SAND2011-6176C

Fundamental issues in the representation and propagation of uncertain equation-of-state information in shock hydrodynamics

Allen Robinson
John Carpenter, Richard Drake, Ann Mattsson, Bill Rider
Computational Shock and Multiphysics

Robert Berry and Bert Debusschere
Reacting Flow Research

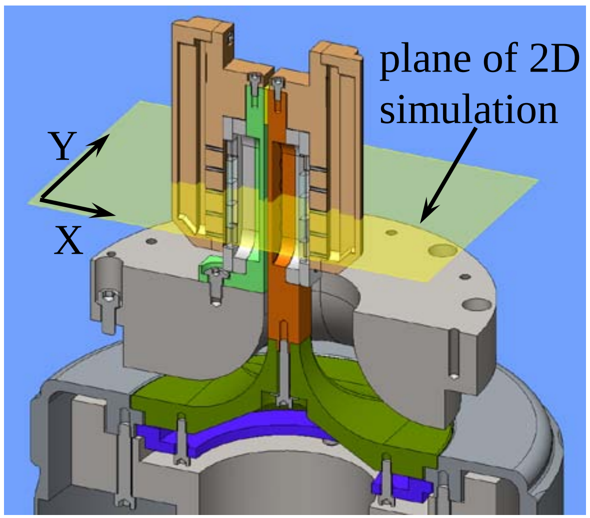
Sandia National Laboratories

MULTIMAT 2011
Arcachon, France
September 5-9, 2011

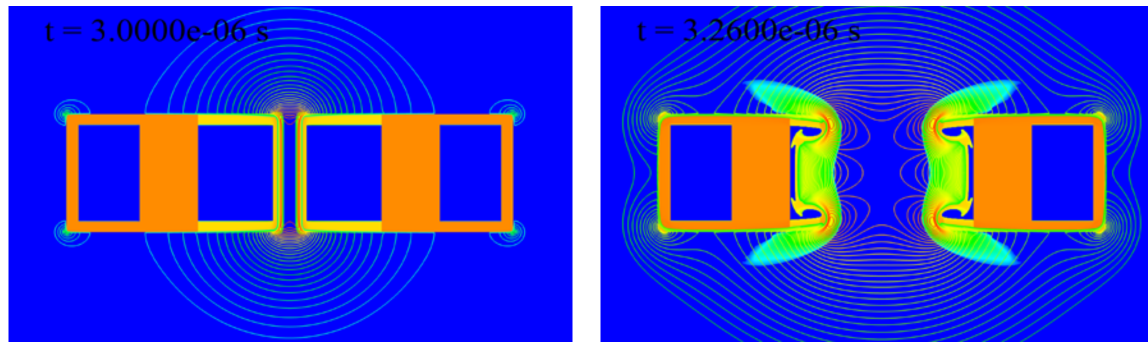
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Predictive Design of Z Experiments (Lemke)

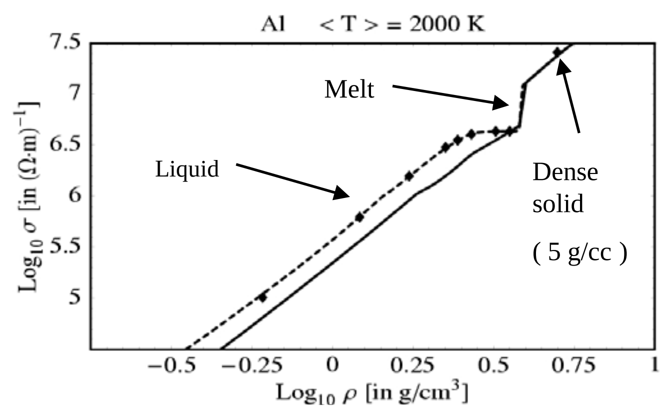
Two-sided Strip-line Flyer Plate Experiment



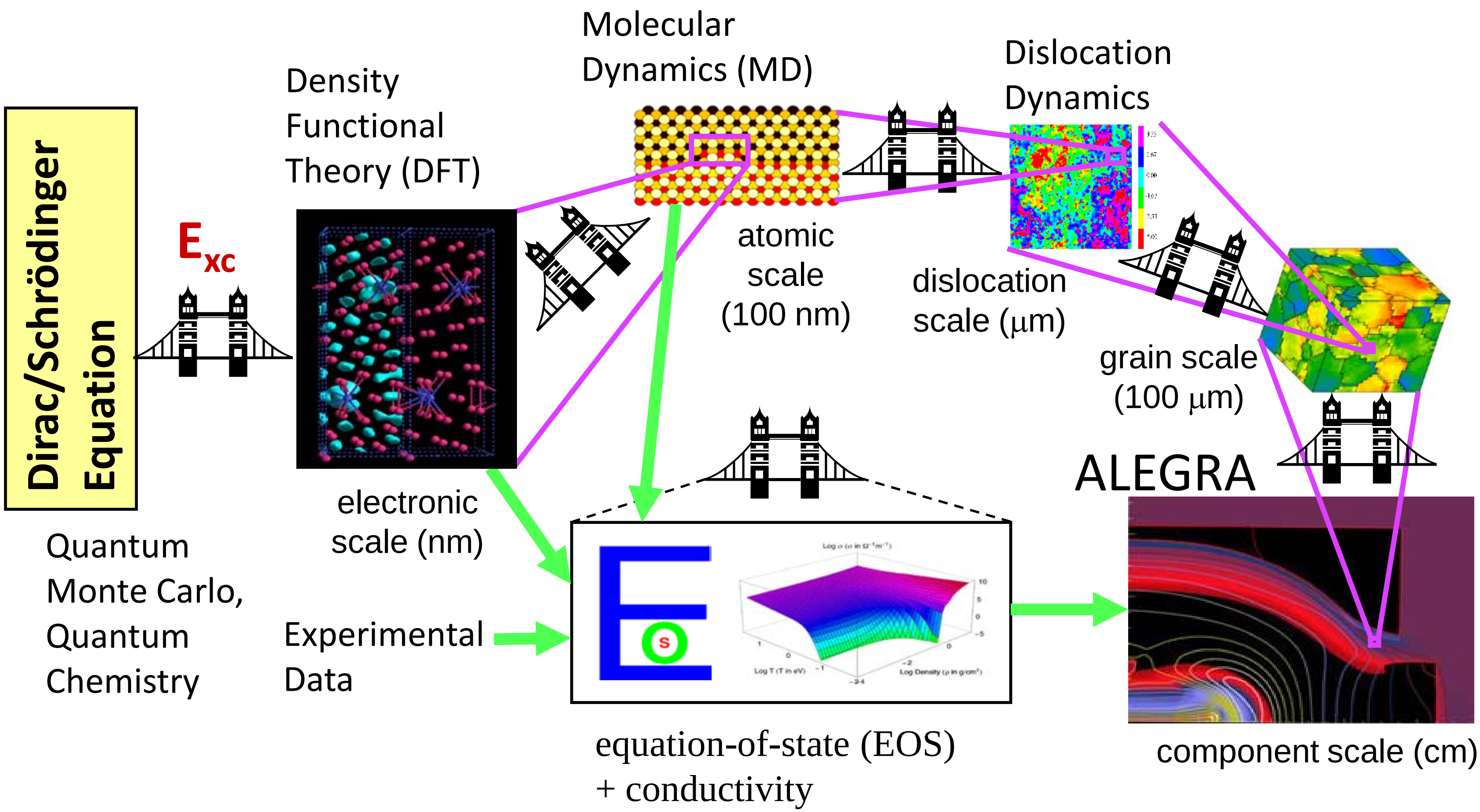
2D Simulation Plane of Two-sided Strip-line



