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Peridynamic Theory: An Approach to Computational Mechanics for High-Impulse Loading and Fragmentation

Presentation for

Workshop on Computational Mechanics and Insensitive Munitions

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Outline of Presentation

- What is Peridynamic Theory?
- Why Use Peridynamics?
- The Fundamental Equation of Peridynamic Theory
- Material Modeling in Peridynamics
- Numerical Method for Solving the Fundamental Equation of Peridynamics
- Implementation of Peridynamic Theory in the EMU Computer Code
- High-Impulse Impact Loading of a Structure
- Detonation Modeling in Peridynamic Theory
- High-Impulse Explosive Loading of Structures
- Verification and Validation (V&V) Process for Warhead Fragmentation Using EMU
- Concluding Remarks

What is Peridynamic Theory?

- ***Peridynamic theory*** **is a theory of continuum mechanics that uses differo-integral equations without spatial derivatives rather than partial differential equations.**
  - **Reformulation of fundamental equations that applies everywhere regardless of discontinuities**
  - **Peridynamic means "near force".**
  - **Theory first published in 2000 by Stewart A. Silling**

PERGAMON

Journal of the Mechanics and Physics of Solids
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JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS

Reformulation of elasticity theory for discontinuities and long-range forces

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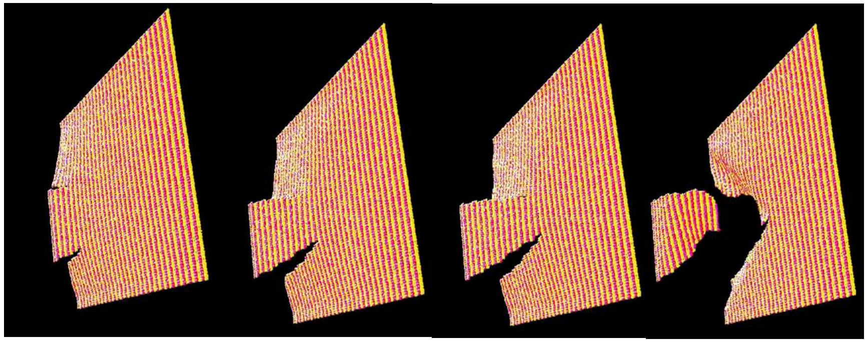
Why Use Peridynamics?

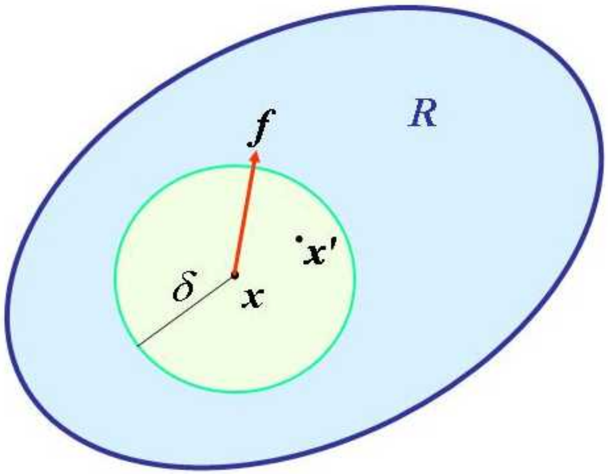
- The fundamental partial differential equations used in conventional finite element codes do not apply at discontinuities such as cracks.

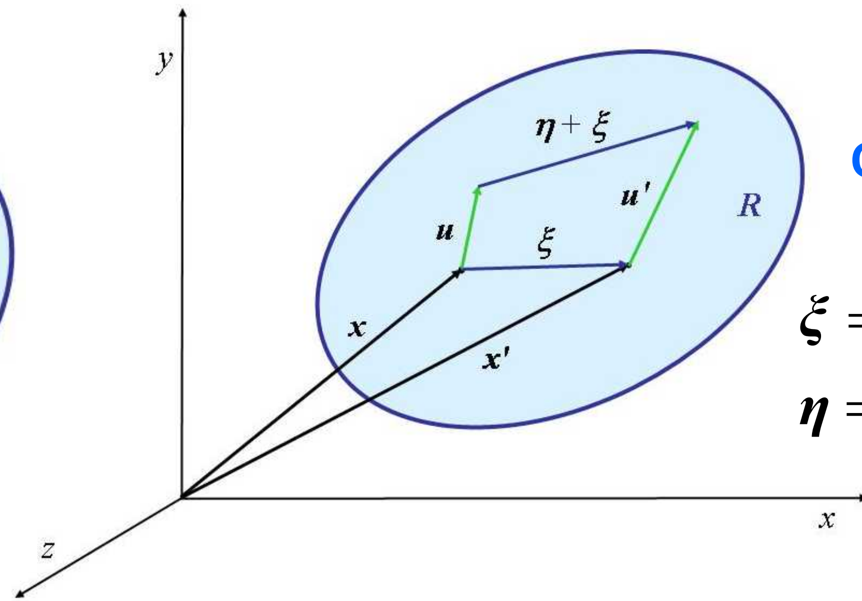


Real life:
Discontinuities can evolve in complex patterns not known in advance.

- With peridynamics, cracks initiate and grow spontaneously and there is no need for externally supplied "crack growth laws".

Fundamental Peridynamics Equation





Configuration Variables

$$\xi = \boldsymbol{x}' - \boldsymbol{x}$$

$$\boldsymbol{\eta} = \boldsymbol{u}(\boldsymbol{x}', t) - \boldsymbol{u}(\boldsymbol{x}, t)$$

$$\rho(\boldsymbol{x}) \frac{d^2}{dt^2} \boldsymbol{u}(\boldsymbol{x}, t) = \iiint_R \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{x}', t) - \boldsymbol{u}(\boldsymbol{x}, t), \boldsymbol{x}' - \boldsymbol{x}) dV' + \boldsymbol{b}(\boldsymbol{x}, t)$$

where

ρ is the density at $\boldsymbol{x}$,
$\boldsymbol{x}$ is the position vector,
t is the time,
$\boldsymbol{u}$ is the displacement vector,
R is the computational domain,
$\boldsymbol{f}$ is the pairwise force function, and
$\boldsymbol{b}$ is the body force.

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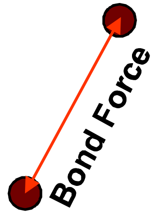
Material Modeling in Peridynamics

- The force per unit volume squared between particles located a two points is given by the ***pairwise force function*** (*PFF*) f.
  - Peridynamic interaction between two points is called a ***bond***.



- **Constitutive properties** of materials are given by specifying the *PFF*.
  - Thus, material response, damage, and failure are determined at the bond level.
- **Bond properties** are derivable from measured material properties including:
  - elastic modulus, yield properties, and fracture toughness.

Properties of the Pairwise Force Function

- Newton's third law of motion implies that the *PFF* satisfies

$$\boldsymbol{f}(-\boldsymbol{\eta},-\boldsymbol{\xi}) = -\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) \quad \forall\, \boldsymbol{\eta},\boldsymbol{\xi}$$

- Furthermore, conservation of angular momentum implies that the *PFF* satisfies

$$(\boldsymbol{\eta}+\boldsymbol{\xi})\times \boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = 0$$

- These properties imply that the *PFF* is of the form

$$\boldsymbol{f}(\boldsymbol{\eta},\boldsymbol{\xi}) = F(\boldsymbol{\eta},\boldsymbol{\xi})(\boldsymbol{\eta}+\boldsymbol{\xi}) \quad \text{where} \quad F(-\boldsymbol{\eta},-\boldsymbol{\xi}) = F(\boldsymbol{\eta},\boldsymbol{\xi})$$

- For isotropic materials, F has the form

$$F(\boldsymbol{\eta},\boldsymbol{\xi}) = I(p,q,r) \quad \text{where} \quad p=\left|\boldsymbol{\eta}+\boldsymbol{\xi}\right|,\ q=\boldsymbol{\eta}\cdot\boldsymbol{\xi},\ r=\left|\boldsymbol{\xi}\right|$$

Micro-Elastic (Plastic) Materials

- A *PFF* is said to be ***micro-elastic*** (*ME*) ***-plastic*** (*MP*) if and only if there exists a scalar function, w, such that

$$\mathbf{f}(\boldsymbol{\eta},\xi) = \frac{\partial w}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta},\xi)$$

- A *ME* material is said to be ***proportional*** if and only if the *PFF* is proportional to the stretch, s, where $s = (p - r)/r$.
- Failure occurs when s exceeds a value, s_0, called the ***critical or failure stretch (FS)***.
- Isotropic, proportional ME materials have

$$F(\boldsymbol{\eta},\xi) = \frac{1}{p} g(s,r) \quad \begin{cases} \text{where } g(s,r) \text{ is a piecewise} \\ \text{linear function of } s. \end{cases}$$

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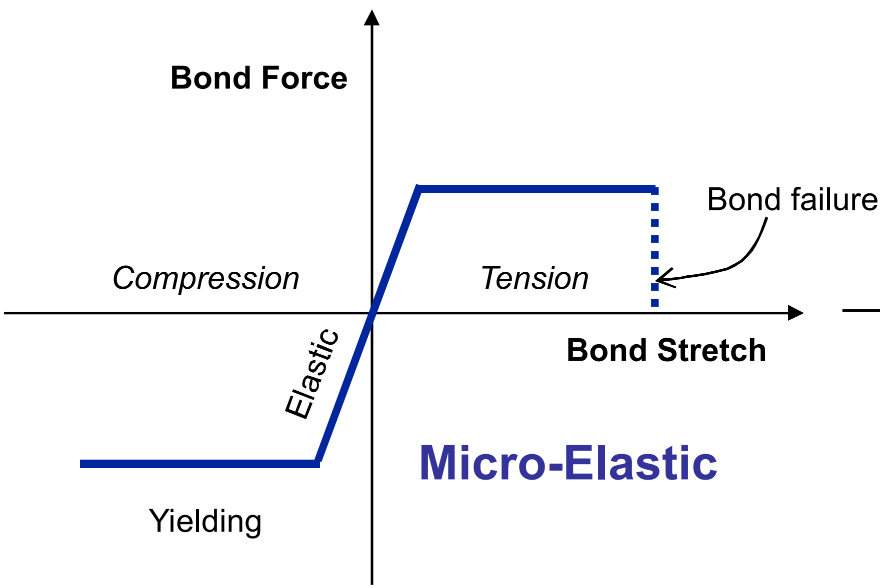
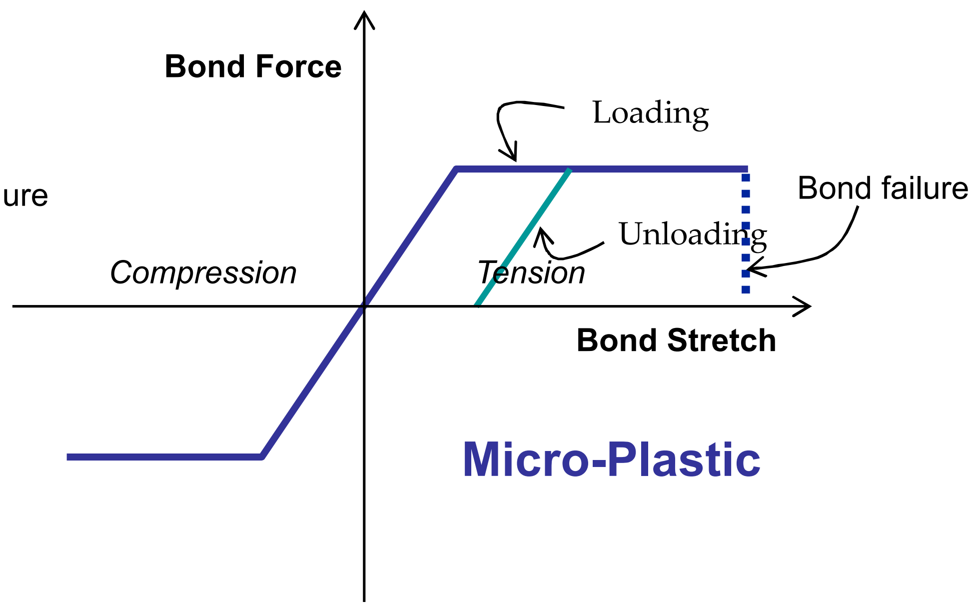
Micro-Elastic and -Plastic Materials

- The difference between isotropic, proportional *micro-elastic* and *micro-plastic* materials is their behavior on unloading.





Bond is a spring in these cases.

- For extreme loading analyses, we use isotropic, proportional, micro-elastic (plastic) materials.

