SAND2007-1669C

Verification and Validation of Fragmentation Modeling with Peridynamics

Presentation for TCG IV Meeting
March 13, 2007

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Purpose and Objectives of Our Work

1) Determine if a particle code such as EMU, that has been used for other fragmentation-fracturing problems, can be successfully adapted for predicting the fragment sizes and velocities in fragmenting munitions.
2) Combine Interior Ballistics and Launch Code with EMU to provide an integrated capability.
3) Transfer the gun launched munition modeling capability to the military labs.

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Outline of Presentation

- What is Peridynamic Theory?
- The Fundamental Peridynamics Equation
- Gases as Peridynamic Materials
- JWL Equation of State
- EMU Detonation Model
- Fragmentation of Exploding Munitions (ALACV)
- Confidence in Predictive Capability of Computer Code
- What are Verification and Validation (V&V)?
- Current and Future Work

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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 48 (2000) 175–209

JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS

Reformulation of elasticity theory for discontinuities and long-range forces

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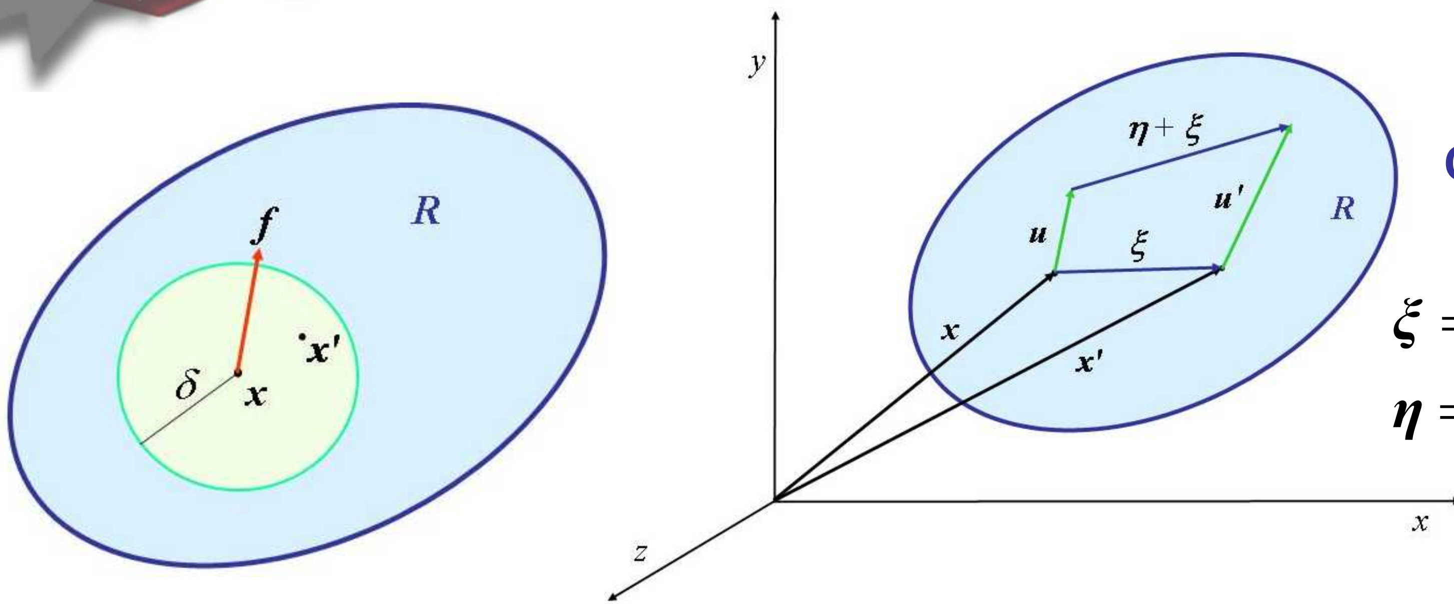
Received 2 October 1998; received in revised form 2 April 1999

Fundamental Peridynamics Equation



Configuration Variables

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

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

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

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.