- **Resistive magnetohydrodynamics.**
- **Accurate electrical conductivities.**
- **Accurate equation of state (EOS).**
- **Circuit model for self-consistent coupling.**
- **DAKOTA optimization loops.**
- **Density functional theory and molecular dynamics (DFT-MD) computations are needed to accurately characterize material response.**



The Upscaling Promise



Current Upscaling Practice and Our Goals

- ***DFT-MD is important to develop accurate EOS and conductivity models.***
- ***Various uncertainties are managed by expert users using long experience and judgment.***

- **UQ=Uncertainty Quantification**
  - ***Epistemic Uncertainty = Reducible or model uncertainty may be improved with additional knowledge or data.***
  - ***Aleatory Uncertainty = Irreducible Uncertainty***
- **What are the practical requirements for a UQ technology for shock physics with upscaling**
  - **Evolutionary, well grounded, accessible and backward compatible**

    "Probability is too important to be left to the experts." – Richard Hamming
- **We want to demonstrate such a system.**

Hydrodynamics

- Conservation of mass,

$$\dot{\rho} + \rho \nabla \cdot \mathbf{u} = 0,$$

- Conservation of momentum,

$$\rho \dot{\mathbf{u}} + \nabla p = 0,$$

- Conservation of energy,

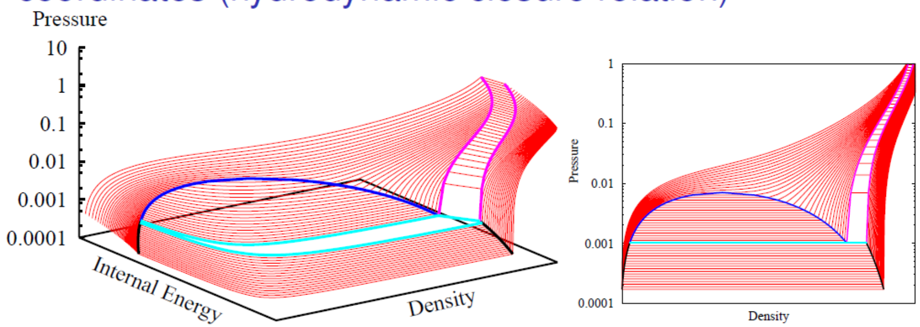
$$\rho \dot{e} + p \nabla \cdot \mathbf{u} = 0,$$

- Equation of state, $p = P(\rho, e)$

These equations are an excellent model for many practical systems.

The wide range EOS closure surface is epistemically uncertain.

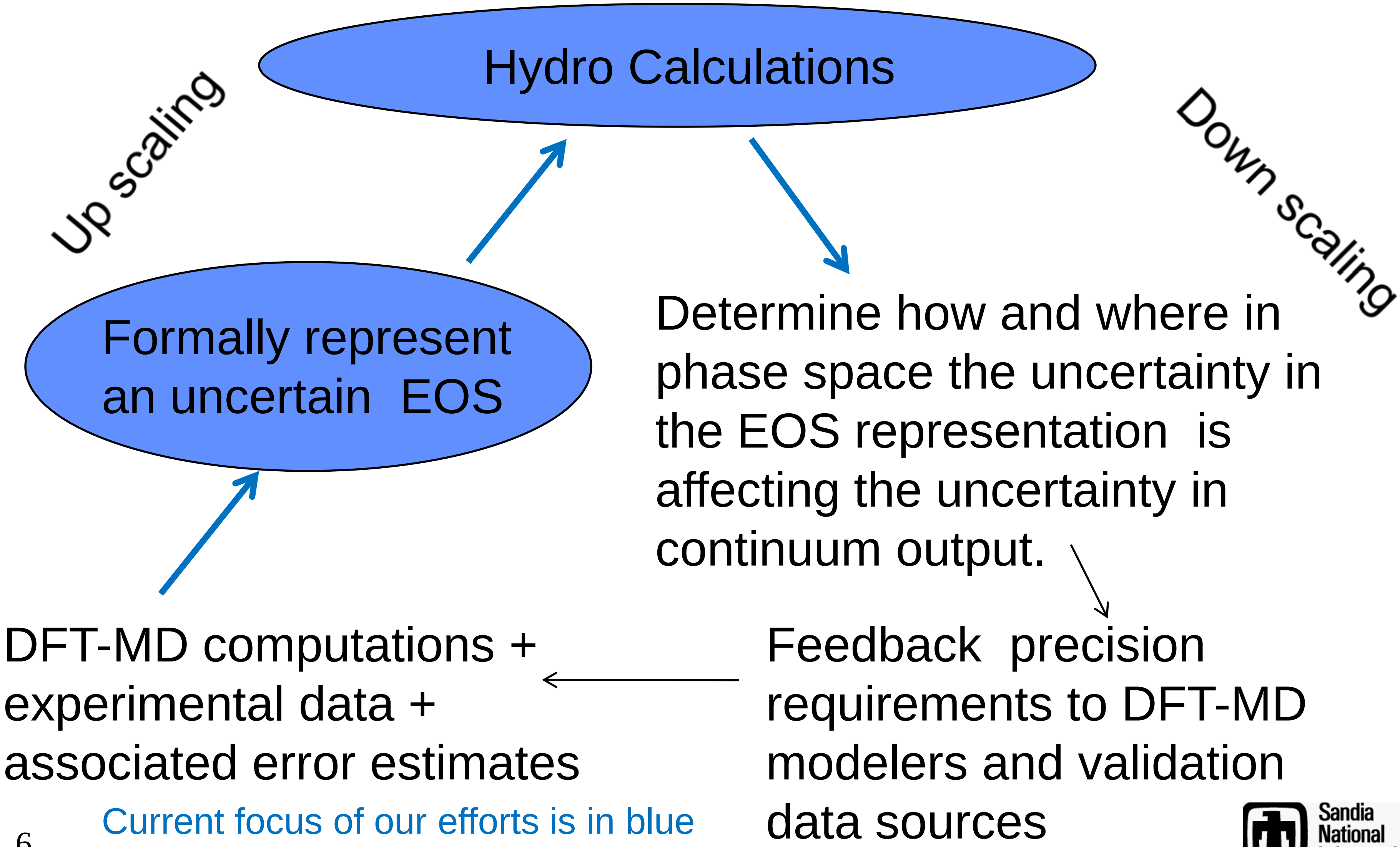
EOS tables: Multi-phase pressure surface in $\rho - E$ coordinates (hydrodynamic closure relation)



Phase boundaries:

Solid-Gas (Sublimation)	Liquid-Gas (Vaporization)	Solid-Liquid (Melt)	Solid-Liquid-Gas (Triple Point)

The Predictive Analysis Cycle



Current focus of our efforts is in blue

Uncertainty in the EOS Bridge

The representation of the uncertainty in the EOS bridge has emerged as a critical issue.