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Damage

- At time t, consider a node at position $\boldsymbol{x}$.
- Let $V_d(\boldsymbol{x},t)$ denote the volume of the material initially connected to $\boldsymbol{x}$ but whose bonds with $\boldsymbol{x}$ have been broken and let $V_0(\boldsymbol{x})$ denote the volume of material initially connected to $\boldsymbol{x}$.
- Then the ***damage*** $D(\boldsymbol{x},t)$ is defined as

$$D(\boldsymbol{x},t) = V_d(\boldsymbol{x},t) / V_0(\boldsymbol{x})$$

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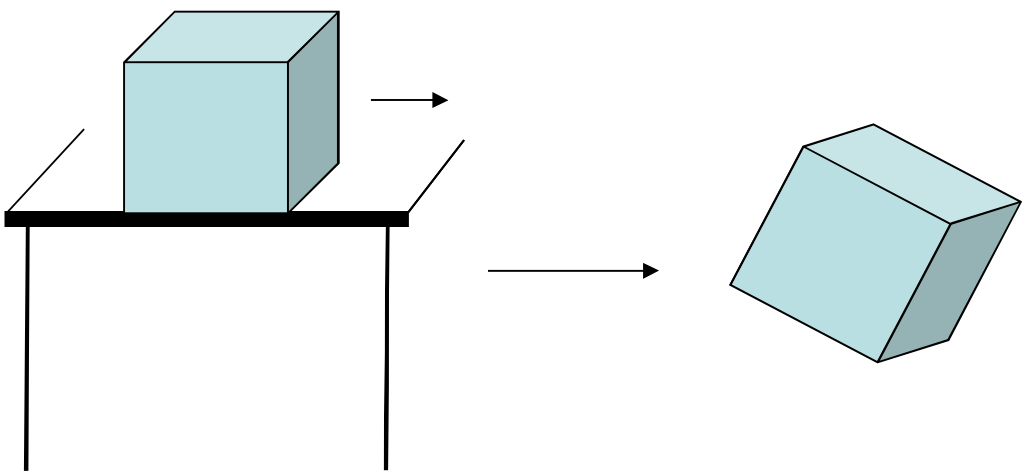
Gravitational Forces

- Gravity is important to determine the long term consequences of impacts to structures.
- We include gravity as a body force

$$\boldsymbol{b}(\boldsymbol{x},t) = \rho(\boldsymbol{x})\,\boldsymbol{g}$$

  - $\rho(\boldsymbol{x})$ is the density and
  - $\boldsymbol{g}$ is the acceleration due to gravity, g = 9.814 m/s^2.



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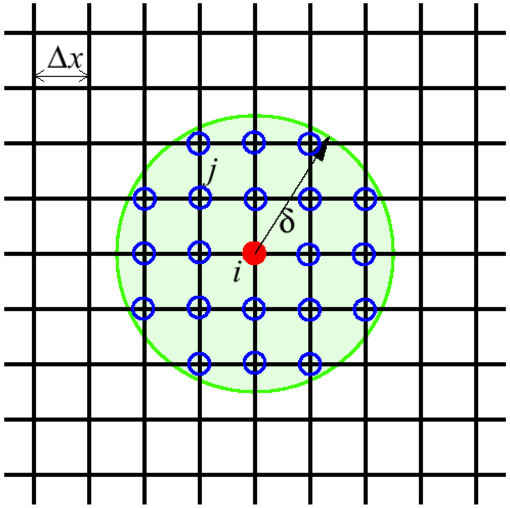
Numerical Method



- The computational region is discretized into nodes with a known volume in the reference configuration, forming a *grid of nodes*.
- The fundamental equation is replaced by a finite sum, which at time t_n is

$$\rho_i \frac{d^2}{dt^2}\boldsymbol{u}_i^n = \sum_p \boldsymbol{f}(\boldsymbol{u}_p^n - \boldsymbol{u}_i^n, \boldsymbol{x}_p - \boldsymbol{x}_i)V_p + \boldsymbol{b}_i^n, \quad \boldsymbol{u}_i^n = \boldsymbol{u}(\boldsymbol{x}_i, t_n)$$

- For each node, the peridynamic interaction is assumed to be zero outside a distance δ called the *horizon*.

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Implementation in EMU Computer Code

- Peridynamic theory is implemented in the EMU computer code.
- EMU is
  - *mesh free* (no elements, just generate a grid of nodes),
  - *Lagrangian* (each node represents a fixed amount of material),
  - *explicit* (simple, reliable time-integration method),
  - *parallel* (executes on multiple processors).

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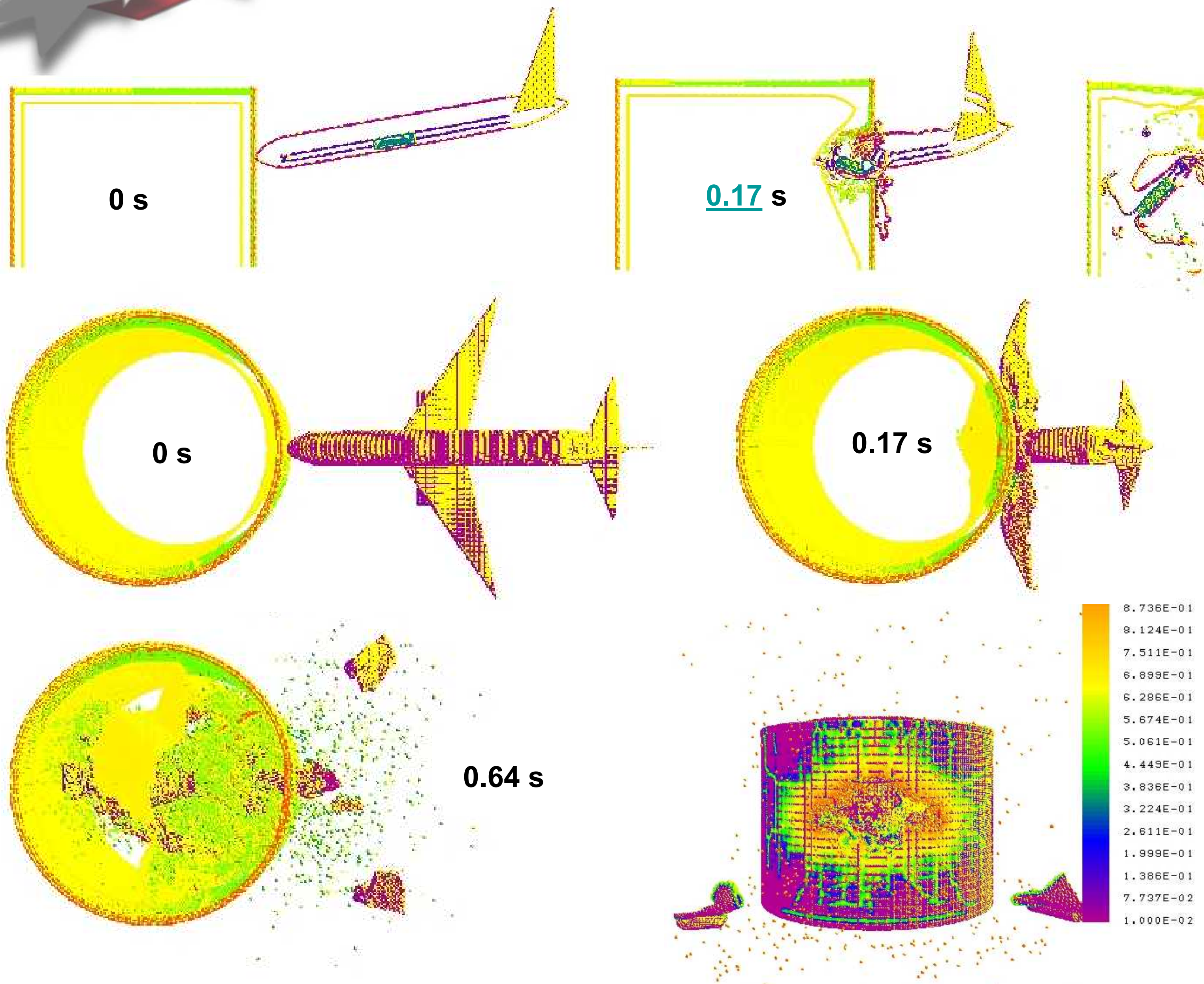
High-Impulse Impact Loading of a Structure



Damage at 0.64 s

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EMU Detonation Model

$(x_{det}, y_{det}, z_{det}, t_{det}), \rho_{unreacted}, v_{det}$

- **Detonation model inputs:**
  - Location of detonation point(s) and initial detonation time(s), density of unreacted explosive, and detonation speed.
  - Parameters for equation of state (ideal gas or JWL).
- **Program burn model for detonation times.**
  - Detonation times computed prior to time advancement using Huygen's construction.
  - Detonations can propagate around obstacles.
- **Upon detonation:**
  - Reaction products are treated as ideal or JWL gas undergoing an adiabatic expansion.
  - Energy conserved using volume-burn algorithm.

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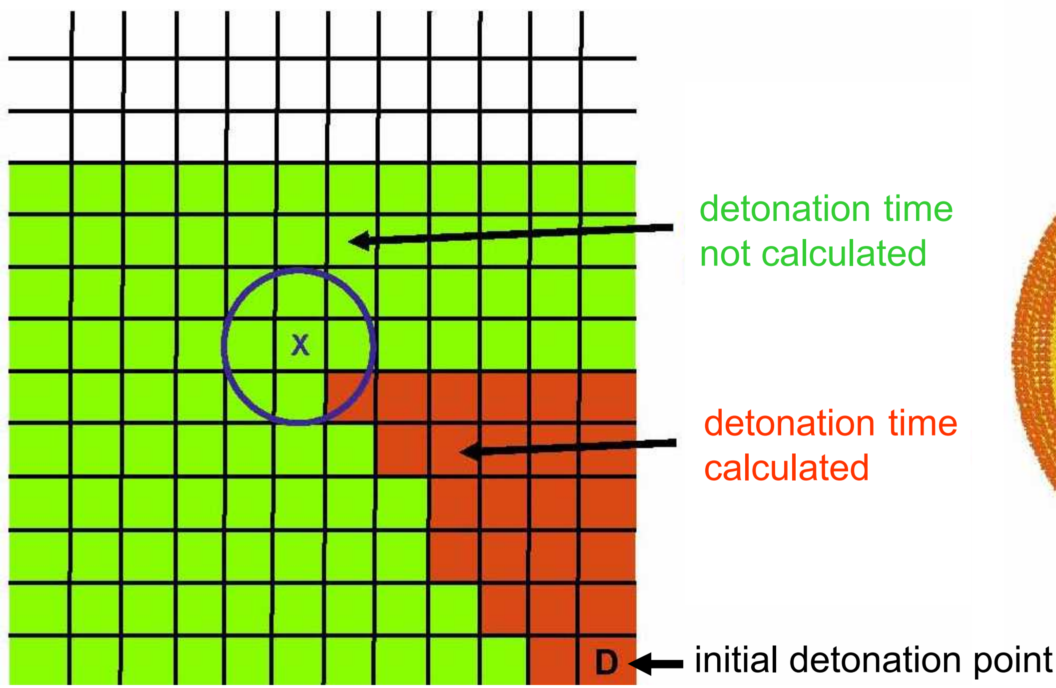
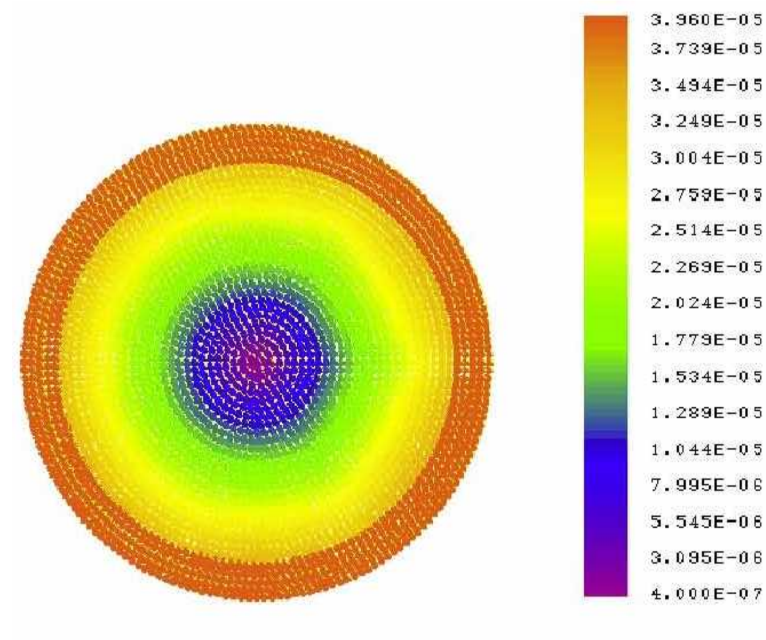
Program Burn

- **Huygen’s Construction**
- **Reliable, time-tested method used since 1950’s)**





Detonation Times

Huygen’s Construction illustrated in Two Dimensions

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Gases as Peridynamic Materials

- Since detonation products are gases, gases must be modeled as peridynamic materials.
- Consideration of the energy required to stretch a bond leads to the following *PFF* for a gas:

$$f_k = -\frac{6P}{r_k V}\left(\frac{r_k}{p_k}\right)^{m+1} X^{1+m/3}$$

where

$p = |\boldsymbol{\eta} + \boldsymbol{\xi}|$, $r = |\boldsymbol{\xi}|$, V is volume, P is pressure,

$$X = \frac{\rho_0}{\rho} = \left[\frac{1}{V}\sum_j \left(\frac{r_j}{p_j}\right)^m \Delta V_j\right]^{-3/m}, \quad V = \sum_i \Delta V_i$$

In the present version of EMU, m = 1.