Micro-Elastic Materials

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

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

- 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 stretch***.
- Isotropic, proportional ME materials have

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

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Damage

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

$$D(x,t) = V_d(x,t)/V_0(x)$$

The EMU Computer Code

- **Peridynamics 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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Gases as Peridynamic Materials

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

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

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

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

ρ is the density in deformed configuration,

ρ_0 is the density in undeformed configuration

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Comments on Peridynamic Gas Model

- This expression for the *PFF* of a gas applies to any gas.
- There are many ways to approximate the expansion, X.
- In the present version of EMU, $m = 1$.
  - We have not investigated the consequences of using a different value or an alternate formulation.
  - The purpose of including $m \neq 1$ is to allow for the possibility that bonds of different length could sustain different forces even if the deformation is an isotropic expansion. This form can be helpful, for example, in preventing nodes in a numerical grid from getting so close to each other that they overlap.

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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**

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

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EMU Detonation Model

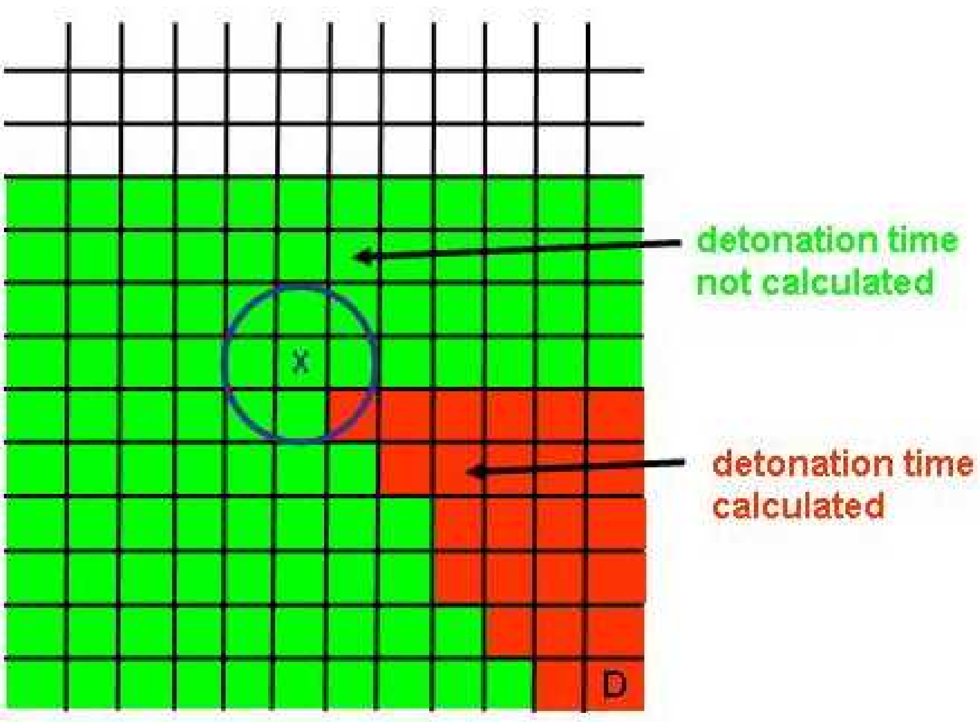
(funded by Joint DOE/DOD Munitions Technology Program)