- Uncertain parametric EOS
  - Model form with several to tens of EOS parameters as random variables.

- Uncertain tabular EOS
  - Option 1: Deliver separate tables at evaluations points in probability space.
  - Option 2: Build a compressed representation of the uncertain EOS.

- All techniques should be consistent but will have different performance characteristics

Sandia National Laboratories

Bayesian Viewpoint

- Uncertain quantities are represented as random variables.

- The Bayesian view of probability
  - Probability is inherently the degree of belief in a proposition
  - Not necessarily derived from sampling or observations
  - Handles both aleatory and epistemic uncertainty

- Bayes' Theorem:

likelihood

prior

posterior

$$p(\beta \mid d) = \frac{p(d \mid \beta)\, \pi(\beta)}{p(d)}$$

normalization

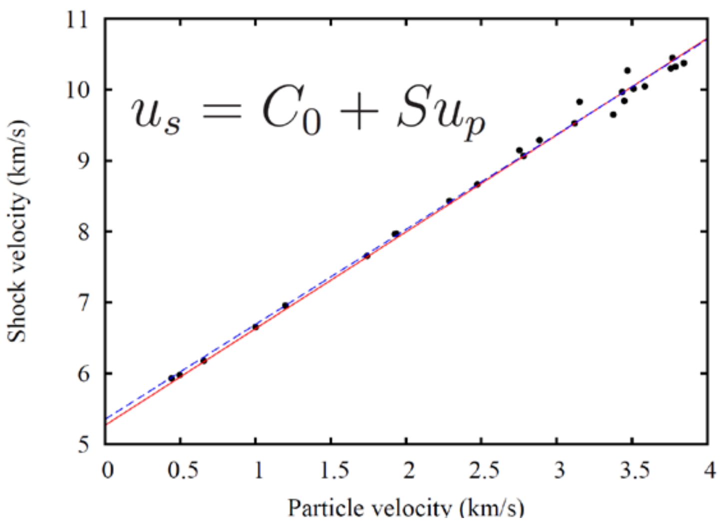
- The likelihood is usually a composite of fit and noise models.

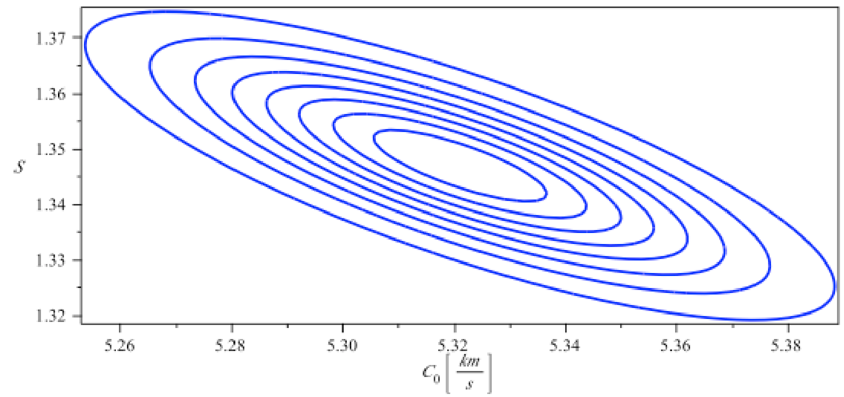
Sandia National Laboratories

Direct Parametric EOS Representation

- The vector of parameters λ is inferred from experimental data
- Noise in data implies uncertainty in parameters
- Bayesian inference provides a (joint) probability density for λ (Markov Chain Monte Carlo)
- Pressure and temperature become random variables (for fixed density and internal energy).
- Poor scaling as uncertain parametric dimension becomes large

$$P = P(\rho, E; \lambda) \qquad T = T(\rho, E; \lambda)$$





Sandia National Laboratories

Tabular Option I

- An ensemble of EOS tables can represent uncertainties.
  - Sample uncertain parameters
  - Ensemble of models
  - Each table given a weight

- Expensive to store and distribute and manage a sufficient number of tables to represent uncertainties.

- However it does satisfy production efficiency requirements except for memory storage.

- Could be used to get off the ground in the short term and as a baseline.

Tabular Option II

•Starting with a table $\tau = \{(\rho_i, E_i, P_i, T_i) : i \in I\}$
consider a perturbation $D = \{(\Delta\rho_i, \Delta E_i, \Delta P_i, \Delta T_i) : i \in I\}$

•We would like to build a joint density *μ* for *D* so that a sample $d \sim \mu$ provides a new table $\tau + d$ which is "reasonable."

- •Consistency: all perturbations are thermodynamically consistent
- •Stability: *μ* should disallow an unstable EOS

•Stochastic process techniques allow for reduction of dimensionality in representing model uncertainties. However, these would require a metric on (ρ, E, P, T) in order to gauge the "size" of *D*, or provide a sense of "correlation length." Is there a natural one?

•Similarly, techniques such as the Karhunen-Loève decomposition require a Hilbert space structure.

Sandia National Laboratories

Karhunen-Loève Representation

- Given a (vector valued) process, find an optimal separated representation

$$F(x,\xi) = F_0(x) + \sum_{i=1} \sigma_i\, \varphi_i(\xi)\, F_i(x)$$

  - $(\sigma_i^2, F_i(x))$ are eigenvalue/functions (o.n.) for the kernel

$$C(x,y) = \int F(x,\xi) F^T(y,\xi)\, d\mu(\xi)$$

  - $(\sigma_i^2, \varphi_i(\xi))$ are eigenvalue/functions (o.n.) for the kernel

$$K(\xi,\theta) = \int \langle F(x,\xi), F(x,\theta)\rangle\, dm(x)$$

- For a discrete process and standard inner product, KL = Principal Component Analysis (PCA) = subtract mean and then calculate the singular value decomposition (SVD)

$$x\left\{\overbrace{\begin{bmatrix} F - \bar{F} \end{bmatrix}}^{\xi}\right. = \begin{bmatrix} \quad F_i \quad \end{bmatrix} \begin{bmatrix} \mathrm{Diag}(\sigma_i) \end{bmatrix} \begin{bmatrix} \quad \varphi_i \quad \end{bmatrix}$$

