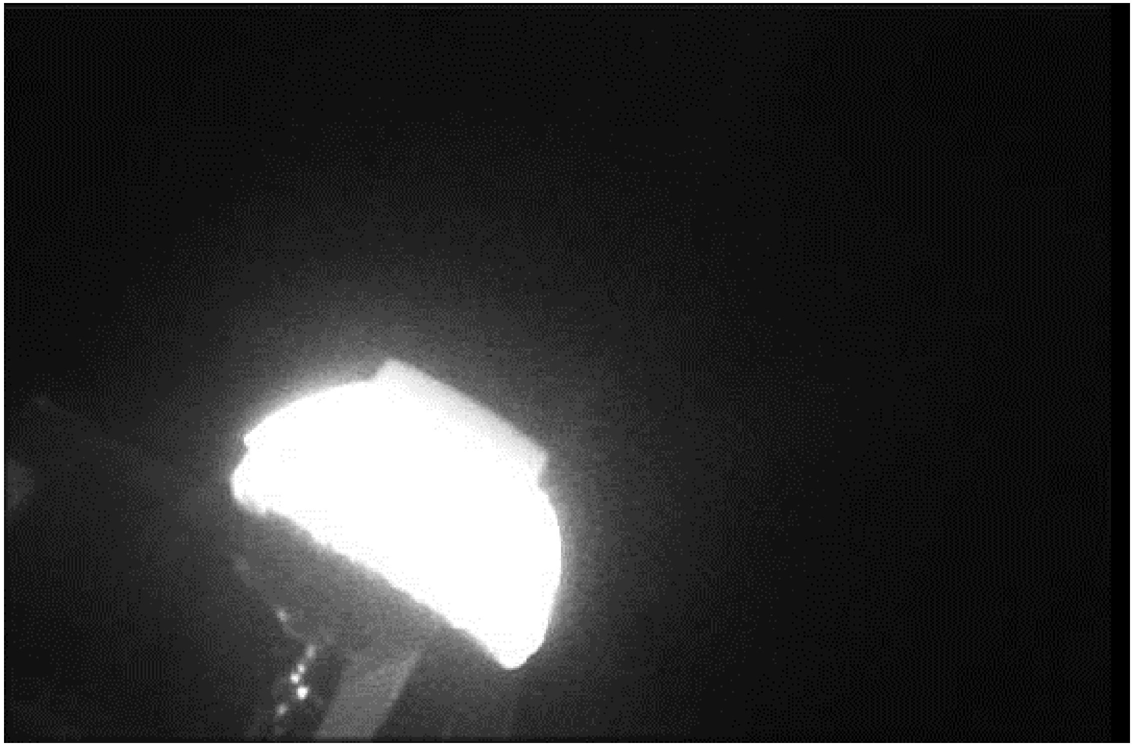

HMX Pellet Test

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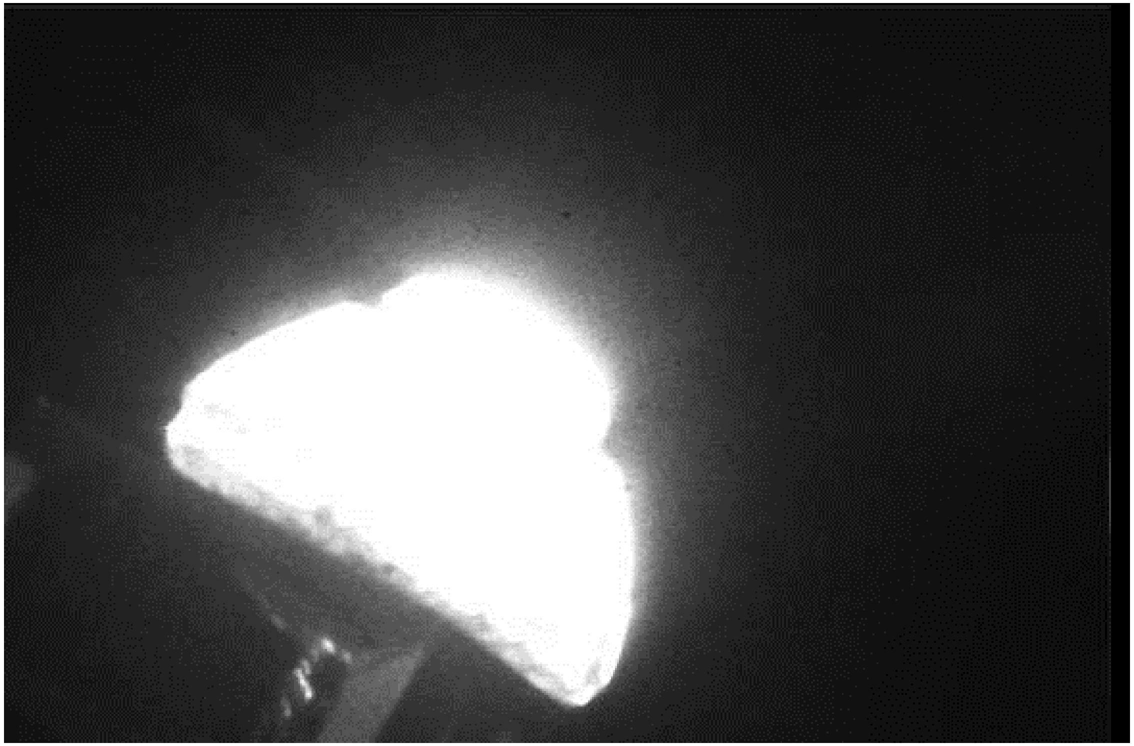