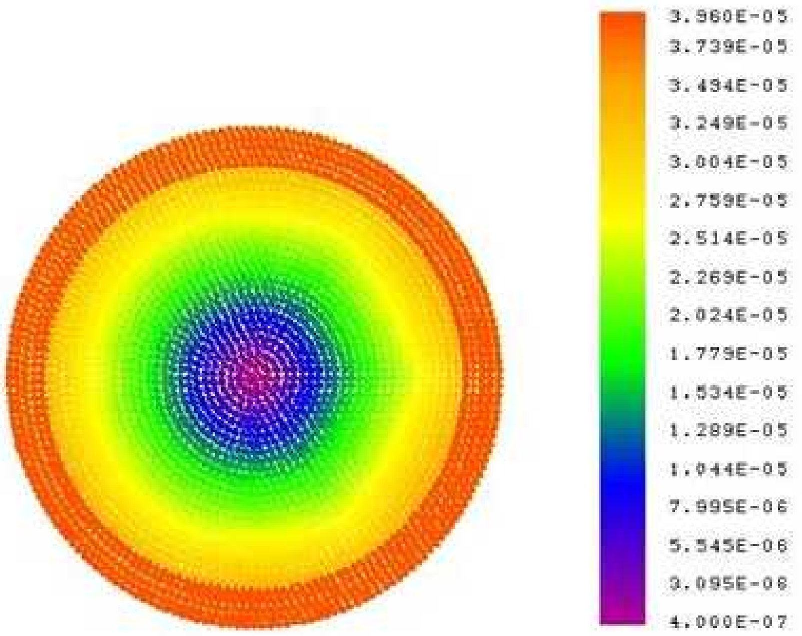
$$(x_{det}, y_{det}, z_{det}, t_{det}), \rho_{unreacted}, v_{det}$$

- **Detonation model inputs:**
  - Location of detonation point and time of initial detonation, density of unreacted explosive, and detonation speed are specified.
  - Inputs for ideal gas or JWL equation of state (EOS) parameters are specified.
- **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 an ideal gas or JWL gas undergoing an adiabatic expansion (volume burn).

Program Burn

- Reliable, time-tested method (since 1950's)
- Huygen's Construction (in two dimensions)





Detonation Times

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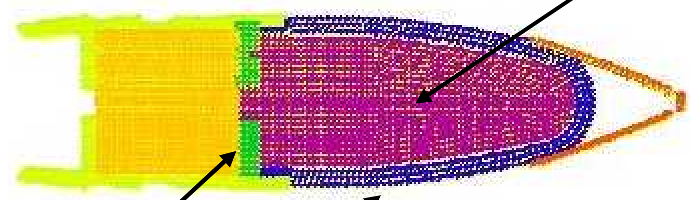
Fragmentation of Exploding Munitions (ALACV)