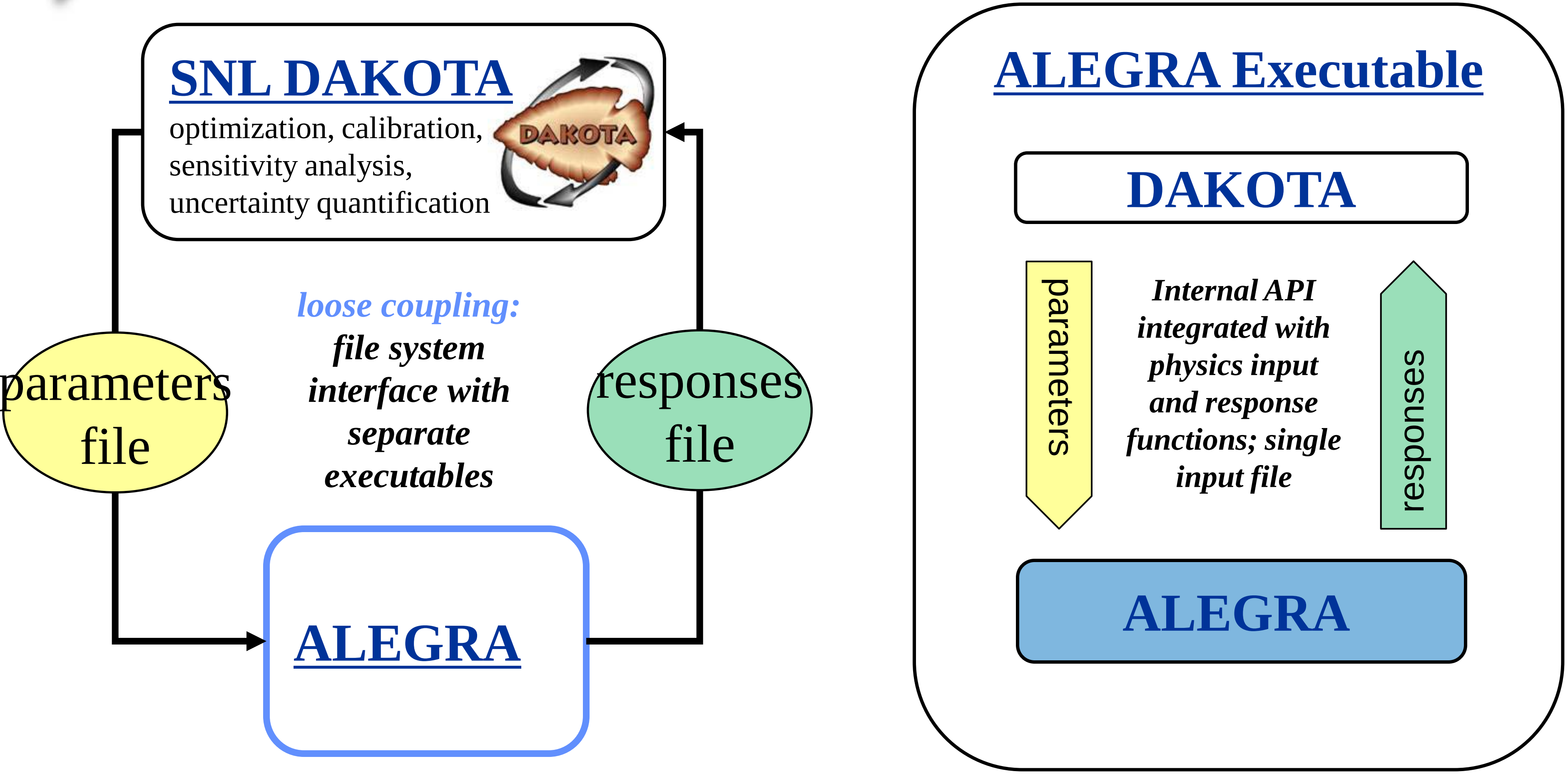
DAKOTA UQ Toolbox

- DAKOTA is a well-known toolkit for black box large scale engineering optimization and uncertainty analysis.

- The historical interface between DAKOTA and analysis codes is based on specialized file based communication interfaces controlled by user scripting.
  - This interface permits usage by analysts with modest scripting skills and determination.

- Making the UQ enabled analysis standard engineering practice requires a much smaller "user energy barrier" at multiple points.

Embedded UQ Interface ALEGRA

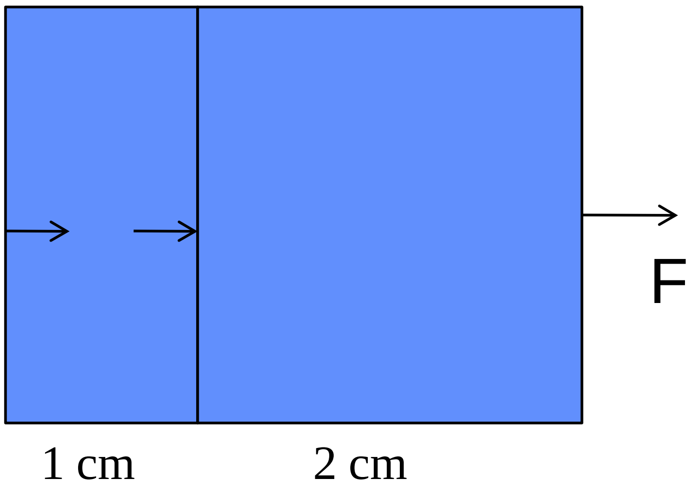


Current → **Moving from potentially fragile, study-specific script interfaces to a unified, user-friendly capability** → Future

AL Flyer/Target Impact Test Case

We are using the new embedded interface for the results presented here.