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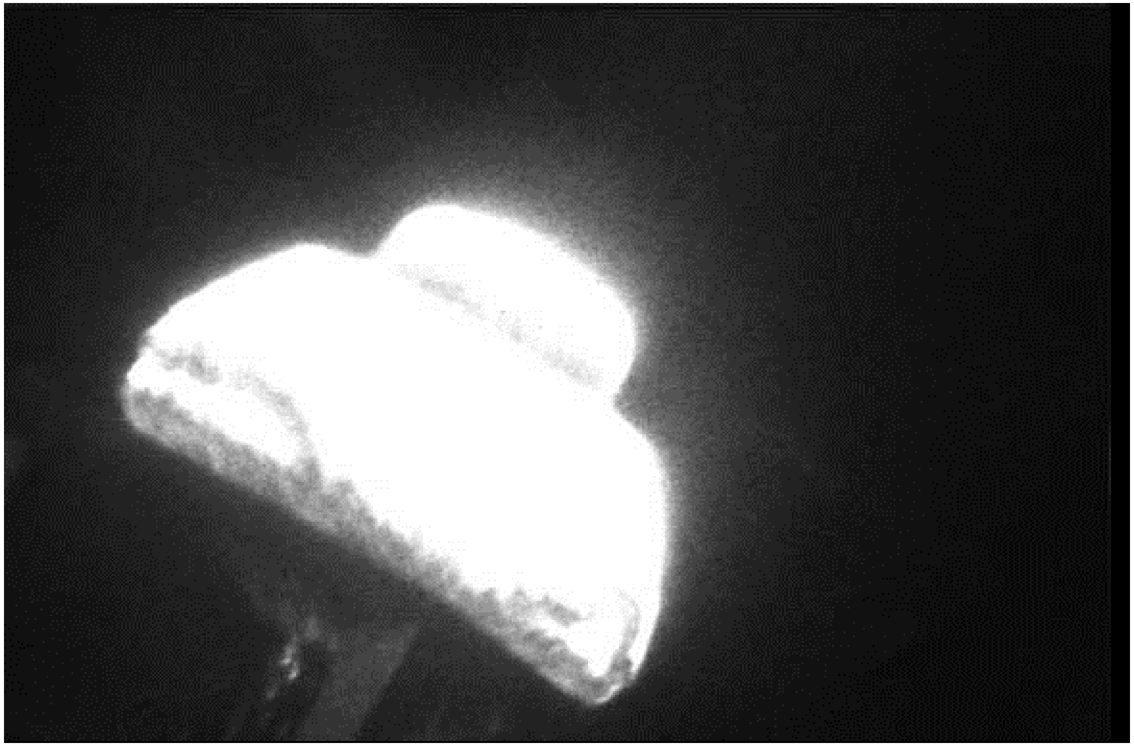
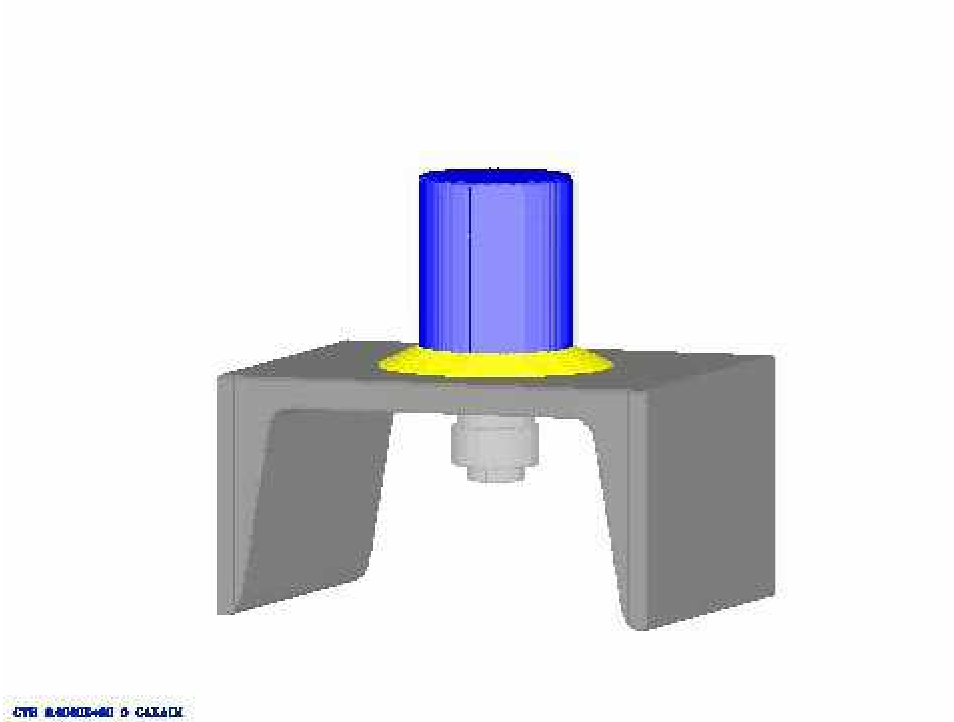
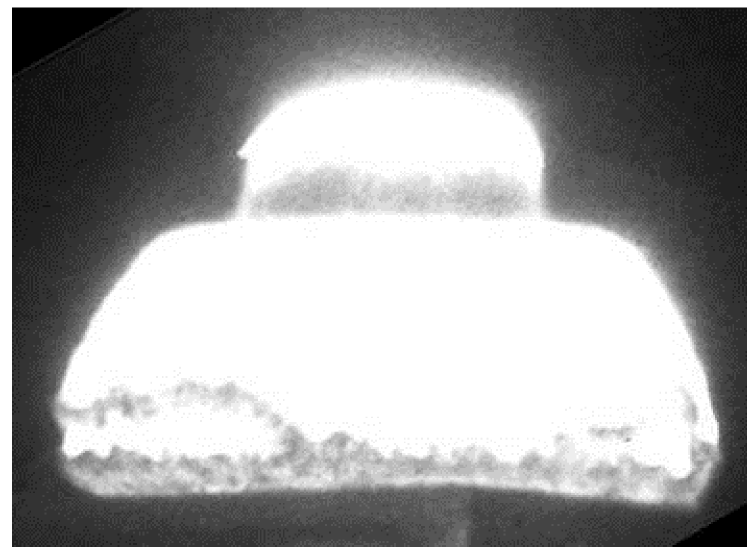