ρ is the density in deformed configuration,

ρ_0 is the density in undeformed configuration

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Jones-Wilkins-Lee (JWL) Equation of State

- JWL Equation of State (EOS), pressure

$$P = \sum_i A_i \left(1 - \frac{\omega}{R_i X}\right) e^{-R_i X} + \frac{\omega E}{X}$$

energy

expansion

Remaining quantities are JWL parameters.

- Expansion Isentrope: pressure

$$P_S(X) = \sum_i A_i e^{-R_i X} + C X^{-(\omega+1)}$$

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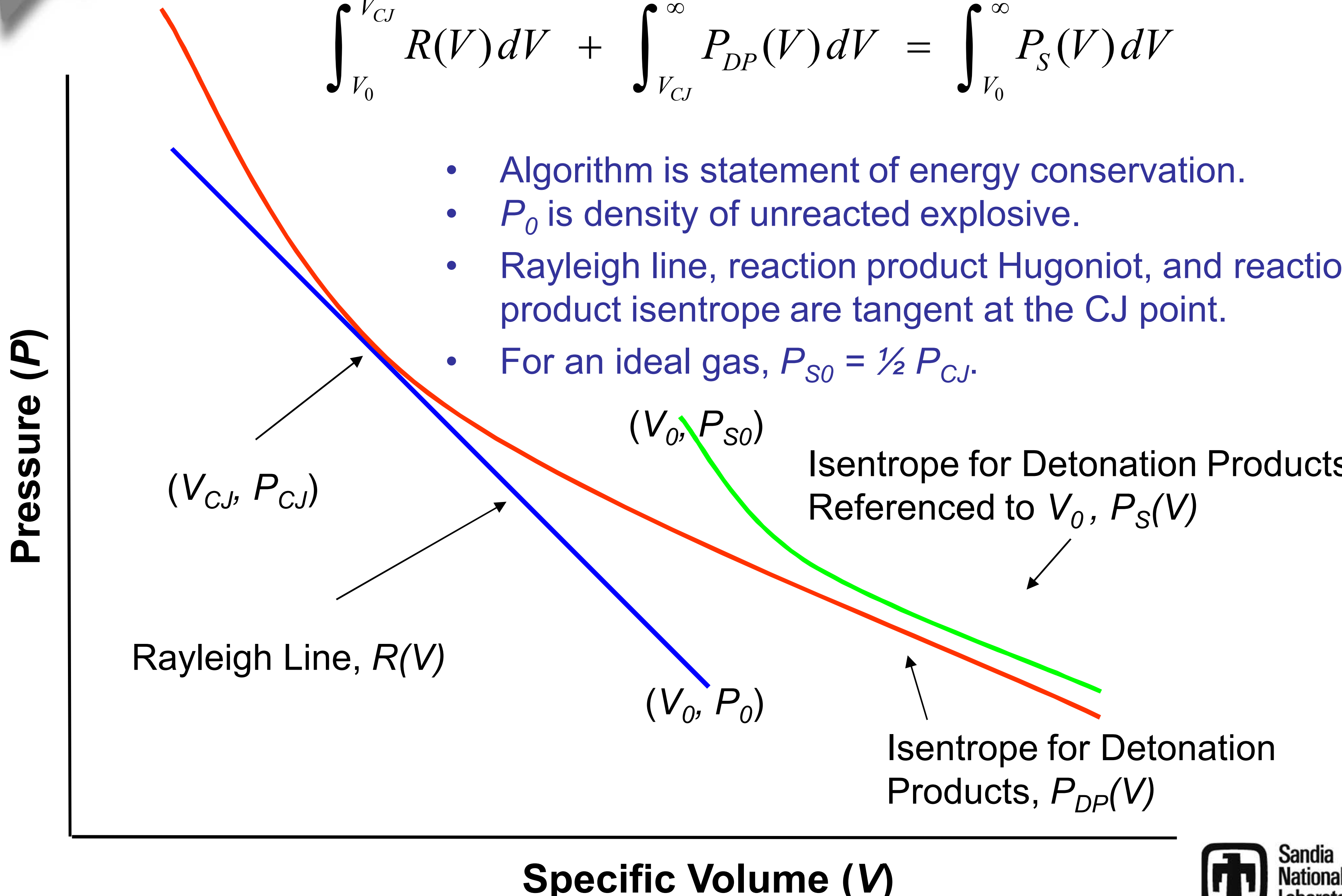
Volume Burn Algorithm

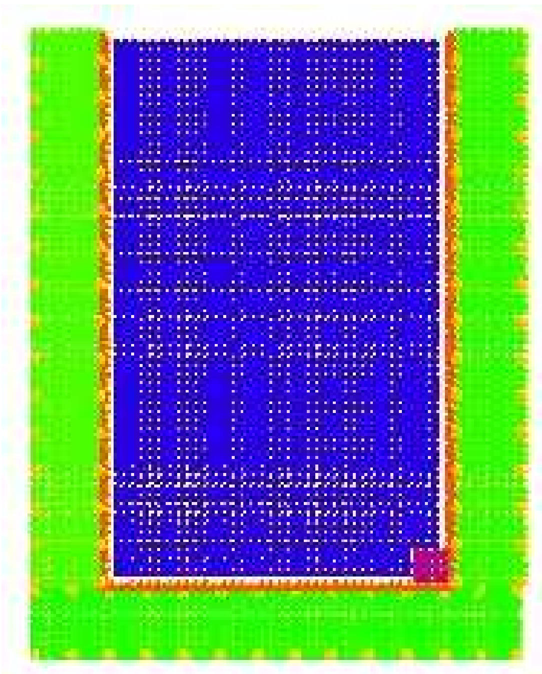
$$\int_{V_0}^{V_{CJ}} R(V)\,dV + \int_{V_{CJ}}^{\infty} P_{DP}(V)\,dV = \int_{V_0}^{\infty} P_S(V)\,dV$$

- Algorithm is statement of energy conservation.
- P_0 is density of unreacted explosive.
- Rayleigh line, reaction product Hugoniot, and reaction product isentrope are tangent at the CJ point.
- For an ideal gas, P_{S0} = ½ P_{CJ}.

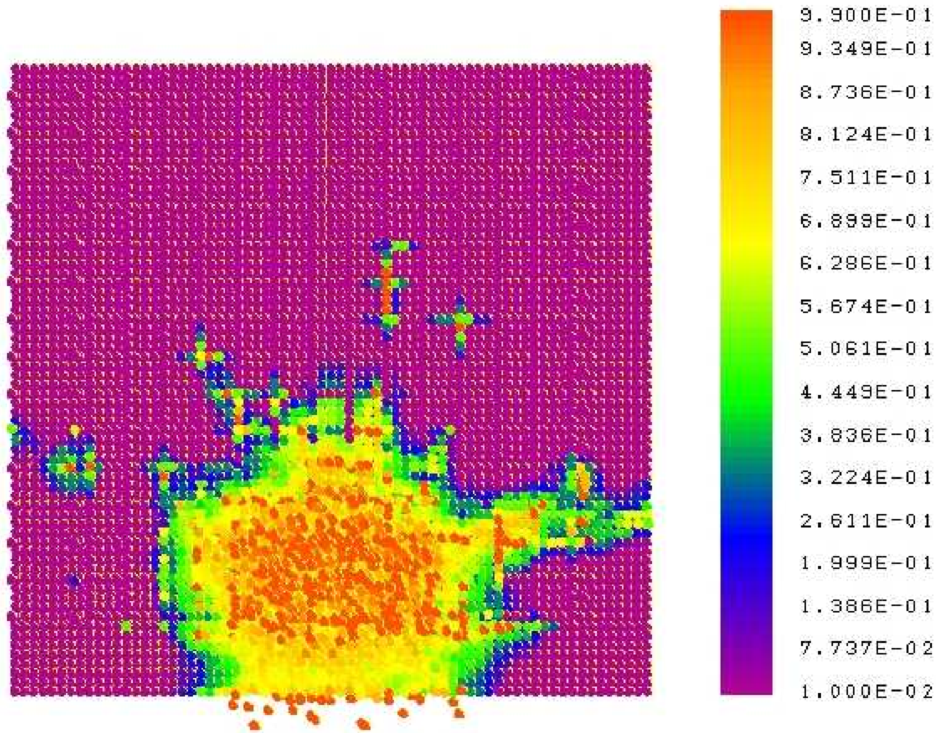


Blast Loading of a Structure

Structure has 6-ft thick walls and floor slab. The floor slab is 40 ft by 52 ft. The walls are 45 ft above the floor. All concrete is reinforced with #18 rebar at 12-in spacing. A cubic yard of explosive with unreacted density 1785 kg/m^3 and detonation speed 8747 m/s is placed on the floor at the center of the wall and detonated at time zero.



Materials



Internal Damage

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Verification and Validation (V&V) Process

- Objective of V&V Process
  - To obtain confidence in the predictive capabilities of EMU for warhead fragmentation.
- What are Verification and Validation?
- A V&V Process for Warhead Fragmentation using EMU
  - Comparison with Fragmentation Tests of an Exploding Munition (ALACV)
  - Predictions for an Exploding Cylinder
  - Sensitivity of Mass Distributions to Sound Speed and Yield Stress
  - Future V&V Work

What are Verification and Validation?

- ***Verification***: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.
  - ***Code Verification***: Activities directed toward:
    - Finding and removing mistakes in the source code
    - Finding and removing errors in numerical algorithms
    - Improving software using software quality assurance practices
  - ***Solution Verification***: Activities directed toward:
    - Assuring the accuracy of input and output data for the problem of interest
    - Estimating the numerical solution error
- ***Validation***: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

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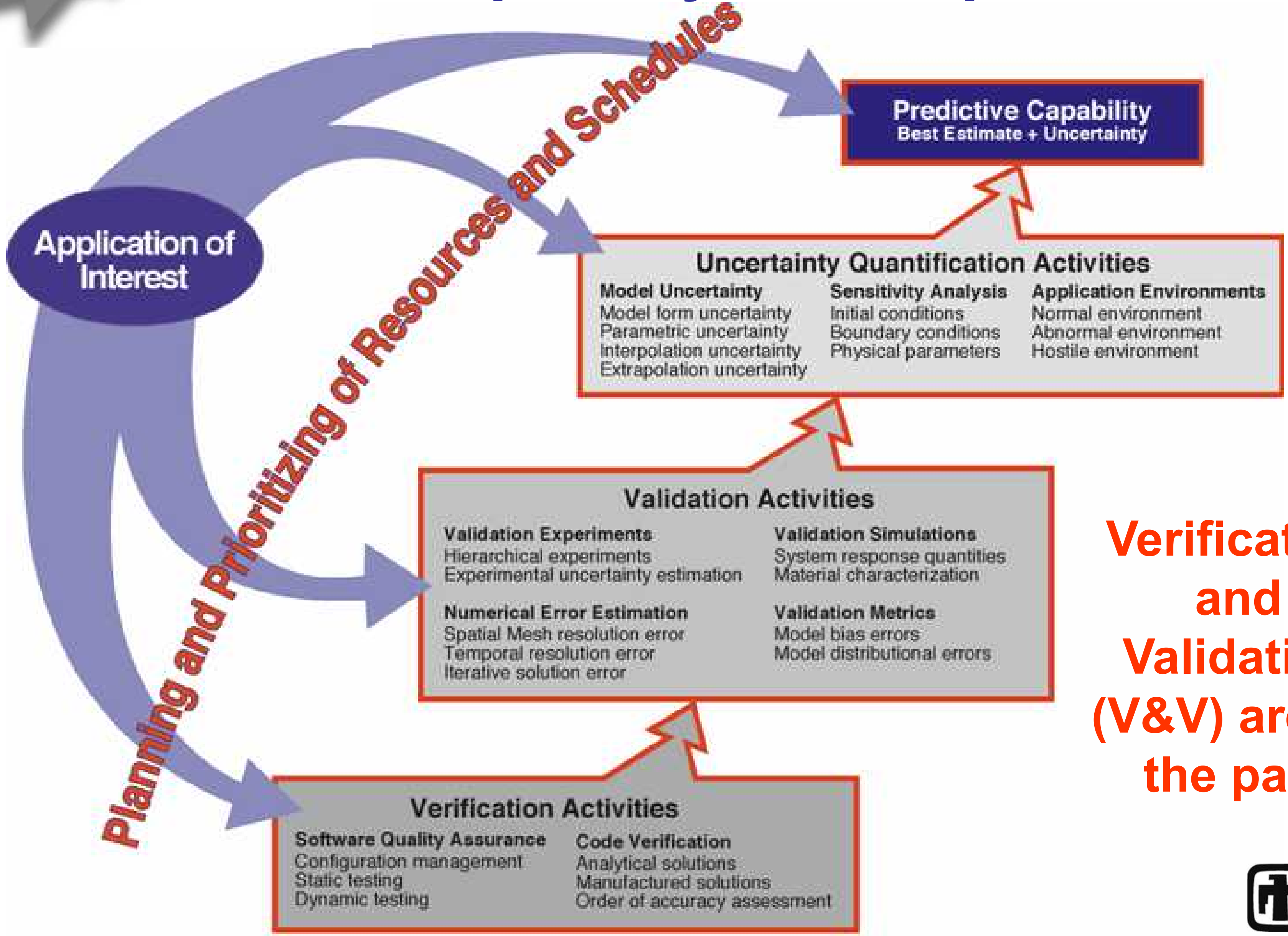
Objective: Confidence in Predictive Capability of Computer Codes