Impact velocity



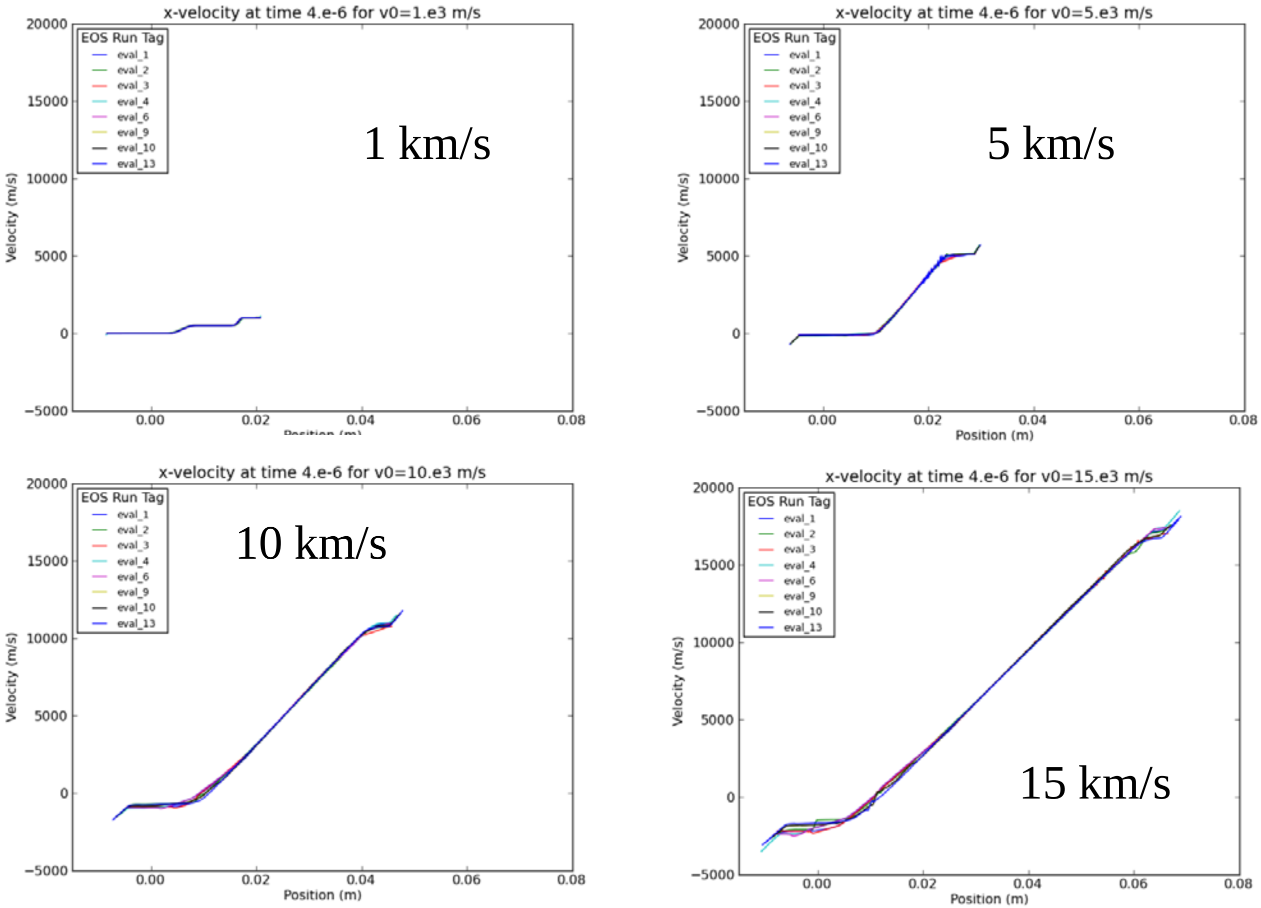
Free surface velocity

Simple shock analysis says that the free surface velocity should be slightly larger than the impact velocity for convex Hugoniots and release isentropes.

Sandia National Laboratories

A Computational Experiment

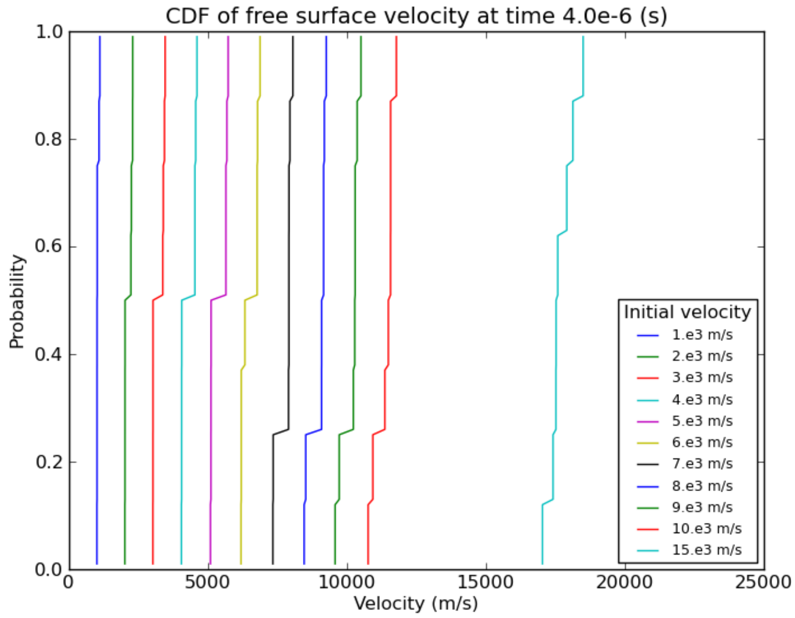
Current tabular models do not come with a UQ representation. Can we get a feel for the variation to be expected from different wide range tabular models with varying provenance, for a given interpolation scheme? 8 wide range tables were used as a surrogate for the drawing of realizations from a random field EOS.



These results are indicative of what we expect to see from a more formal uncertain EOS modeling approach. e.g. small uncertainty at low impact velocities and high uncertainty when traversing off Hugoniot states.

A UQ View of the Experiment

Assume that the 8 tables each occur with a .125 probability

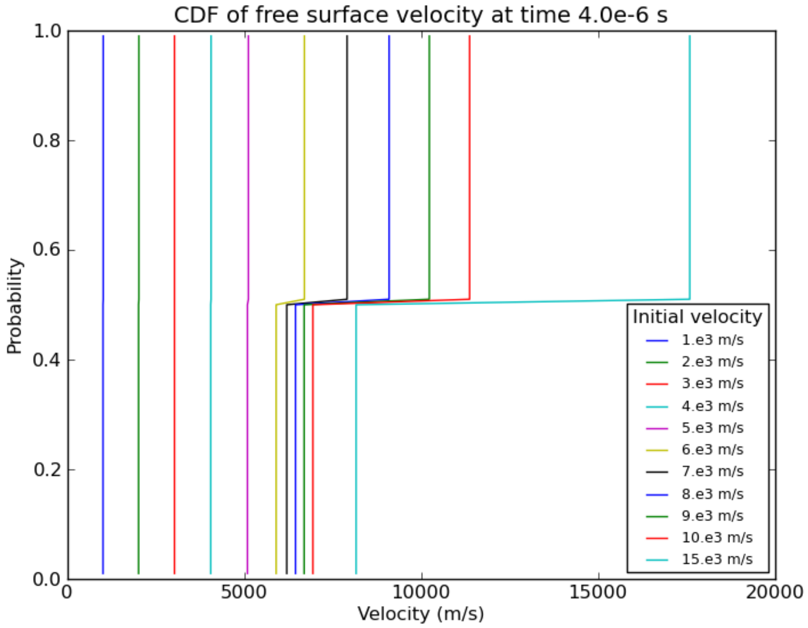


•We see in the plots of the output cumulative distribution function (CDF) evidence of small uncertainty at low impact velocities and high uncertainty when traversing off Hugoniot states.
•Note that the physical information content is not as rich as the previous slide.
•We shall see that this simplistic distribution assumption is unacceptable.