HMX Pellet Test

HMX Pellet Test

- Movie of Simulation (from CTH code)
- Typical simulation (14 cm x 14 cm x 12 cm) to 100 ms with 0.5 mm resolution (~19 million computational cells) requires 3-4 hrs with 512 processors on a parallel computing platform (Janus) (*i.e.*, 2,000 cpu processor hours)





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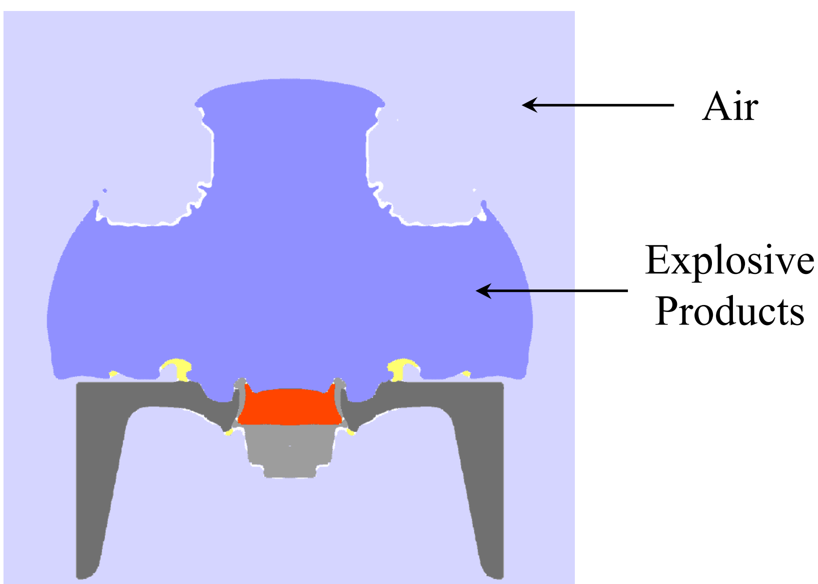
HMX Pellet Test Comparisons