Verification and Validation (V&V) are on the path

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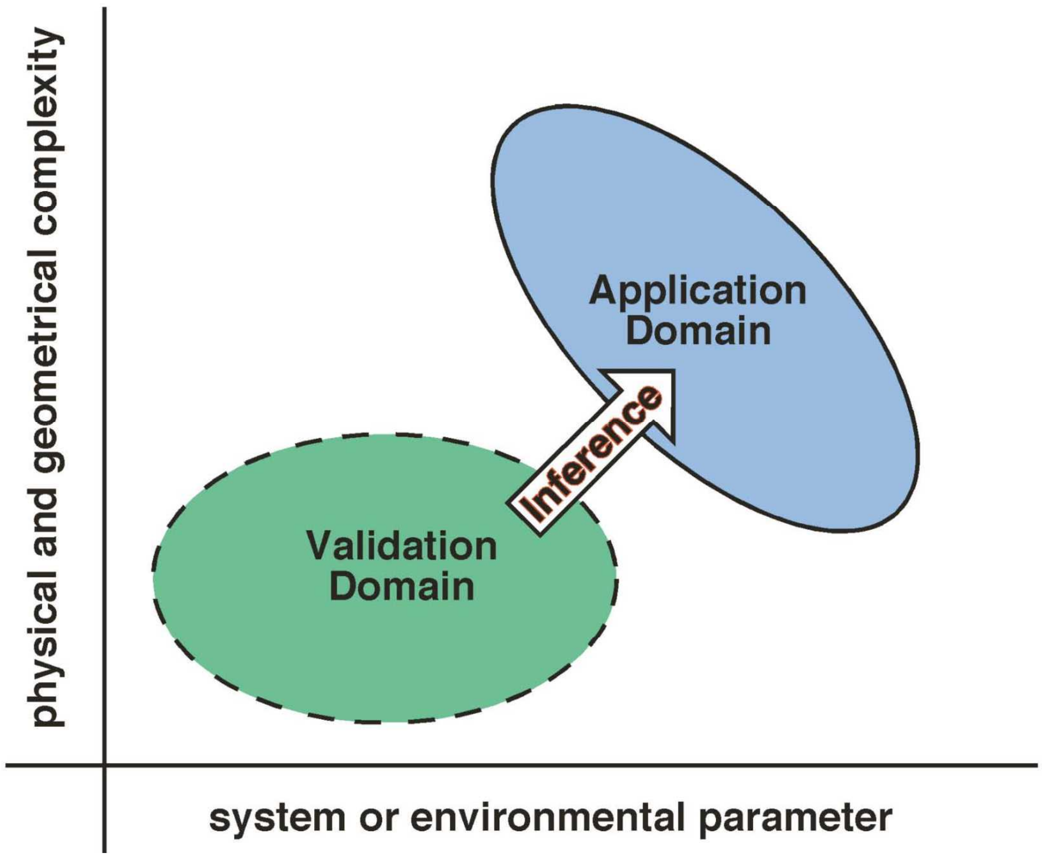
V&V Problems

1. The real world is harsh – neither verification or validation is likely to be completed given finite resources and the complexity of the problems we care about.
2. Weak inference; large extrapolation



- No overlap of application domain and validation database
- Large extrapolations typically occur in terms of meta-coordinate directions, such as:
  - Large changes in physical complexity
  - Introduction of new physics coupling
  - Introduction of coupling between subsystems or components

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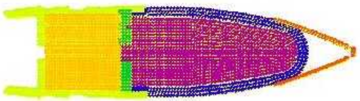
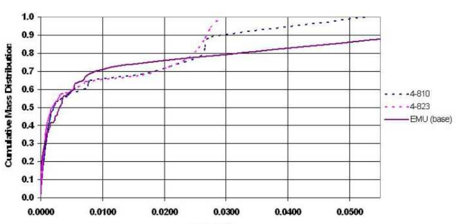
Validation Is An Iterative Process

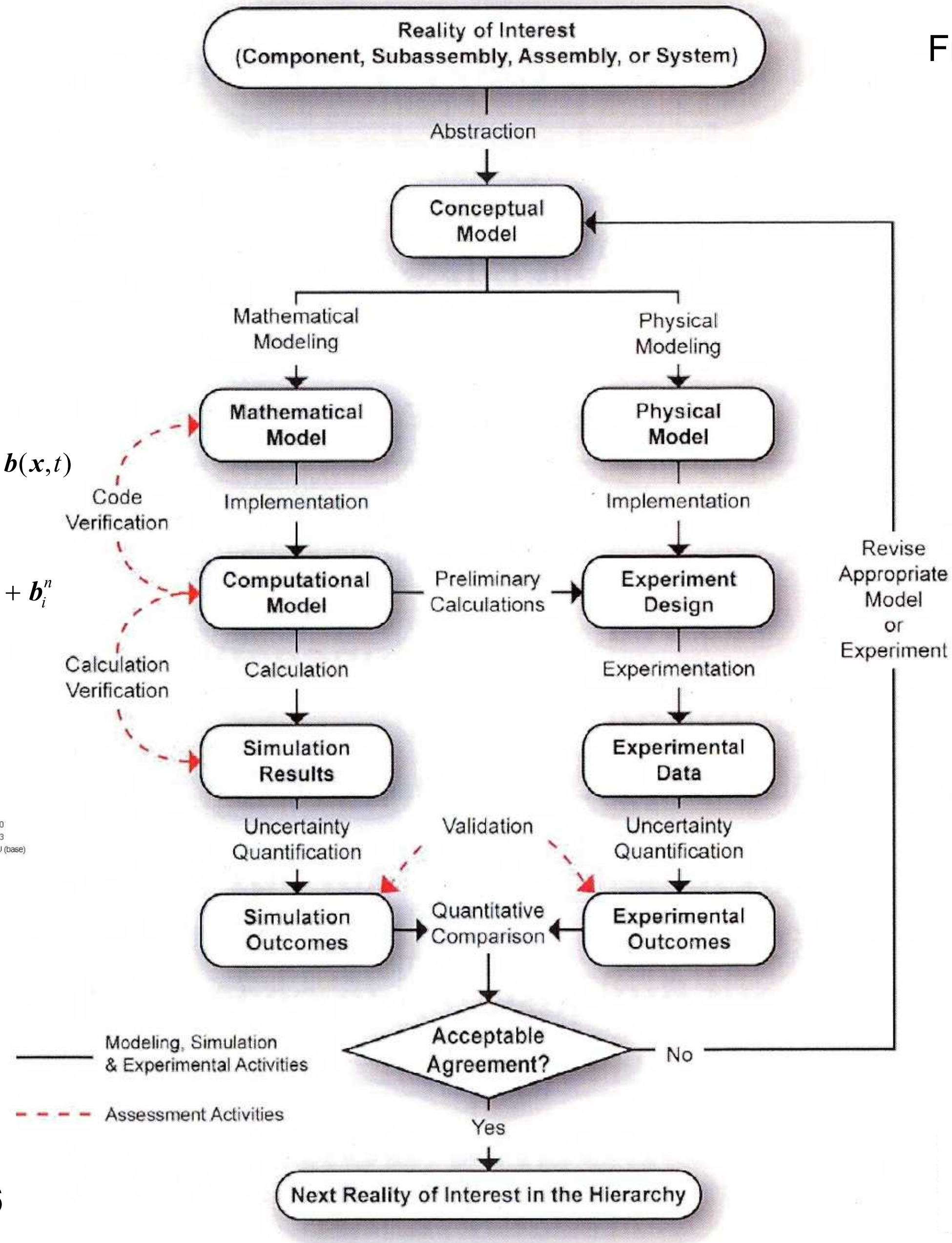
Fragmentation of Munitions

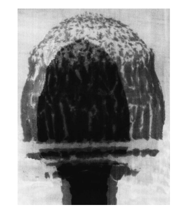


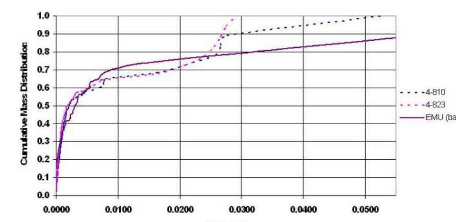
$$\rho(\mathbf{x})\frac{d^2}{dt^2}\mathbf{u}(\mathbf{x},t) = \iiint_R \mathbf{f}(\mathbf{u}(\mathbf{x}',t)-\mathbf{u}(\mathbf{x},t),\mathbf{x}'-\mathbf{x})\,dV' + \mathbf{b}(\mathbf{x},t)$$

$$\rho_i \frac{d^2}{dt^2}\mathbf{u}_i^n = \sum_p \mathbf{f}(\mathbf{u}_p^n-\mathbf{u}_i^n, \mathbf{x}_p-\mathbf{x}_i)V_p + \mathbf{b}_i^n$$









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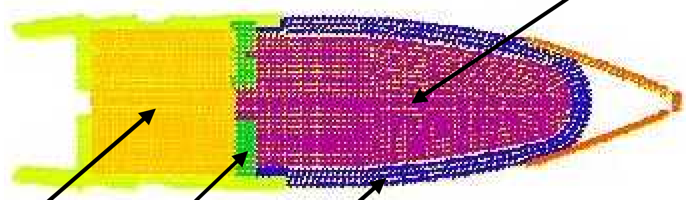
Fragmentation of Exploding Munitions