Sandia National Laboratories

Another UQ Experiment to Emphasize the Point

Pick a simple Mie Gruneisen (MG) model accurate near the primary Hugoniot and a wide range EOS model. Assume that each EOS has a .5 probability. The huge variation at higher velocities is indicative of severe epistemic uncertainty as expected.



The Mie-Gruneisen (MG) Model as a Test Case

Even though we know the MG equation of state is not accurate over a wide range it does have a small number of parameters and we can use this model as a test case for a more formalized approach for a wide range EOS.

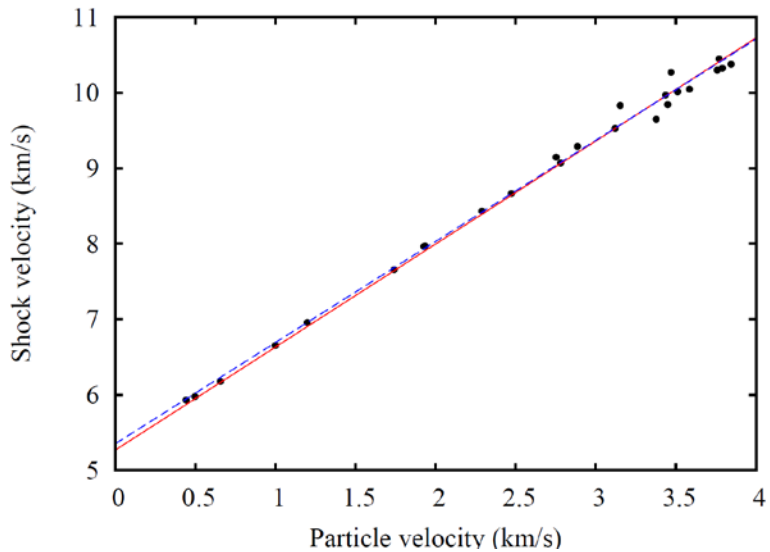
$$
\begin{aligned}
P(\rho, E) &= P_R(\rho) + \Gamma_0 \rho_0 (E - E_R(\rho)) \\
E(\rho, T) &= E_R(\rho) + C_V (T - T_R(\rho)),
\end{aligned}
$$

$$u_s = C_0 + S u_p,$$

$$
\begin{aligned}
P_R(\rho) &= P_H(\rho) = P_0 + \rho_0 u_s u_p \\
E_R(\rho) &= E_H(\rho) = E_0 + (P_H + P_0)\mu / 2\rho_0 \\
T_R(\rho) &= T_H(\rho) = e^{\Gamma_0 \mu} [T_0 + C_V^{-1} \int_0^{\mu} e^{-\Gamma_0 \mu} \mu^2 u_s \frac{du_s}{d\mu} d\mu]
\end{aligned}
$$

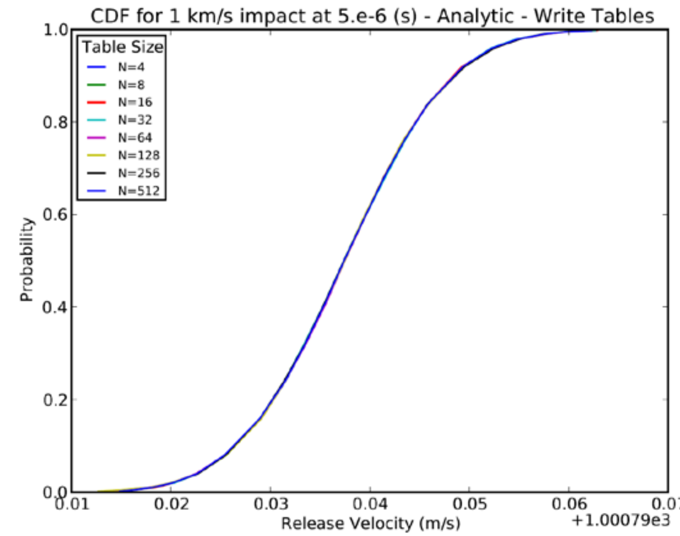
Sandia National Laboratories

MG "Analytic" Model
3x3 Polynomial Chaos Expansion (PCE) UQ



$$
\begin{aligned}
S &= \mu_S + \sigma_S\,\xi_1 \\
&= 1.347 + 0.01322\,\xi_1 \\
C_0 &= \mu_{C_0} + \sigma_{C_0}(r\,\xi_1 + \sqrt{1-r^2}\,\xi_2) \\
&= 5.321 + 0.03213(-.7824\,\xi_1 + 0.6227\,\xi_2)
\end{aligned}
$$

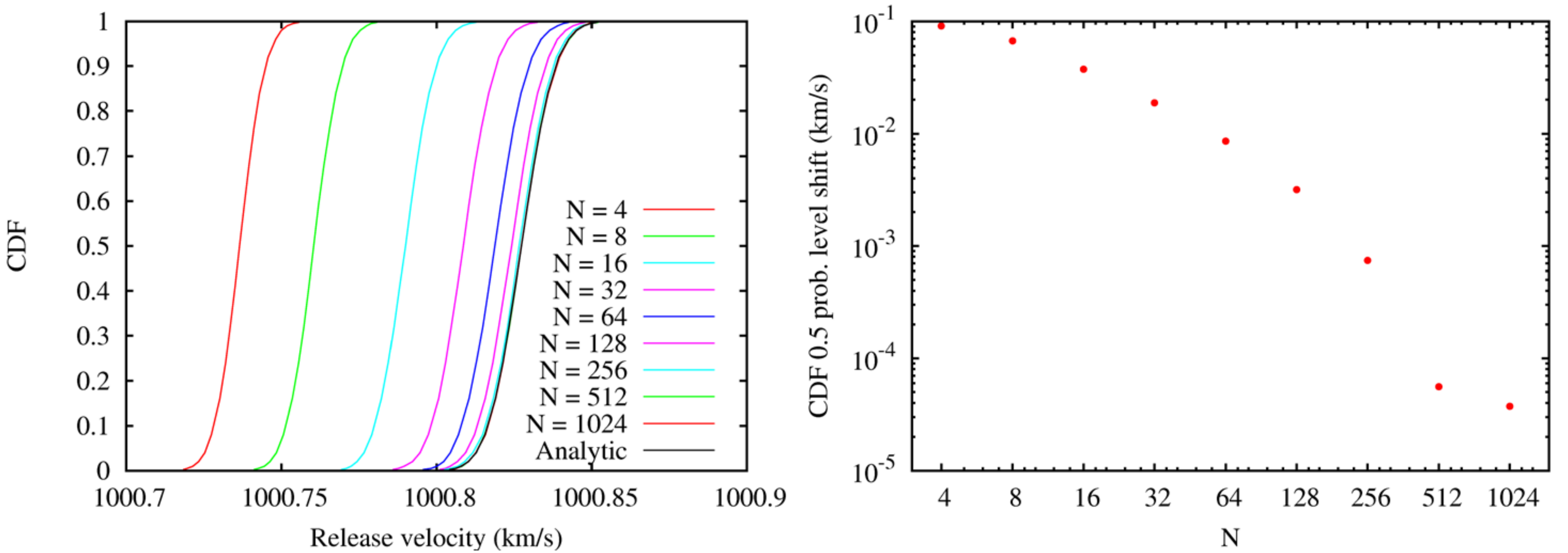
Use Markov Chain Monte Carlo to compute coefficients of random EOS representation.



$$
R = \sum_{n=0}^{N} \alpha_n \psi_n(\xi)
$$

Use tensor product Gauss-Hermite quadrature to compute coefficients of the spectral response representation.