ALACV

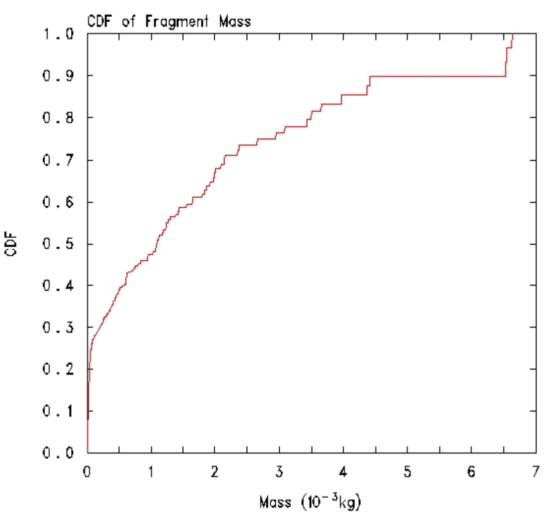
EMU Model



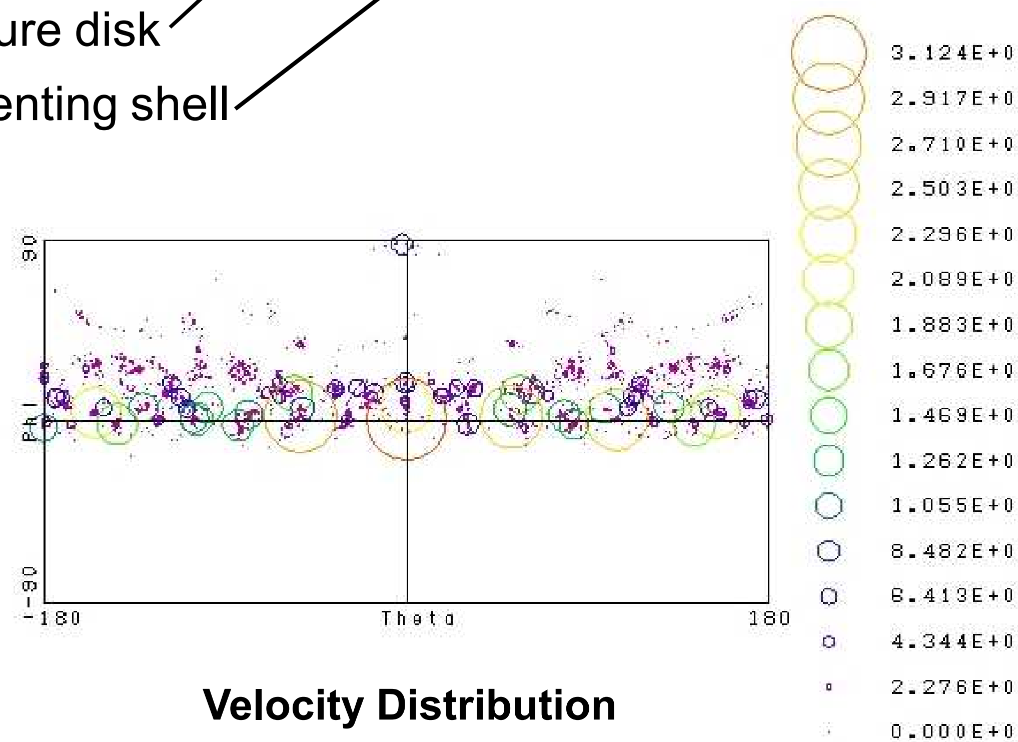
explosive

steel closure disk

steel fragmenting shell



Cumulative Distribution Functions

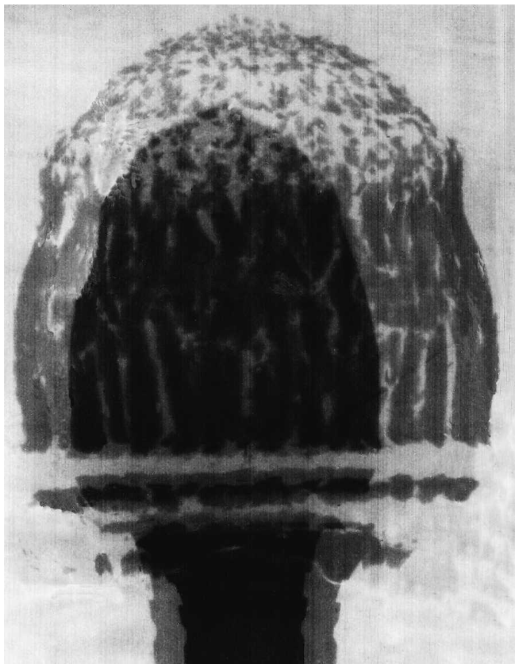


Velocity Distribution

Material Properties of Munition

- **Steel Shell** (4140H Rockwell Hardness C 43)
  - density: 7850 kg/m^3
  - sound speed: 4223 m/s
  - yield strength: 1205 MPa
  - critical stretch (CS): 0.16
- **Explosive**
  - unreacted density: 1770 kg/m^3
  - detonation speed: 8517 m/s
  - CJ pressure: 32.4 GPa
  - JWL Parameters: A_1 = 6540 GPa, R_1 = 9.225, A_2 = 176.9 GPa, R_2 = 2.666, C = 1.322 GPa, ω = 0.3699