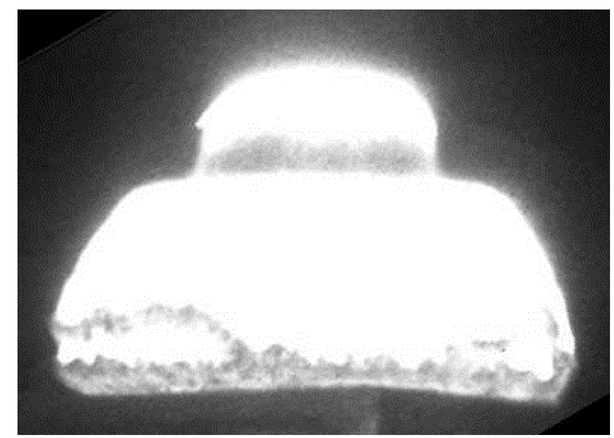
Cross-section material plot (left); experimental image (right)

What seems to be missing from the simulation?

Material Plot



Experimental Image



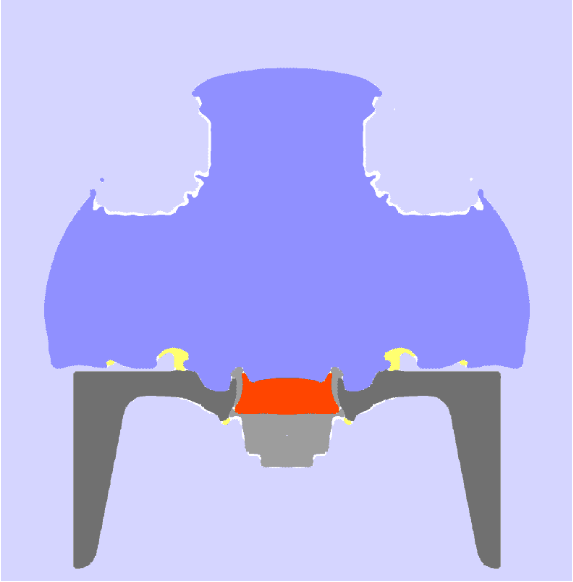
HMX Pellet Test Comparisons

Cross-section material plot (left); experimental image (right)

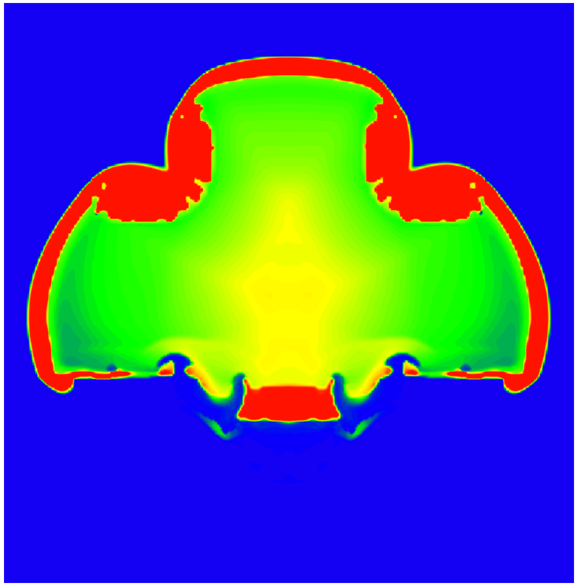
Add air shock temperature (center) (luminous air) – 2500 K