CDF Convergence under Table Refinement using PCE



- CDF converges to analytic result, as expected
  - Shift is converged within sampling error at N=512
  - Convergence appears faster than a power law
- Problem: the converged N=512 produces a very large table for a simple, limited range EOS. Wide range EOS models typically have N~128. Improved tabulation methodologies are needed.

Sandia National Laboratories

Tabular Approach – Option II

Use Principal Component Analysis (PCA) to look for a reduced tabular representation.

Collect a representative sample of tables of (pressure, internal energy) on a fixed (density, temperature) grid

Perform Principal Component Analysis (PCA)

$$A = \{z_1, ..., z_n\} - \bar{z}\mathbf{1}^T = Z - \bar{z}\mathbf{1}^T = U\Sigma V^T$$

$$z = \bar{z} + U\Sigma\xi = \bar{z} + AV\xi$$

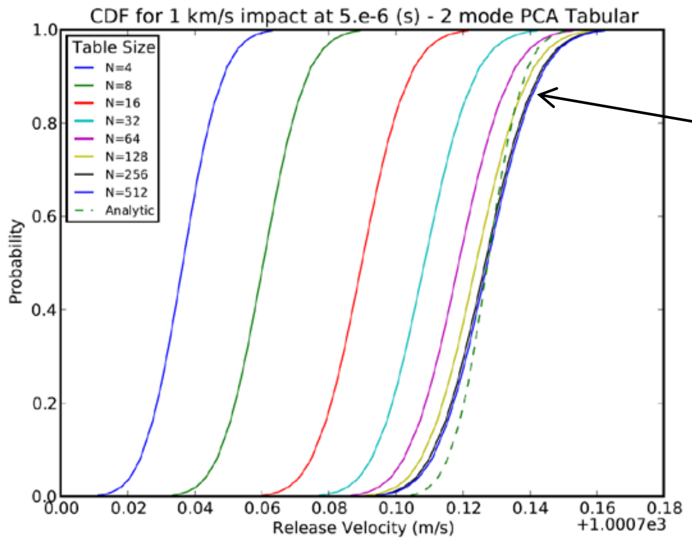
Choose a truncated set of modes.

Compare with previous results.

Sandia National Laboratories

UQ with 2 Mode PCA Tables Taken from PCE Samples

Take 9 tables from PCE as sample data, build a Principal Component Analysis (PCA) representation and use the 2 largest modes



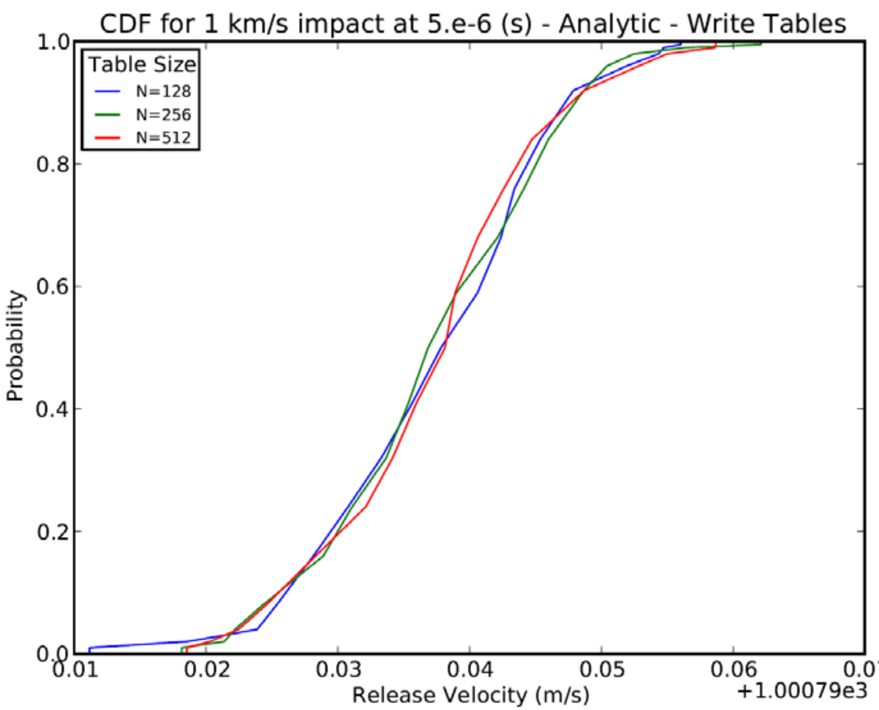
Output distribution is too broad.

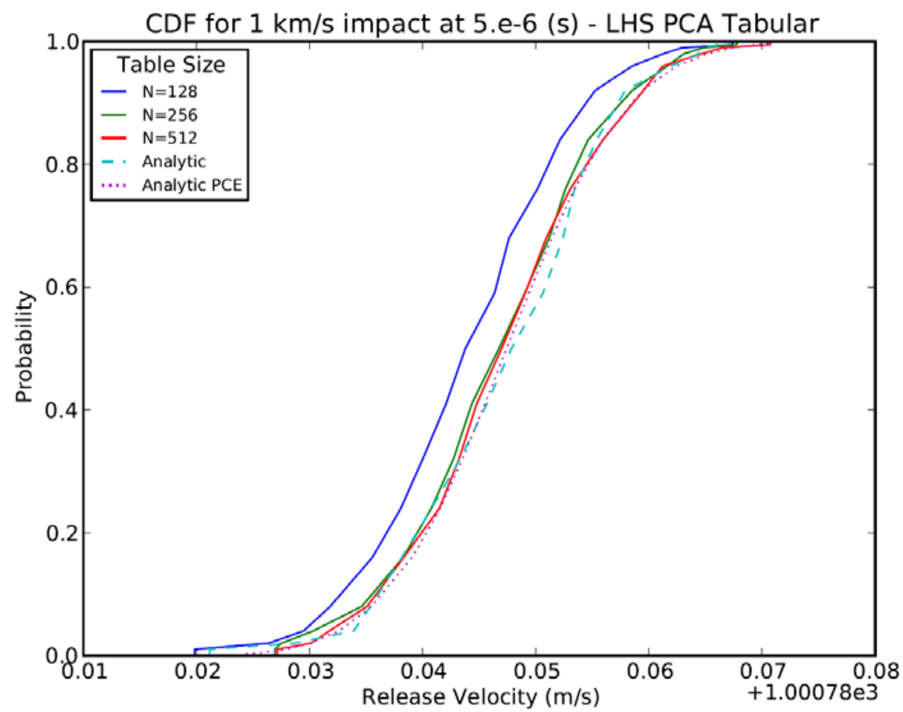
Why?