Explosive Shell

EMU Model

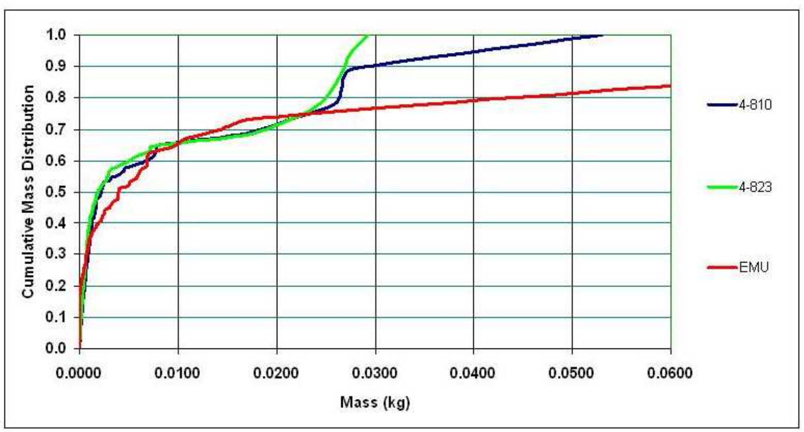


explosive

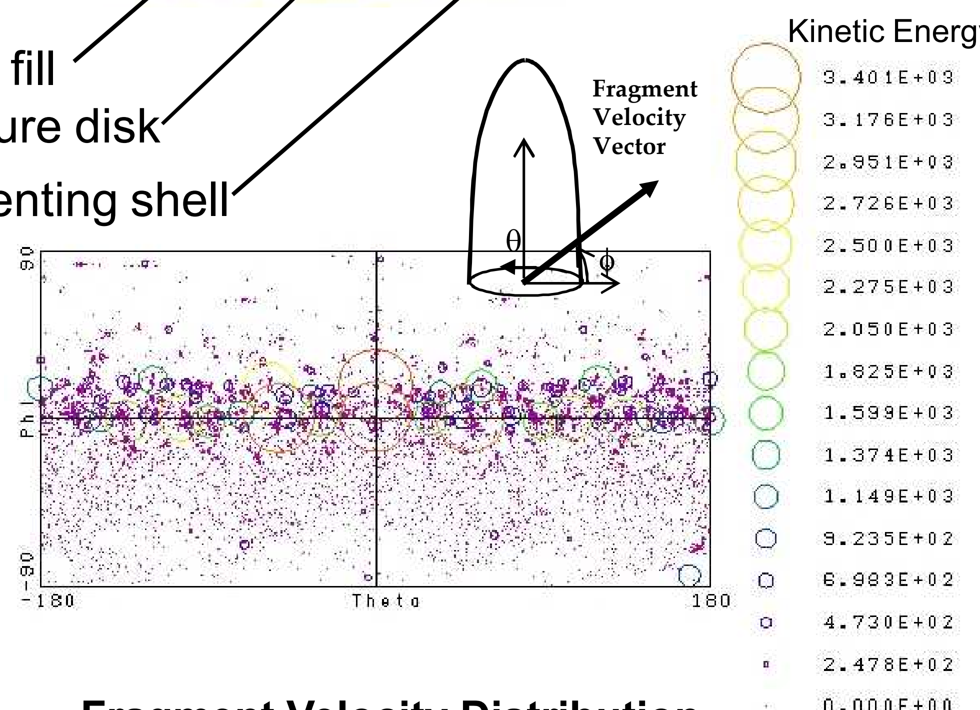
aluminum fill

steel closure disk

steel fragmenting shell



Cumulative Mass Distribution



Fragment Velocity Distribution

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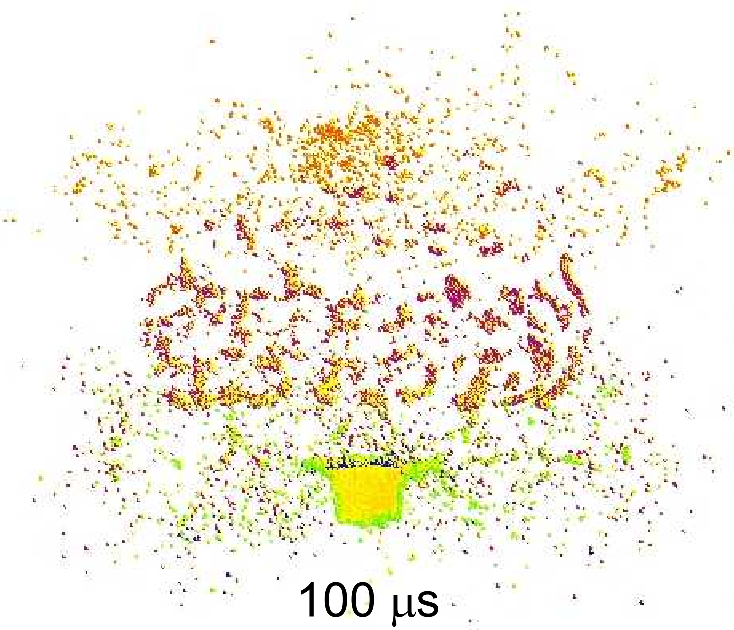
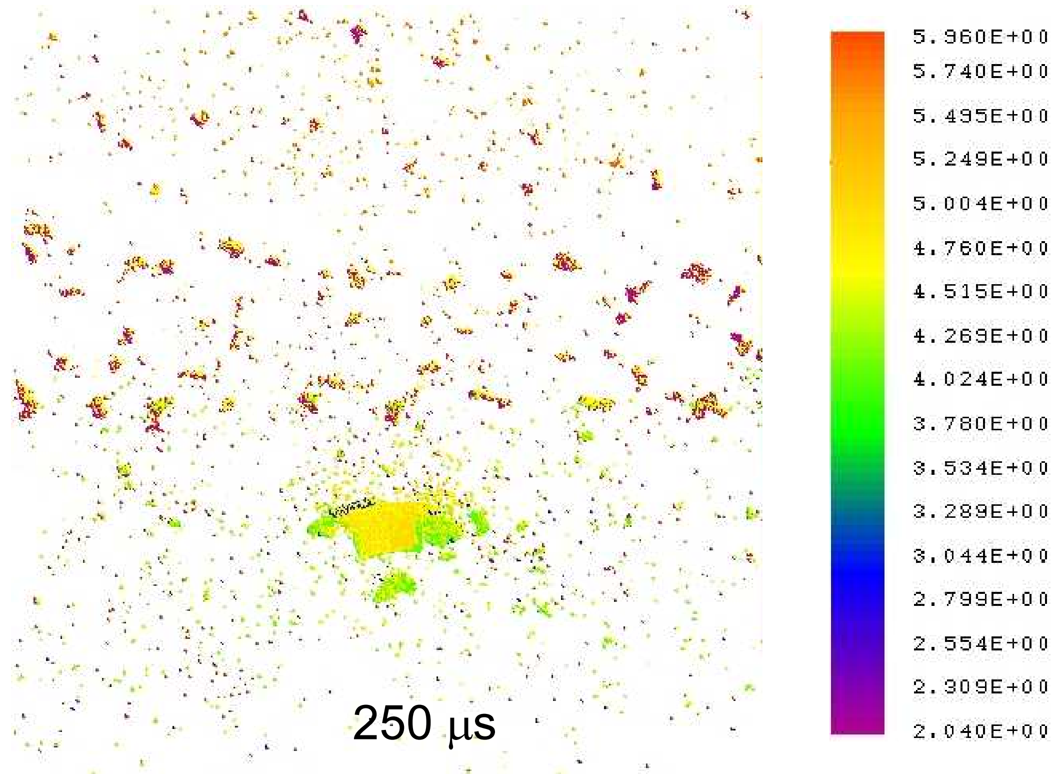
Material States During Simulation

45.7 μs



100 μs



250 μs

Comparisons with Radiographic Data

Test

27.6 μs

45.2 μs

Simulation Results

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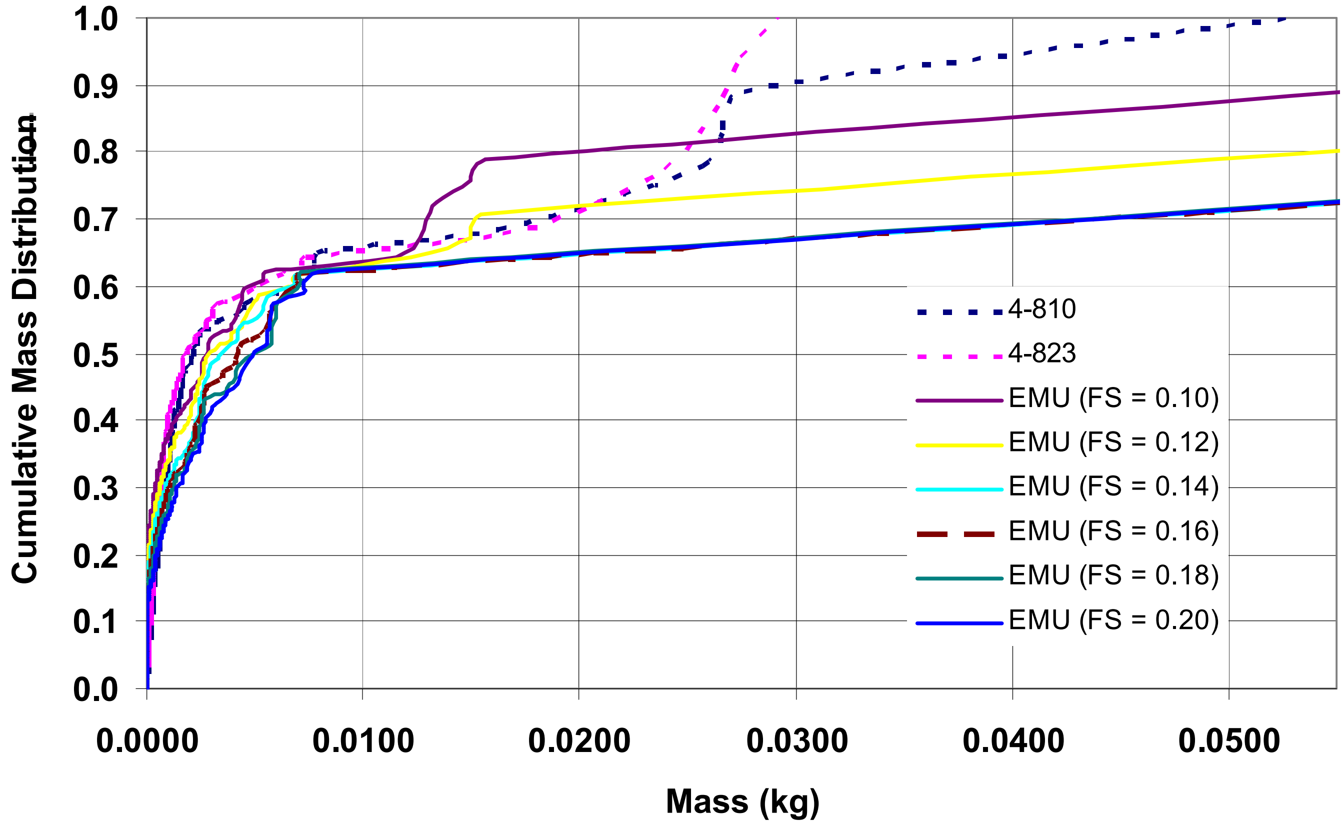
Sensitivity to Failure Stretch

- **Compare data for tests with simulation results with failure stretch varying from 0.10 to 0.20 to show importance of characterizing material properties.**



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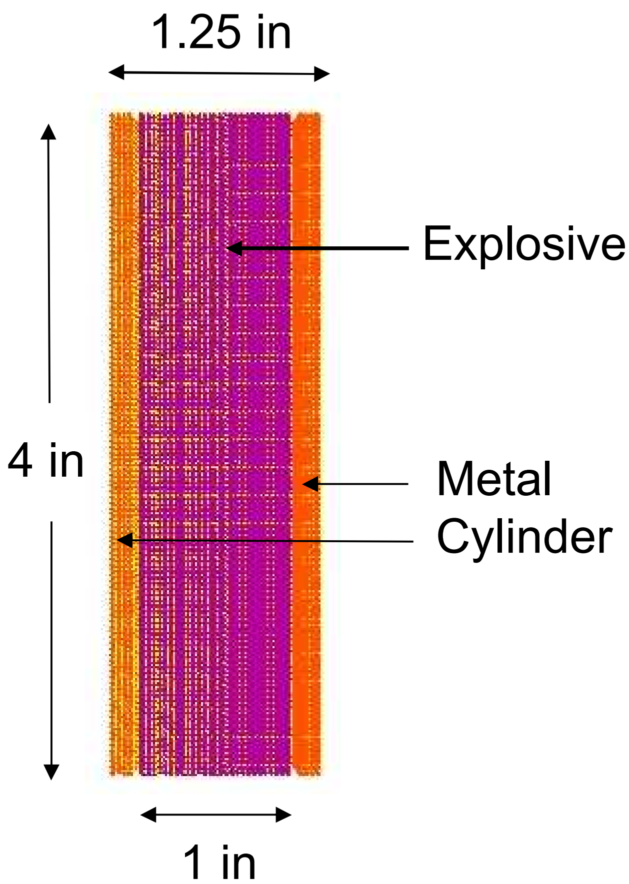
Validation Tests – Exploding Cylinders



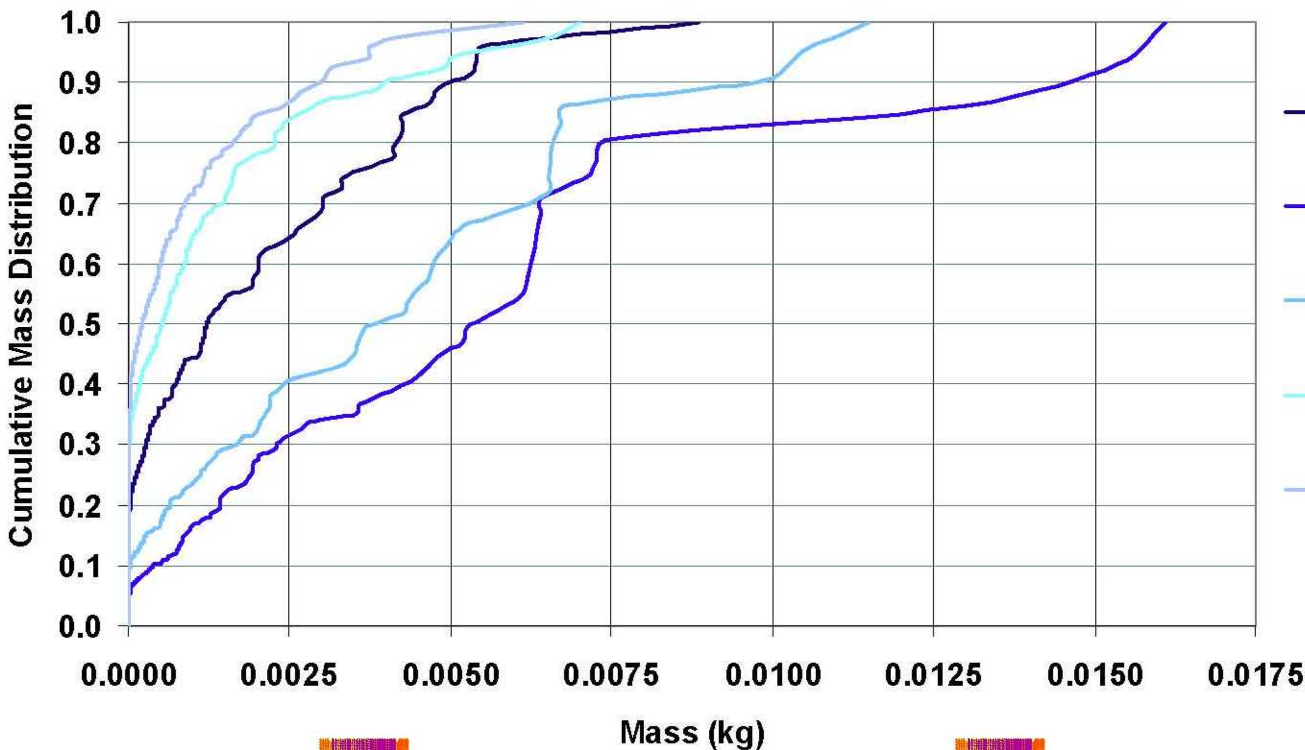
Cross Section of Cylinder
Filled with explosive