- Comparison with data much improved when proper variables examined

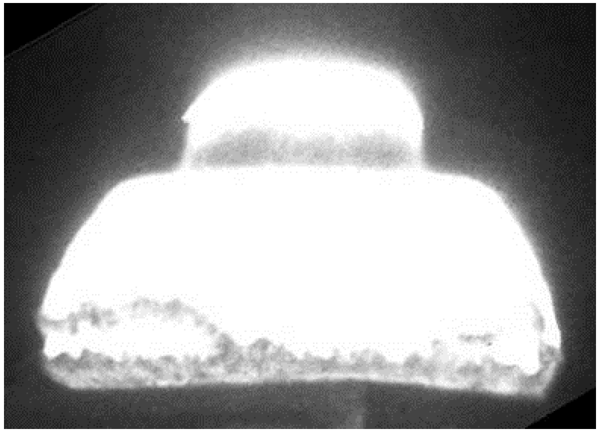
Material Plot



Air Shock Plot (Temperature)

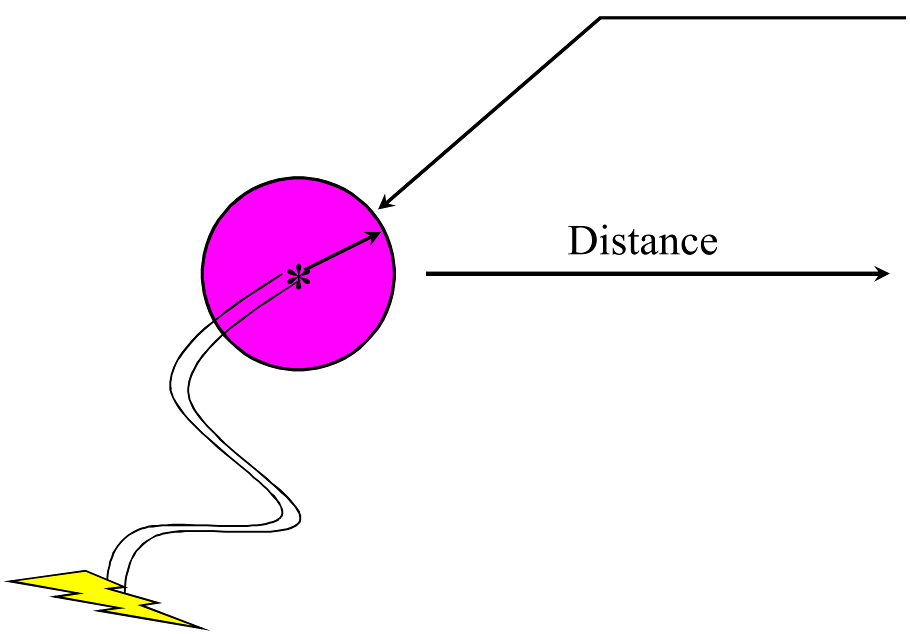


Experimental Image



Explosions in Air – Principles

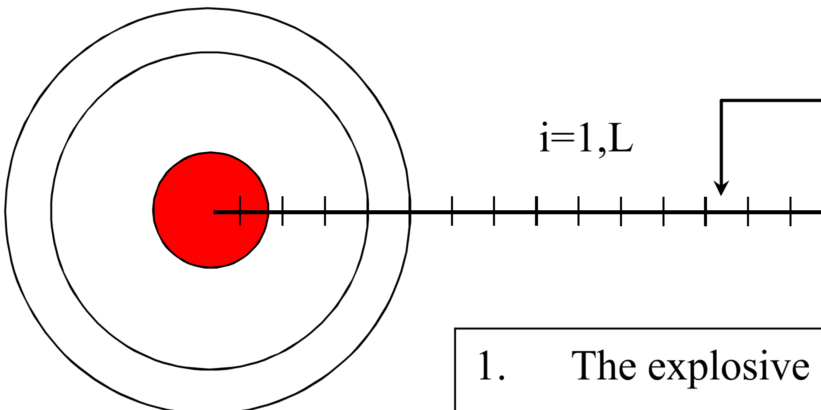
- When an explosion occurs, how much time is available to react? *e.g.*, In movies, see people running and diving to safety as an explosion goes off in the background.
- Example: 10 lbs TNT explosive – a 7 inch diameter sphere (87 mm radius)



1. Time to detonate the explosive = Radius of Charge / Detonation Velocity
2. Detonation velocity = 7 km/s (23,000 ft/s)
   Detonation time = 13 μs
3. Time for shock to arrive at some distance from the explosion = Distance from Charge / Sound Speed in Air
4. Sound speed in air ~ 300 m/s (1000 ft/s)
   At 50 ft, shock arrives in ~ 50 ms
5. A person running at 22 ft/s (4 minute mile) would move a distance of 1 ft in 50 ms