The PCE Gauss quadrature tables should not have equal weights in the PCA analysis!

Parametric UQ with Principal Component Tables - LHS

Take tables from 100 Latin Hypercube Sampling (Monte Carlo) runs as realizations and build a 2 mode Principal Component Analysis representation





CDF shape verifies that proper weighting of the sample realization tables is critical for the PCA representation approach.

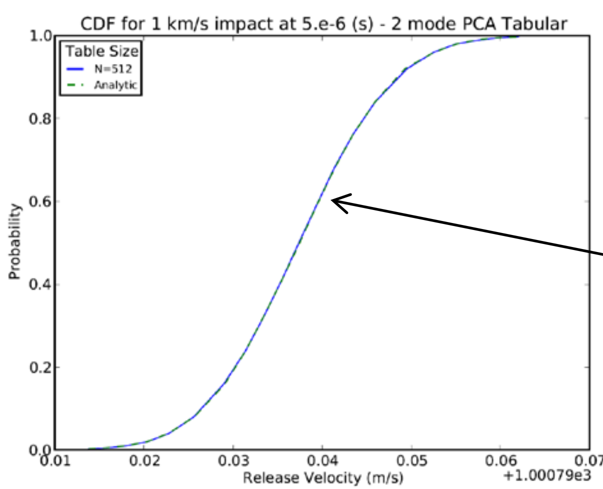
Sandia National Laboratories

UQ with 2 mode PCA Tables Generated with Weighted PCE Samples

$$\bar{z} = Z H^{1/2} \mathbf{1} / \mathbf{1}^T H \mathbf{1} \qquad G^{1/2}(Z - \bar{z}\mathbf{1}^T) H^{1/2} = \tilde{U}\Sigma\tilde{V}^T$$

$$z = \bar{z} + U\Sigma\xi = \bar{z} + G^{-1/2}\tilde{U}\Sigma\xi = \bar{z} + (Z - \bar{z}\mathbf{1}^T) H^{1/2}\tilde{V}\xi$$

Take 9 tables from PCE as data, build a PCA representation using Gauss-Hermite quadrature weights in the PCA analysis (2 largest modes)



Output distribution is now consistent!

Wide Range EOS UQ Representation

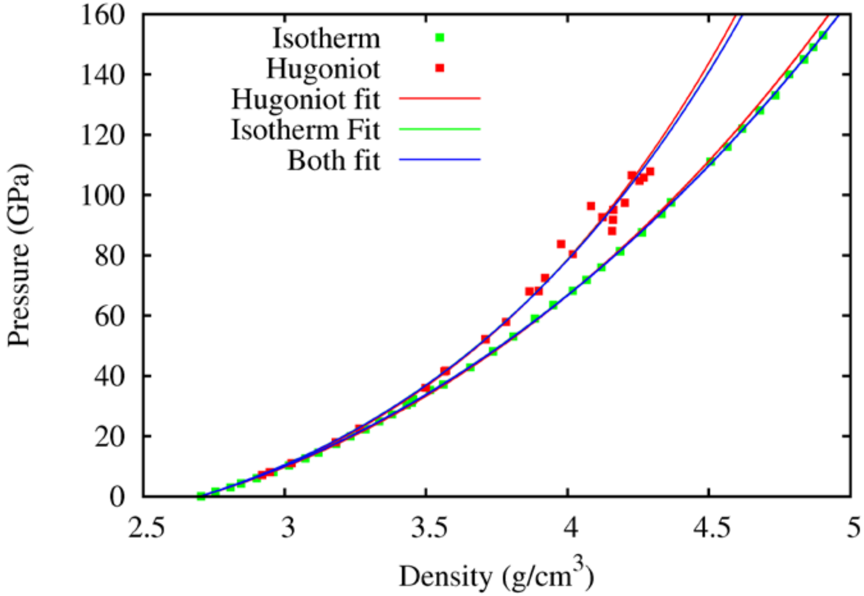
- The PCA approach clearly works for the Mie-Gruneisen EOS for this problem.

- What about wide range EOS?
  - The first thing to try is to add more general coordinates into the PCA analysis.
  - Will we still get useful compression?
  - What about phase boundaries and EOS stability?
  - With large numbers of parameters we will be forced to deal with larger computing requirements for the PCA analysis.

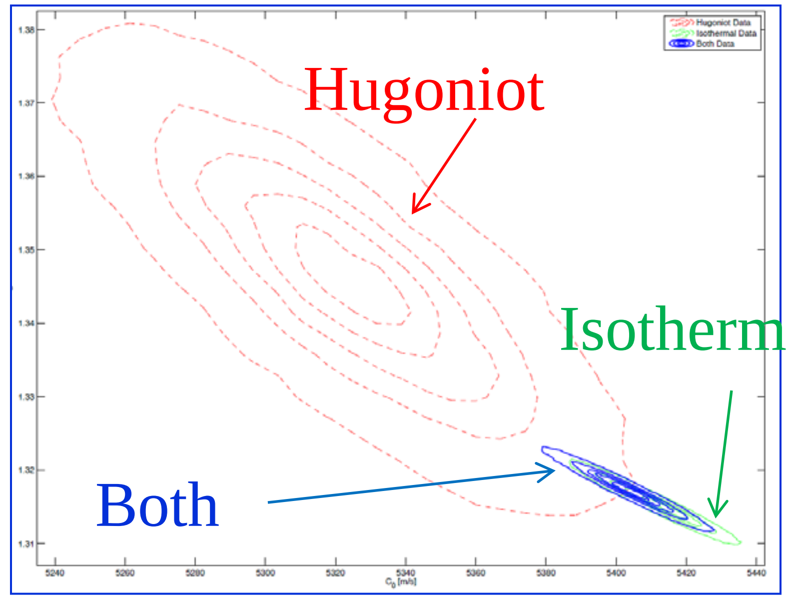
- How do we enable downscale information transfer returning along the bottom of the predictive analysis cycle and the evaluation of epistemic uncertainty?

Looking for Epistemic Uncertainty

Iso-therm and Hugoniot of the inferences relative to the data



Inferred posterior pdf contours



- Mie-Gruneisen model is holding together.
- As we add more data including DFT-MD data, we expect to be able to show using formal UQ methods that the epistemic uncertainty for this model will increase.

Sandia National Laboratories

Summary

- We have outlined a general way of thinking about the upscaling UQ problem for shock hydrodynamics.
- The basic PCA approach shows promise as a workable conceptual framework for tabular delivery of parametric EOS model uncertainty to production users.
- Proper weighting of sample realizations is essential.
- We are experimenting with pulling together the pieces in a way which will be compatible with current technology and a sustainable UQ enabled technology going forward.