Test Configurations Simulated

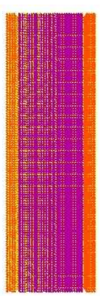
Material	Treatment	Explosive Loading	Mass of Cylinders (g)
4340	HT1	PBXN-9	239.9
4340	HT2	PBXN-9	238.18
4340	HT3	PBXN-9	239.93
1018	None	TNT	250.55
1018	None	PBXN-9	238.61

HT1	Currently unspecified from LLNL
HT2	870 C for 2 hours Oil Quench, 325 C 2 hours Oil Quench
HT3	870 C for 2 hours Oil Quench, 450 C 2 hours Oil Quench

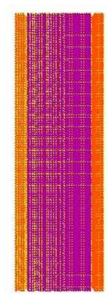
Predicted Cumulative Mass Distributions



	Fragment Mass maximum	Fragment Mass average
4340 HT1 PBXN-9	(8.86 g)	(25.6 mg)
4348 HT2 PBXN-9	(16.1 g)	(92.4 mg)
4340 HT3 PBXN-9	(11.5 g)	(52.3 mg)
1018 TNT	(7.04 g)	(17.1 mg)
1018 PBXN-9	(6.16 g)	(14.5 mg)



Test



EMU Simulation

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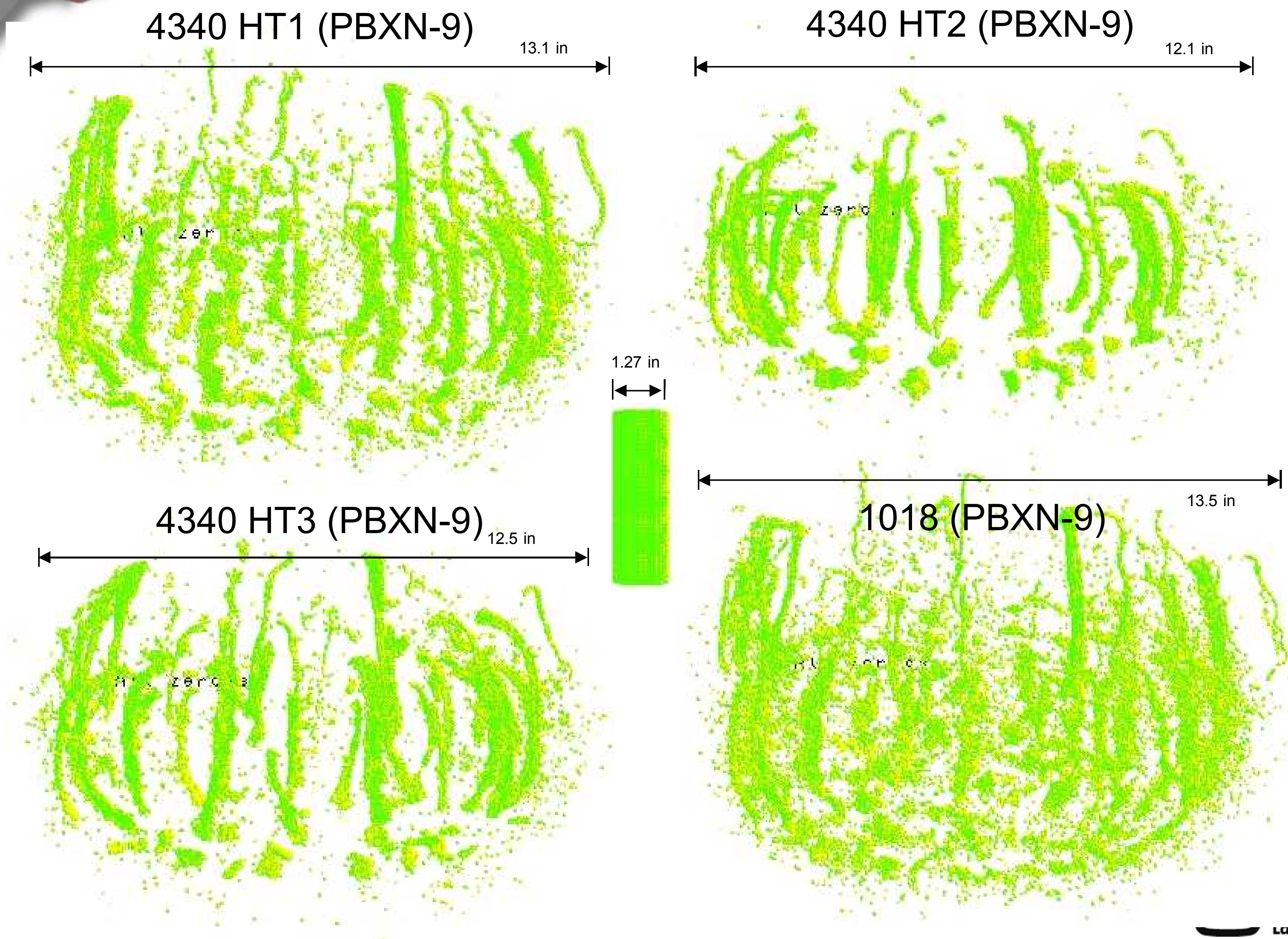
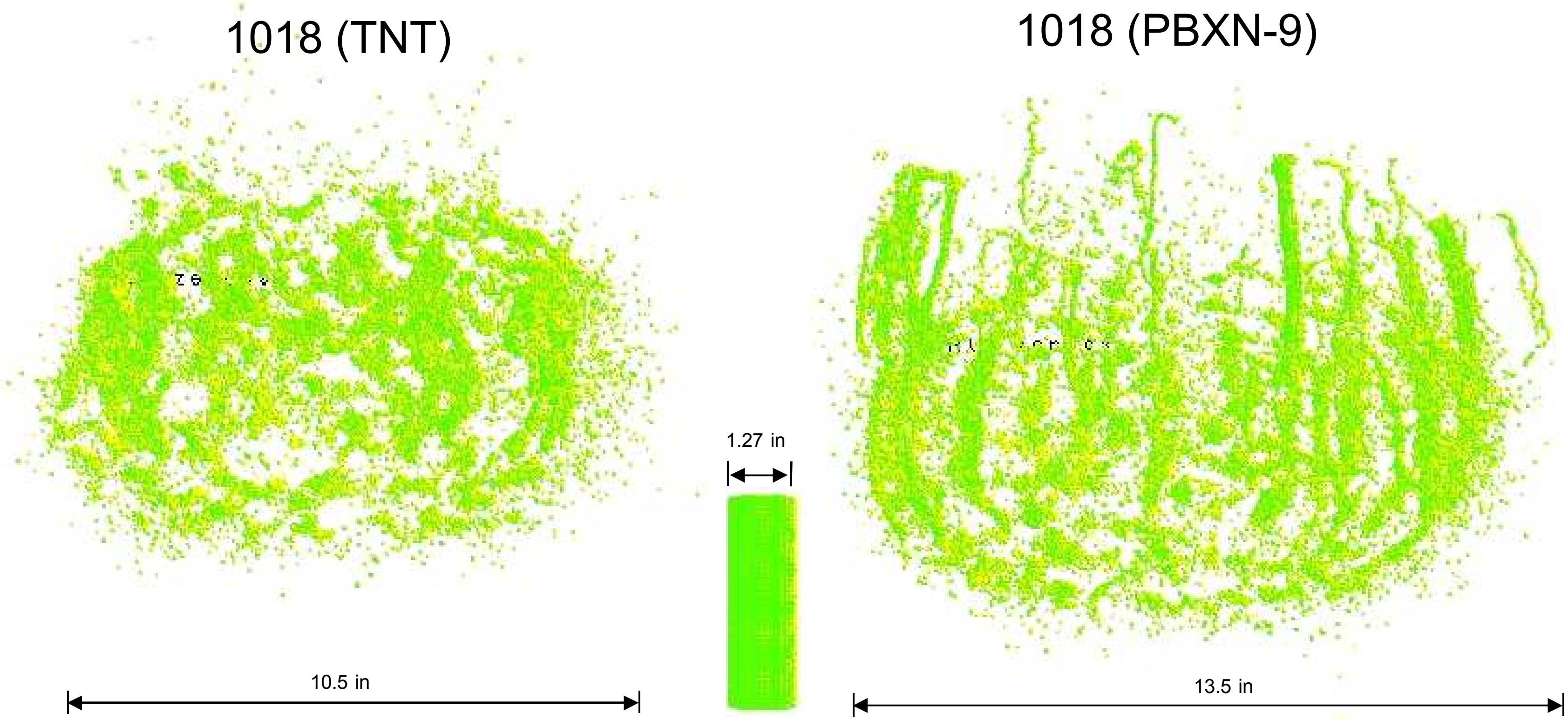
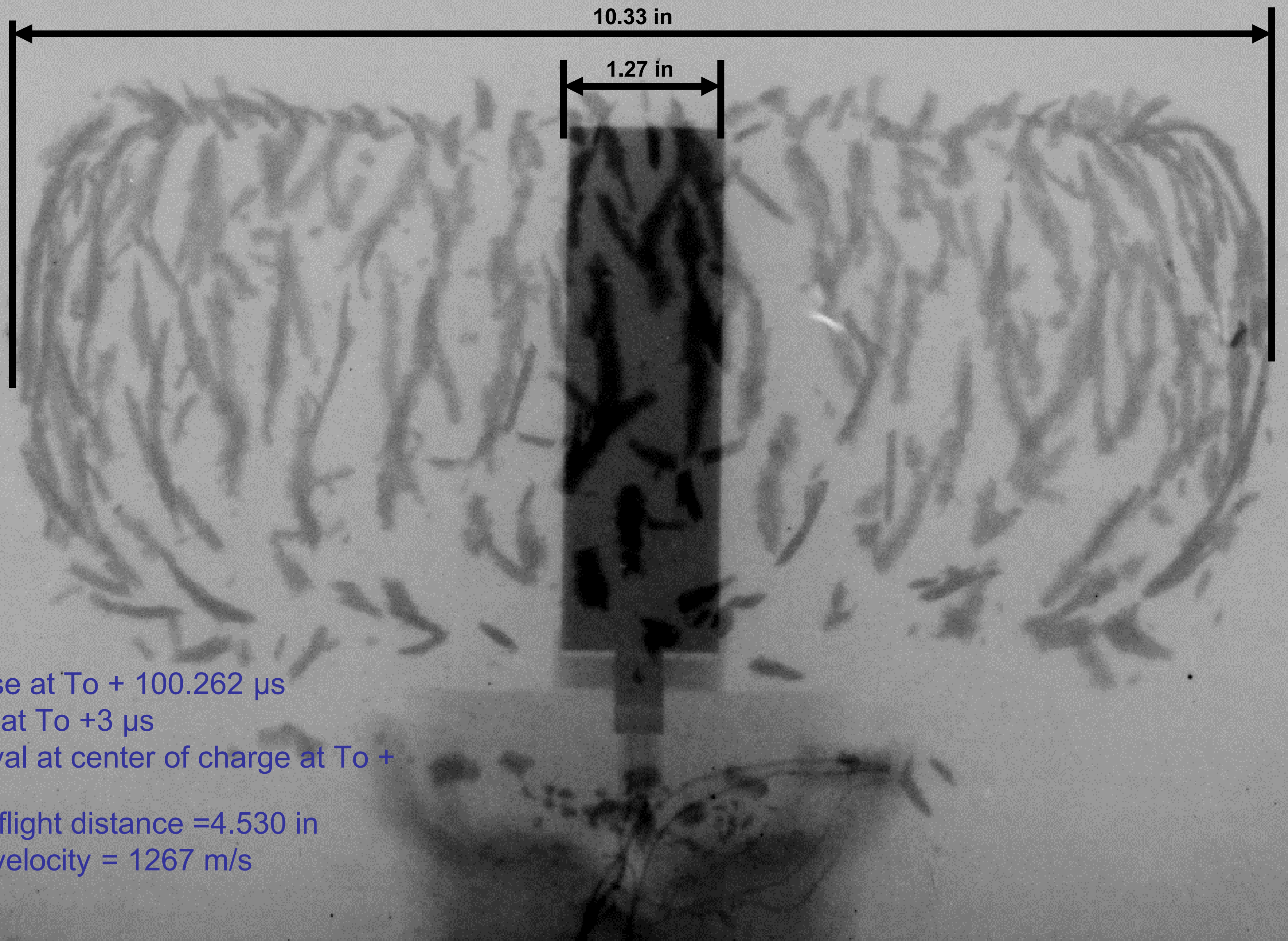
Predicted Fragment Locations (100 μs)



Predicted Fragment Locations (100 μs)