Explosions in Air – Modeling

- To model an explosion in air, discretize one dimension into cells, each cell being a thin spherical shell (identical behavior in all directions from center)
  - Insert explosive at origin of this coordinate system
  - Insert air everywhere else



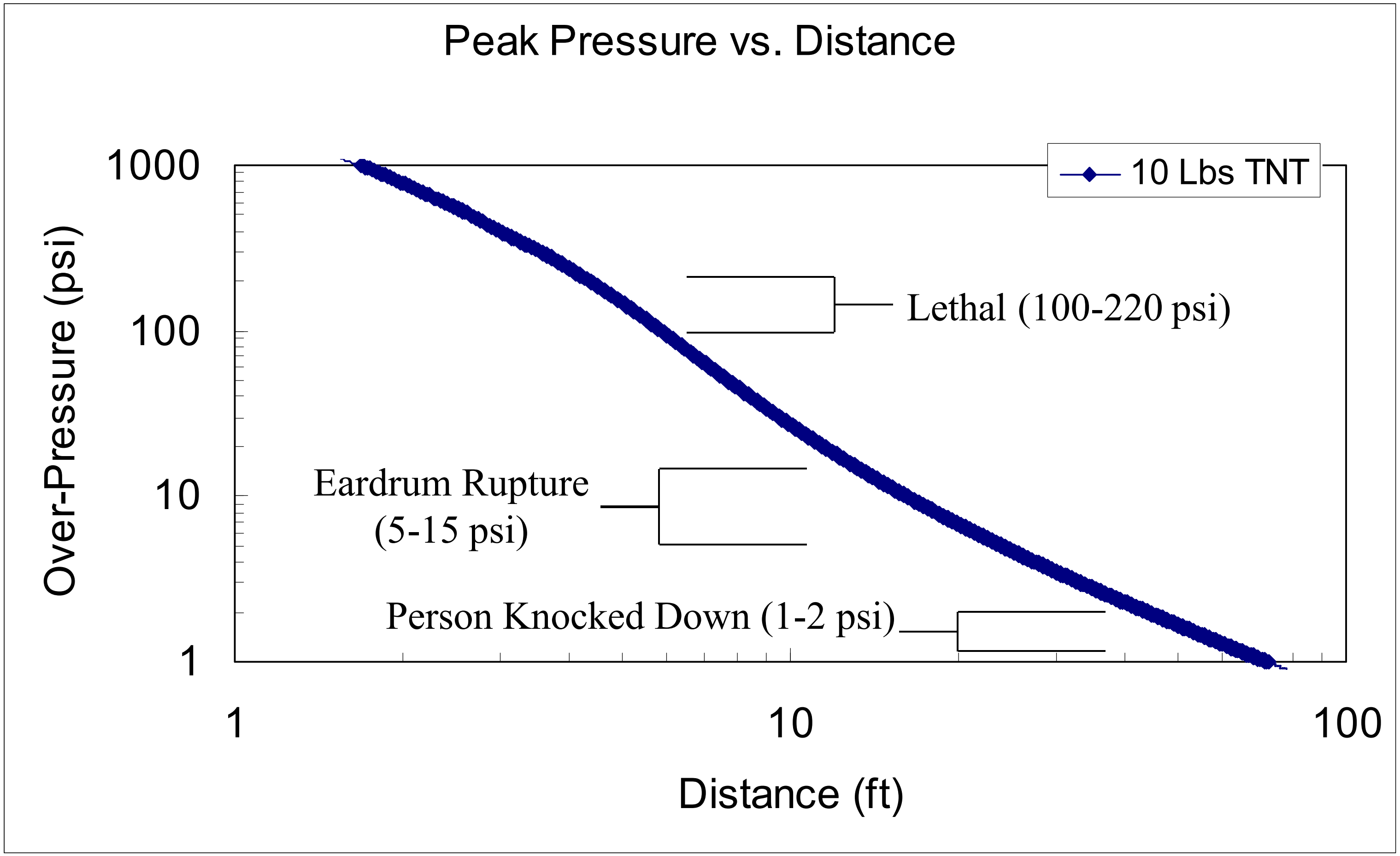
Each cell contains the following data:
Position, velocity, mass, density, energy (temperature), pressure