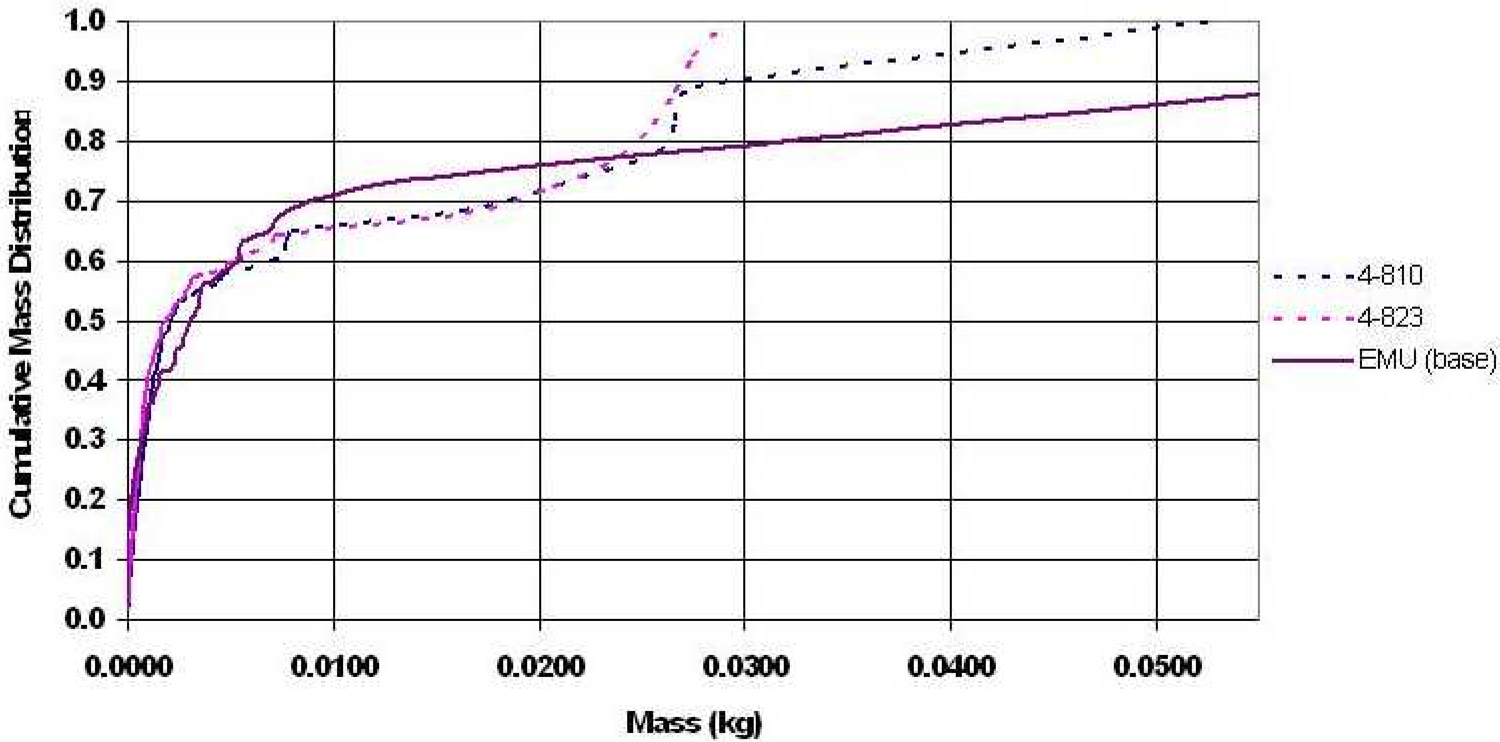
Comparisons with Radiographic Data



27.2 μs

45.5 μs

Fragment Mass Distributions