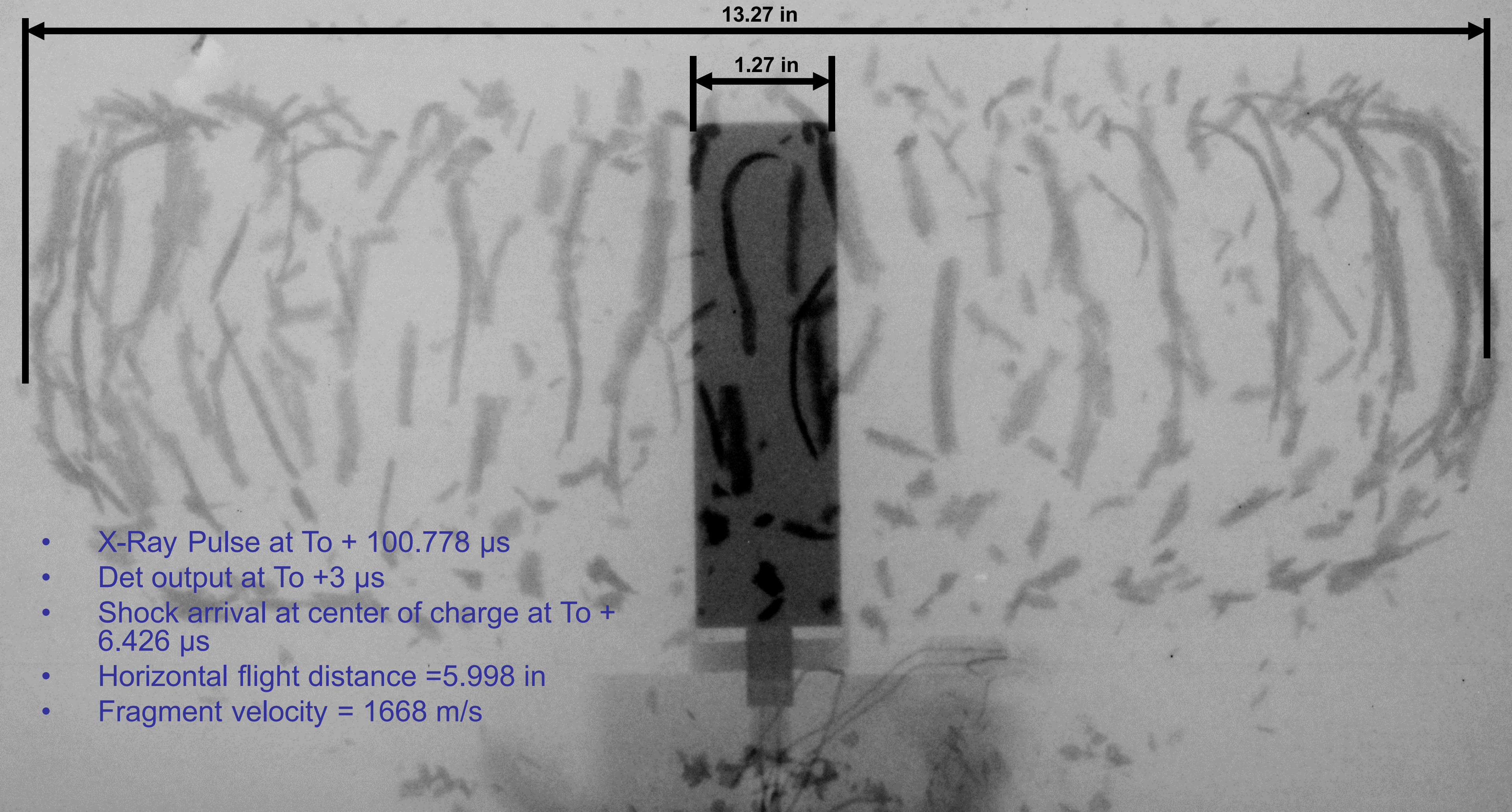


Explosive Testing TNT w/ 1018 Steel



- X-Ray Pulse at To + 100.262 μs
- Det output at To +3 μs
- Shock arrival at center of charge at To + 6.426 μs
- Horizontal flight distance =4.530 in
- Fragment velocity = 1267 m/s

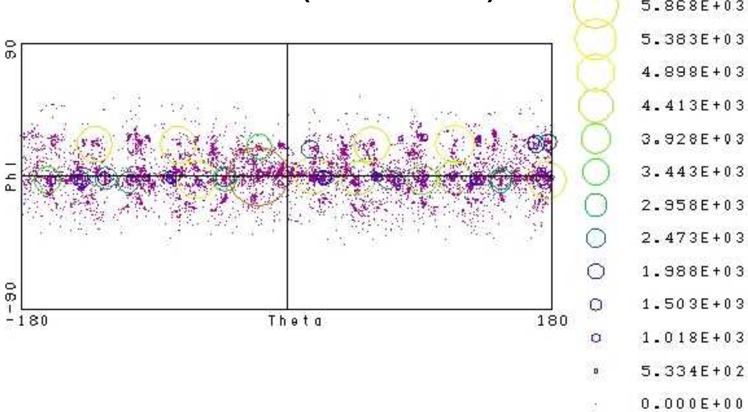
Explosive Testing PBXN-9 w/ 4340 Steel



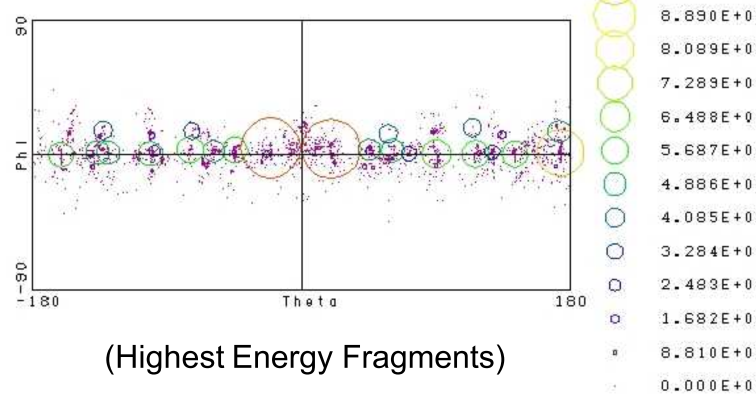
- X-Ray Pulse at To + 100.778 µs
- Det output at To +3 µs
- Shock arrival at center of charge at To + 6.426 µs
- Horizontal flight distance =5.998 in
- Fragment velocity = 1668 m/s

Predicted Velocity Distributions (100 μs)

4340 HT1 (PBXN-9)

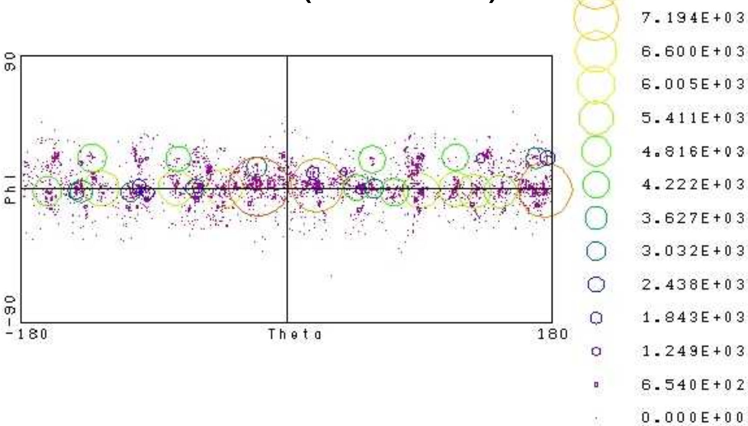


4340 HT2 (PBXN-9)

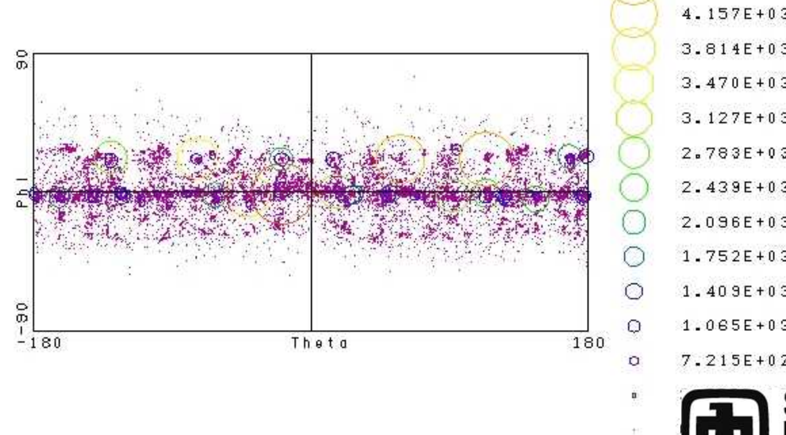


(Highest Energy Fragments)

4340 HT3 (PBXN-9)



1018 (PBXN-9)



Legends are kinetic energy in joules.

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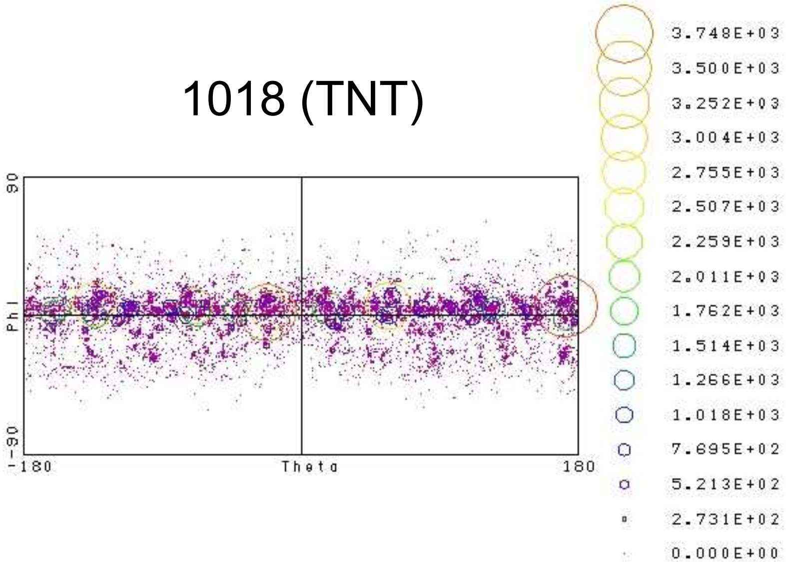
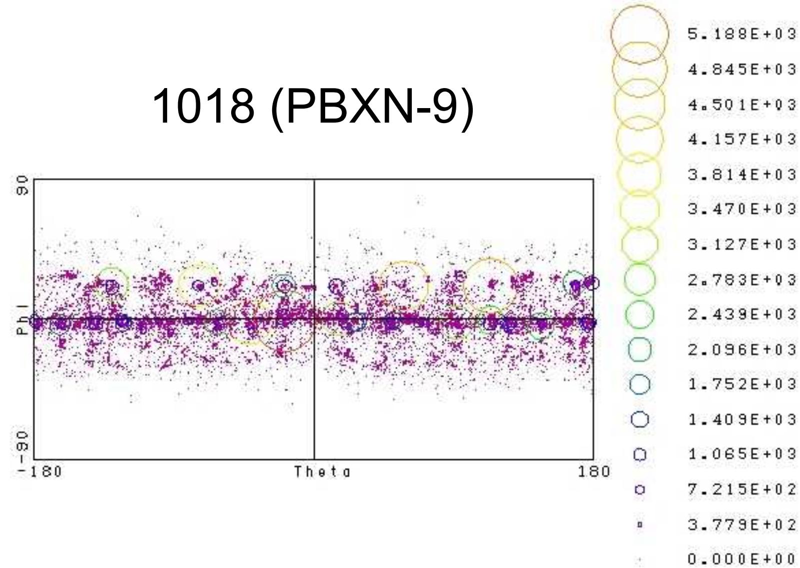
Predicted Velocity Distributions (100 μs)

1018 (TNT)



1018 (PBXN-9)



KE

Legends are kinetic energy in joules.