Data in each cell x number of cells defines the memory requirements for the simulation

1. The explosive is initially an unreacted solid.
2. When it detonates, the solid is transformed into a high-density, high-pressure (200,000 atmospheres), hot gas.
3. The unbalanced forces of this pressure compared with the low pressure of the surrounding air (1 atmosphere) lead to expansion, and a pressure wave (shock) transmitted into the air

10 Lbs TNT – Peak Pressure *vs*. Distance

- Consequences that depend on the distance from this explosive charge



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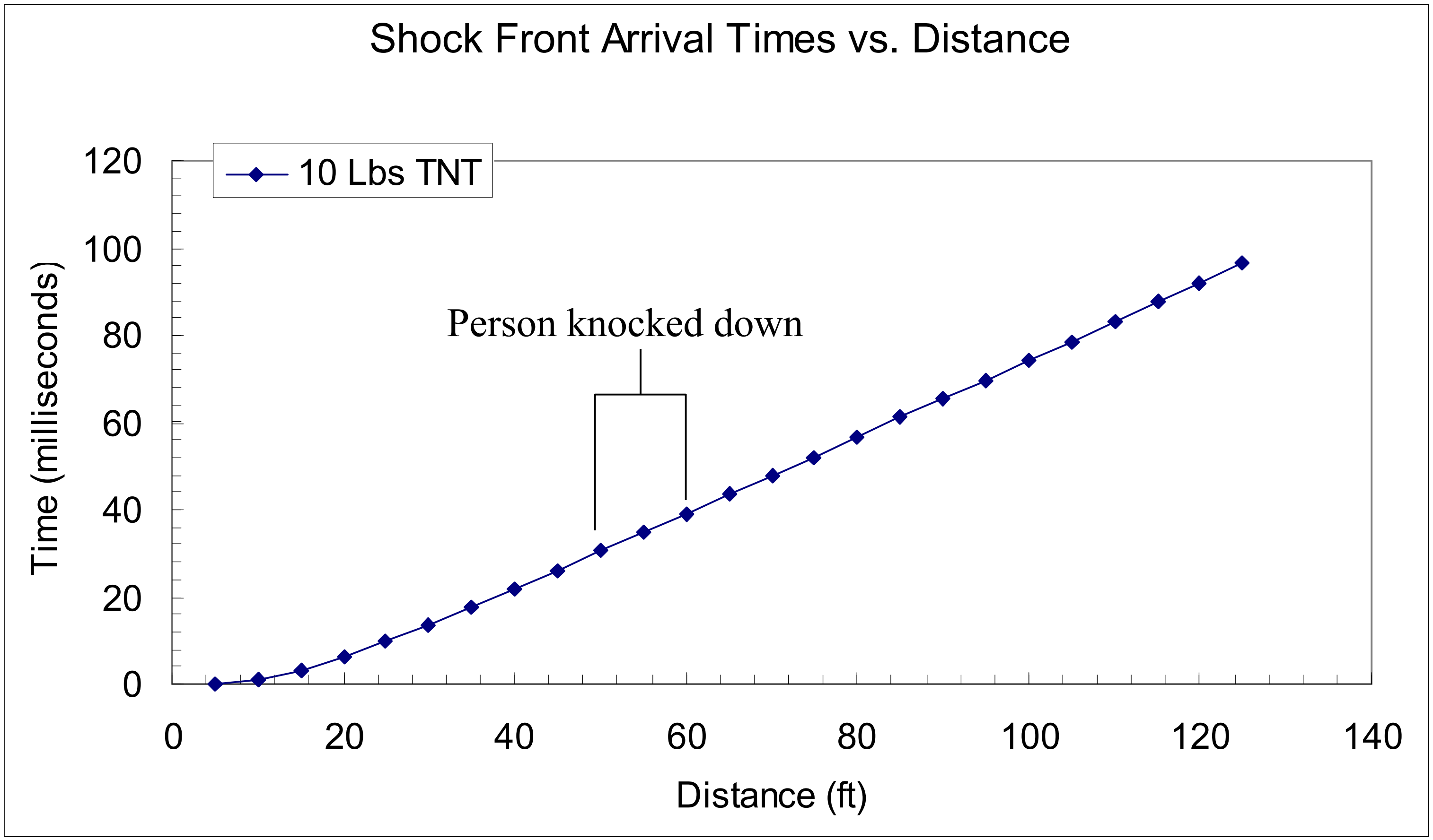
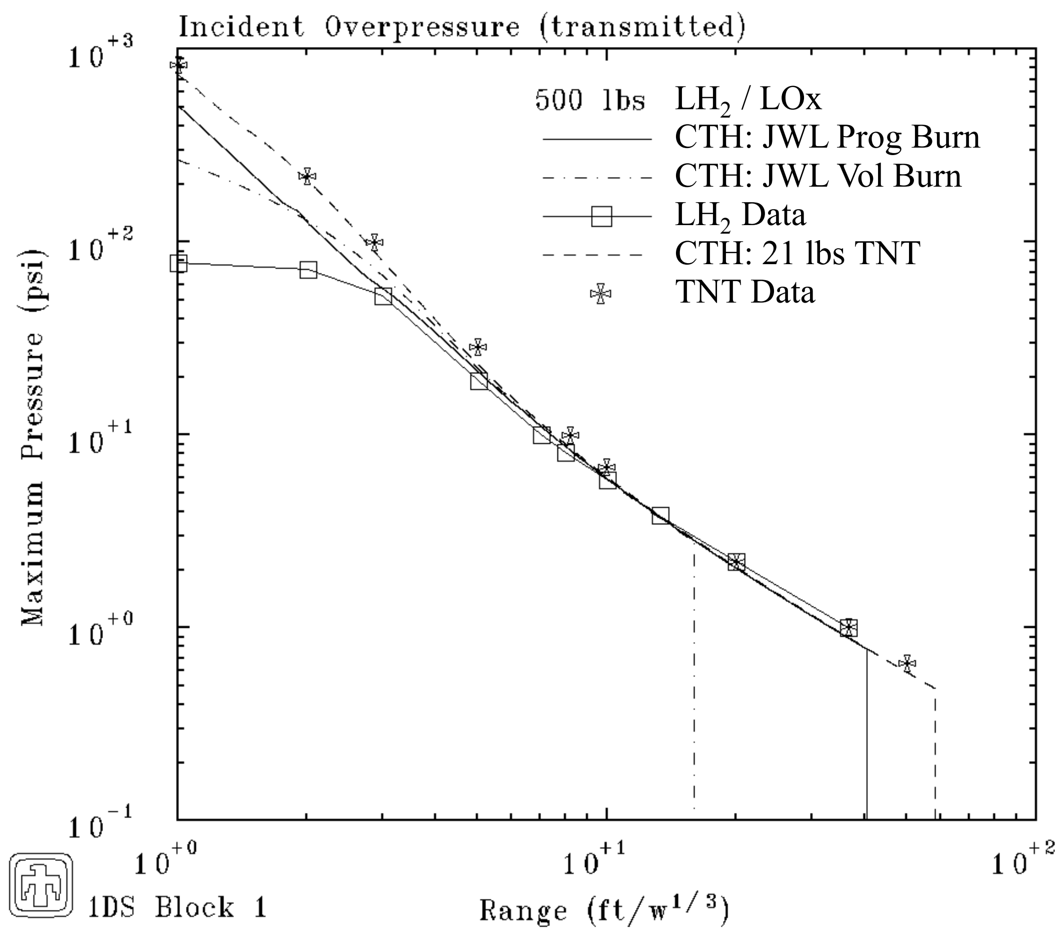
10 Lbs TNT – Shock Arrival Times

- Shock distance from the charge as a function of time after the explosion



Additional Explosive Comparisons

- Peak over-pressure as a function of scaled distance from the charge



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Oxygen Balance

- Explosives are typically oxygen-rich or oxygen-poor relative to the "fuel" in the CHNO molecule (TNT ~ $C_7H_5N_3O_6$)
- After a detonation of an explosive charge, the expanding hot gases mix with the surrounding air
- In an oxygen-poor explosive, these hot gases react with the available oxygen, consuming whatever is required to complete the burn (secondary combustion)
- Example: TNT charges in a tunnel
  - "Small" TNT charge – oxygen in tunnel sufficient to balance the TNT oxygen deficiency
  - "Large" TNT charge – oxygen in tunnel insufficient to balance the TNT oxygen deficiency; oxygen external to tunnel consumed as well
- (Similar to early years of mining with black powder charges, in which miners could suffocate from lack of oxygen, though not injured by the blast)

Oxygen Deficiency Consequences

- TNT is oxygen deficient – After the detonation, the hot, expanding explosive products mix with air and burn to completion

Small TNT Charge

Large TNT Charge

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