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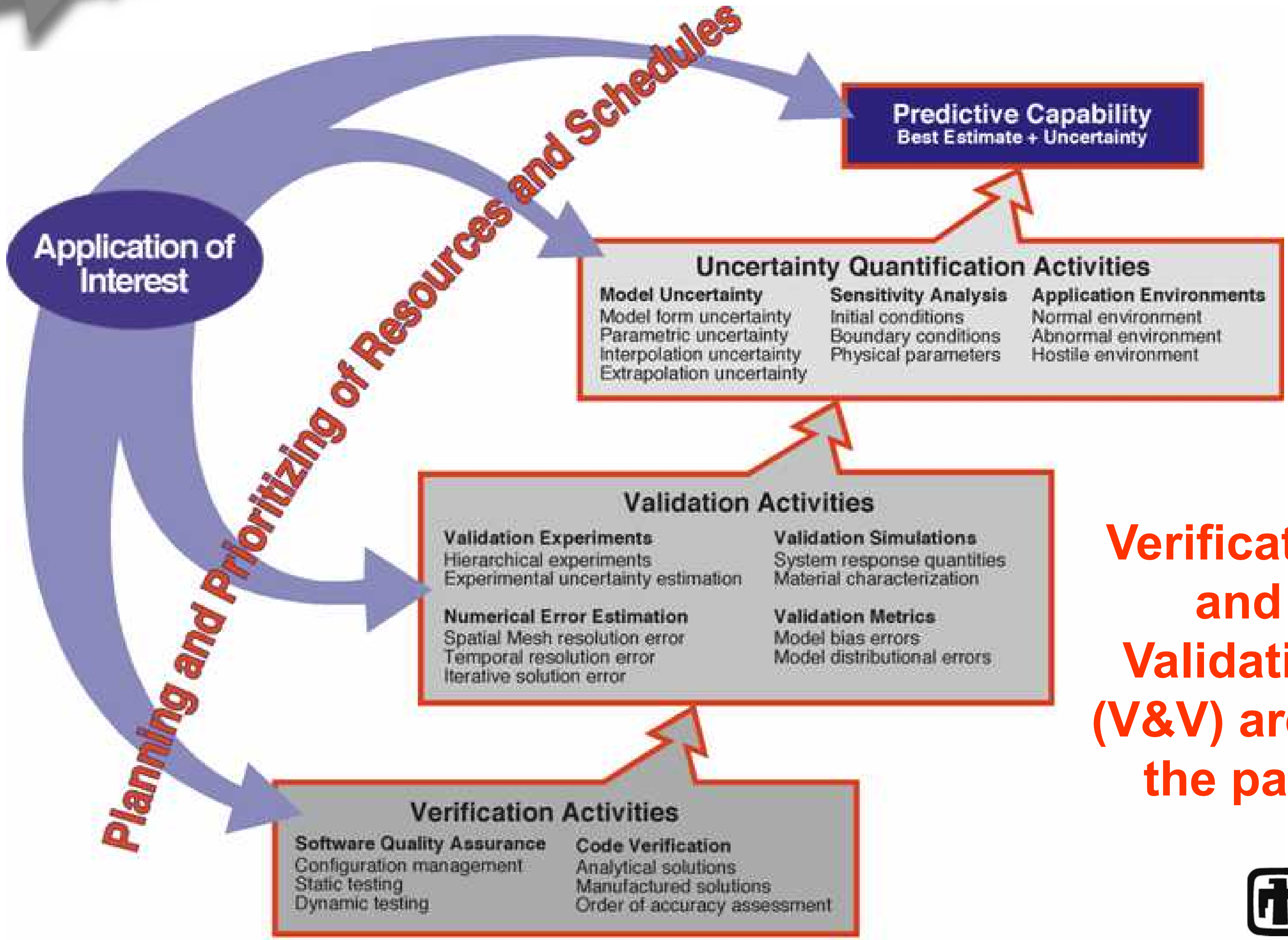
Objective: Confidence in Predictive Capability of Computer Code