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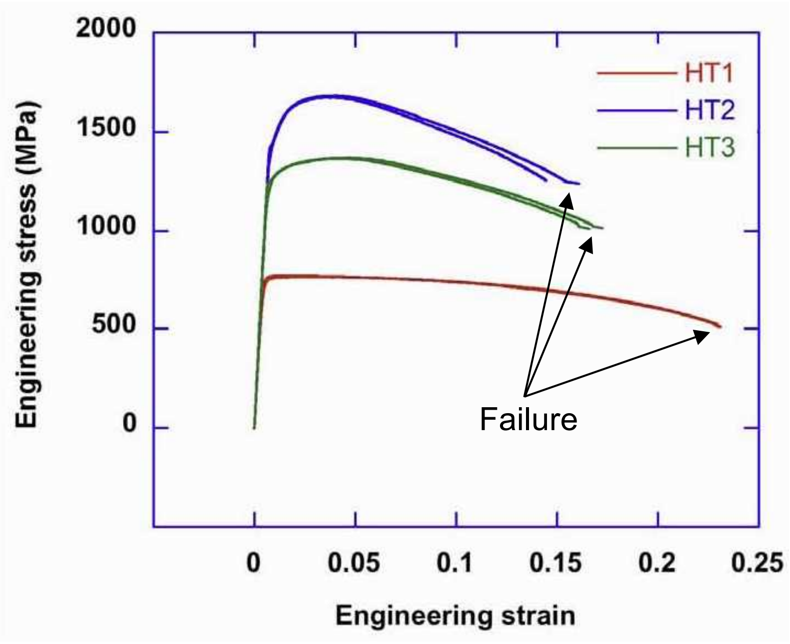
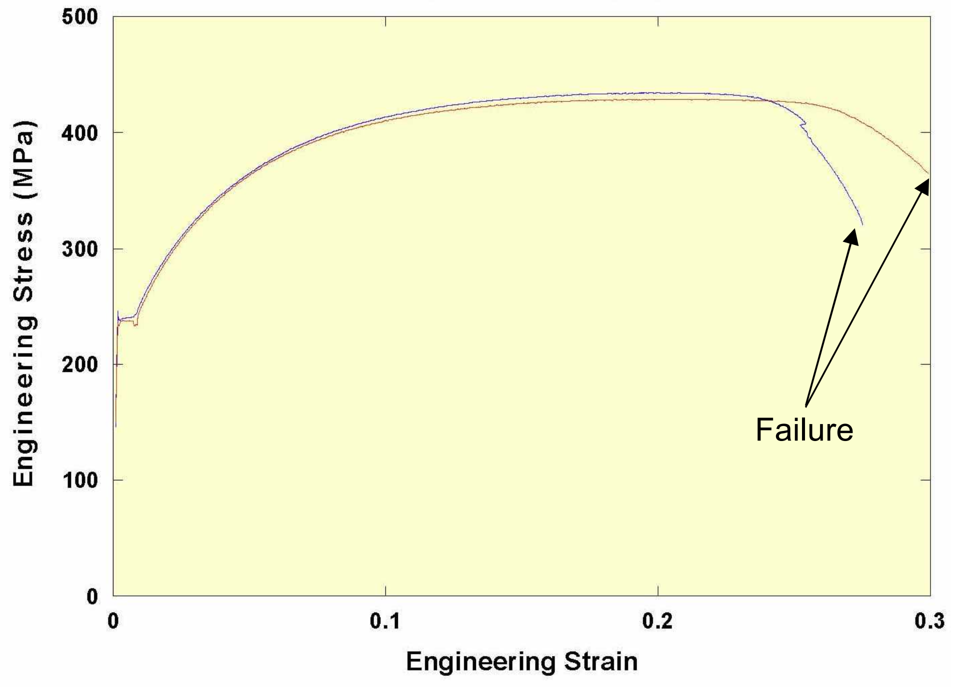
Examples of Stress-Strain Data

Stress Versus Strain for 4340 Steel



Stress Versus Strain for 1018 Steel



What is yield stress from these figures?

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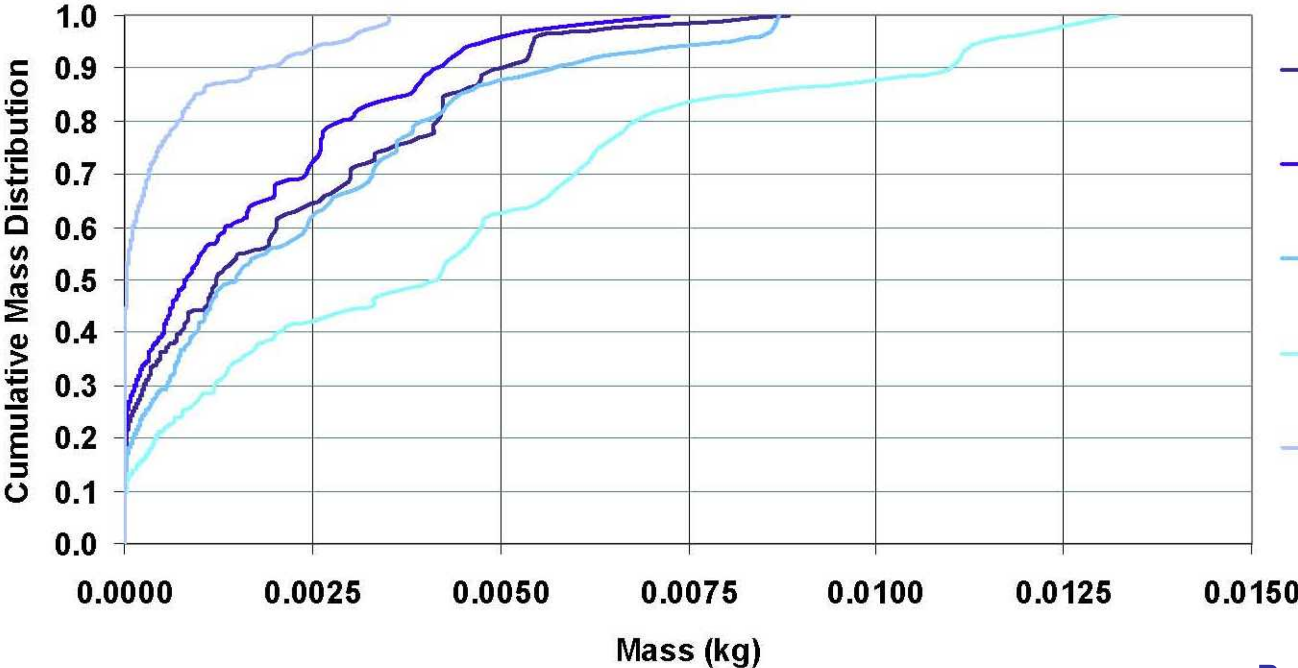
Sensitivity of Mass Distributions to Sound Speed and Yield Stress



Fragment Mass

	maximum	average
4340 HT1 PBXN-9	(8.86 g)	(25.6 mg)
Increased Sound Speed	(7.26 g)	(21.7 mg)
Decreased Sound Speed	(8.70 g)	(33.3 mg)
Increased Yield Stress	(13.2 g)	(47.4 mg)
Decreased Yield Stress	(3.52g)	(10.3 mg)

- **Base case (4340 steel with HT1)**
  - **Sound Speed is 4228 m/s.**
  - **Yield Stress is 750 MPa.**
- **Sound Speed Sensitivity is ± 35%.**
- **Yield Stress Sensitivity is ± 50%.**

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Conclusions from Sensitivity Simulations

- **Purpose**
  - To determine effects on fragmentation of uncertainty in micro-plastic inputs sound speed and yield stress
    - Necessary since material property data is not "text book perfect".
- **Sound Speed** $= \sqrt{(bulk\ modulus)/density}$
  - Average fragment mass decreases and number of fragments increases with increasing sound speed
    - Sound speed varies directly with square root of bulk modulus.
    - Sound speed varies inversely with square root of density.
- **Yield Stress**
  - Average fragment mass increases and number of fragments decrease with increasing yield stress.

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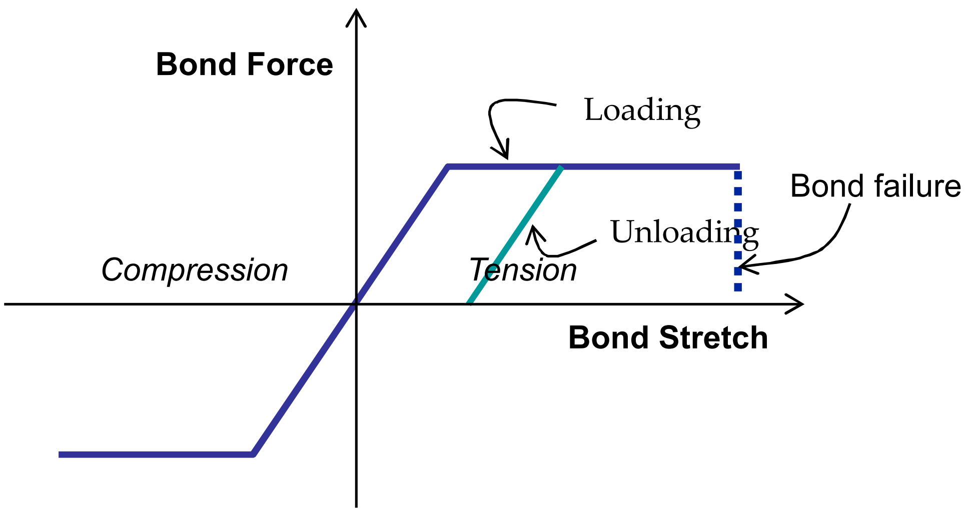
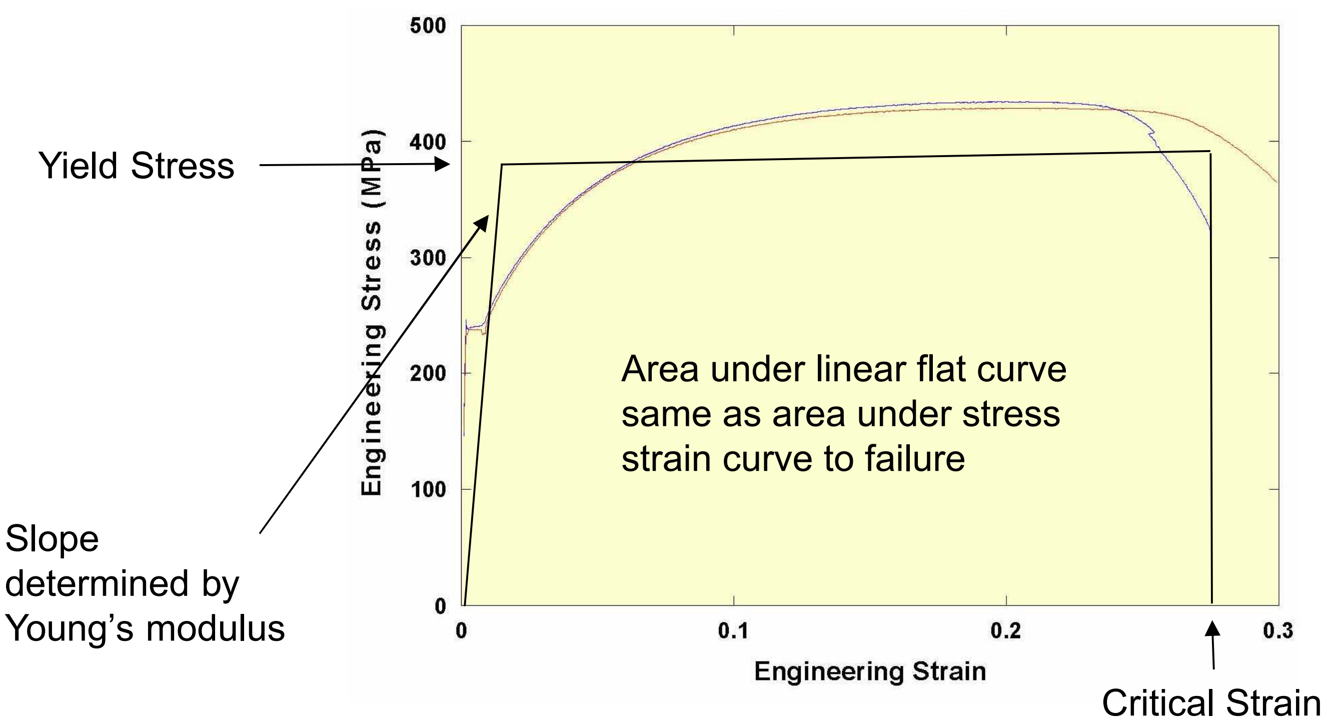
Estimating Yield Stress for Linear Flat MP





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Future Verification and Validation Work

- Perform experiments for validation process.
- Continue V&V iterative process.
- Document V&V process.
- Transfer the EMU fragmentation modeling capability to the military labs.

Peridynamics Research and Development

- Current R&D includes
  - modeling fluids, composite materials, and explosive materials and explosive loading
  - verification and validation
  - modeling shock loading, using adaptive grids and general Poisson ratio
  - software engineering
  - state-based peridynamics
  - nanoscale to continuum coupling
- Future R&D possibilities include
  - peridynamics, finite-element coupling
  - inclusion of additional physical processes to provide a comprehensive methodology for vulnerability assessment of critical structures

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Collaborators and Sponsors

Collaborators

- Stewart Silling (Sandia)
- Paul Taylor (Sandia)
- Bob Cole (Sandia)
- Abe Askari (Boeing)
- Olaf Weckner (MIT, Boeing)
- Mike Epton (Boeing)
- Jifeng Xu (Boeing)
- John Haws (Boeing)
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- Markus Zimmermann (MIT)
- Florin Bobaru (Univ. of Nebraska)
- Simon Kahan (Cray Inc.)
- Walter Gerstle (Univ. of New Mexico)
- Thomas Warren (TLW)

Sponsors

- Joint DOE/DoD Munitions Technology Program
- The Boeing Company
- Nuclear Regulatory Commission (NRC)
- Defense Threat Reduction Agency (DTRA)
- DOE Defense Programs
  - Computer Science Research Foundation
  - Computer Science Research Institute

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References

- URL for EMU at Sandia National Laboratories: http://www.sandia.gov/emu/emu.htm
- Reference on gas and explosive model: Demmie and Silling, "An Approach to Modeling Extreme Loading of Structures using Peridynamics", Published in *Journal of Mechanics of Materials and Structures (JoMMS)*, vol. 2, issue 10, p. 1921 (2007)
- Google on "peridynamic" or access Wikipedia at http://en.wikipedia.org/wiki/Peridynamics to get more information.

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