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

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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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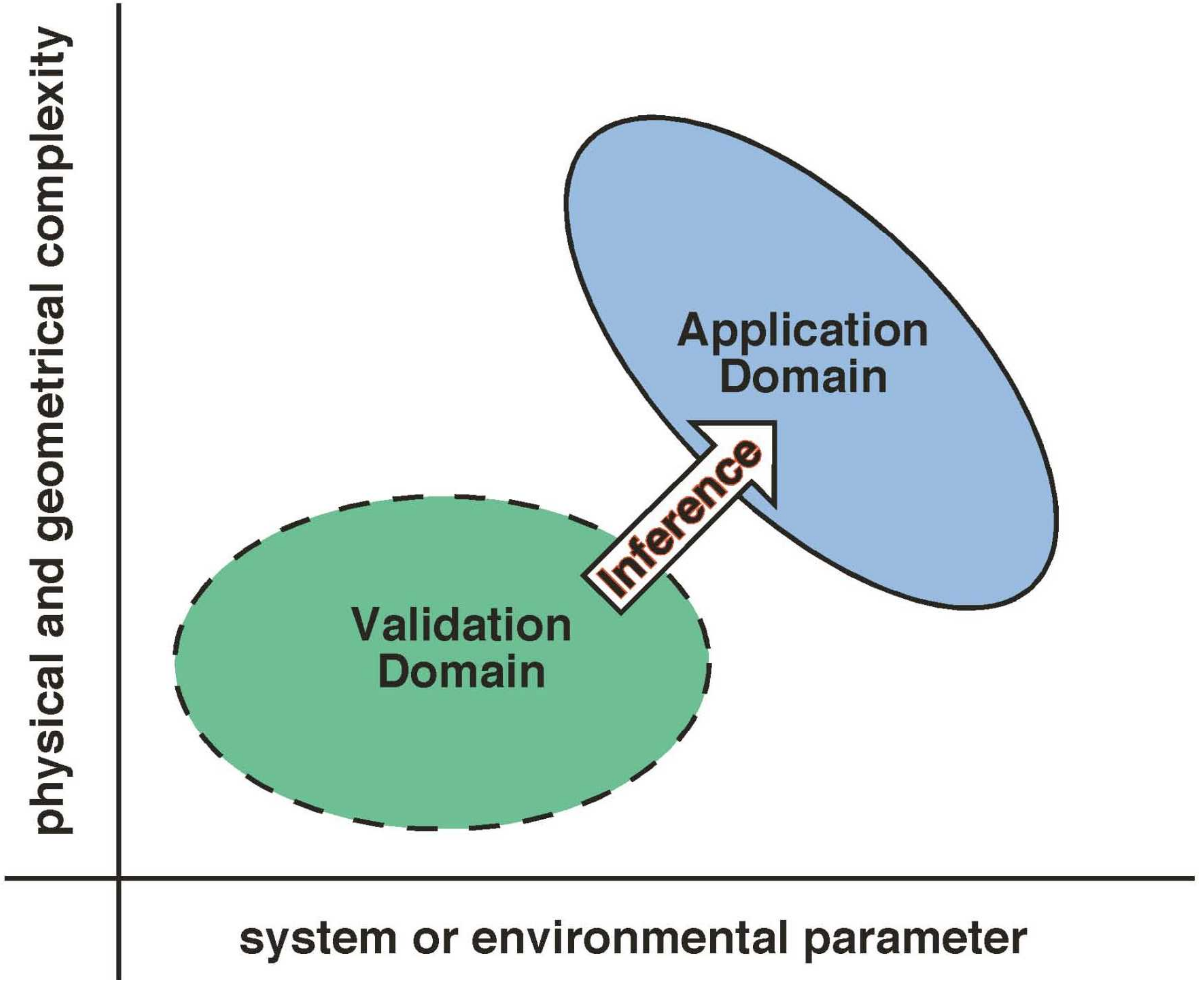
V&V Problems

- 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.

V&V Problems

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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Some Sandia References on V&V

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Current and Future Work

- Continue model calibration for munition materials.
- Understand sensitivity of fragmentation distribution to EMU input parameters.
- Design experiments to validate EMU models.
- Perform experiments for validation process.
- Continue verification and validation (V&V) process.
- Integrate EMU with a ballistics code or extend EMU to provide an integrated capability.

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)
- Rohan Abeyaratne (MIT)
- 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:** **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", submitted to *Journal of Mechanics of Materials and Structures (JoMMS)*.**
- **Google on "peridynamic" to get lots more.**