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Uncertainty quantification of equation-of-state closures and shock hydrodynamics

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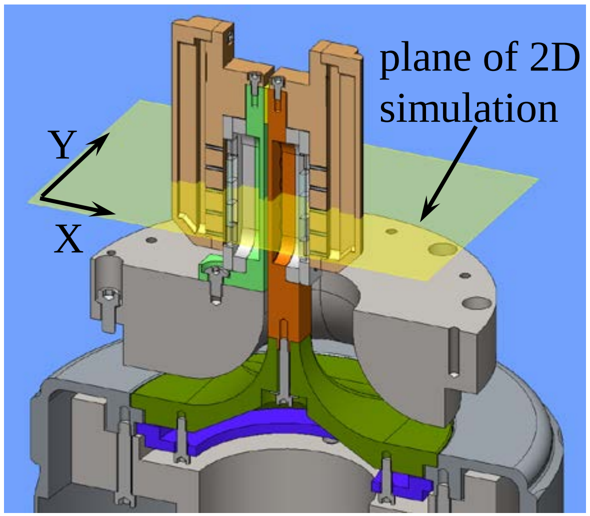
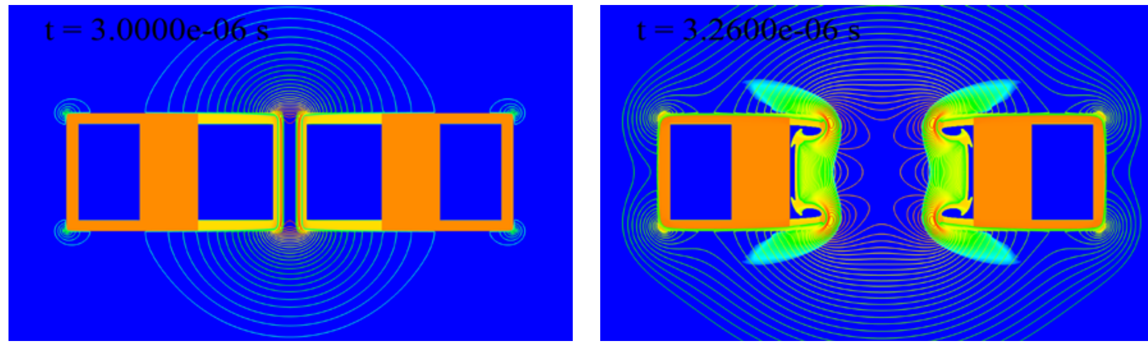
Predictive Design of Z Experiments (Lemke)

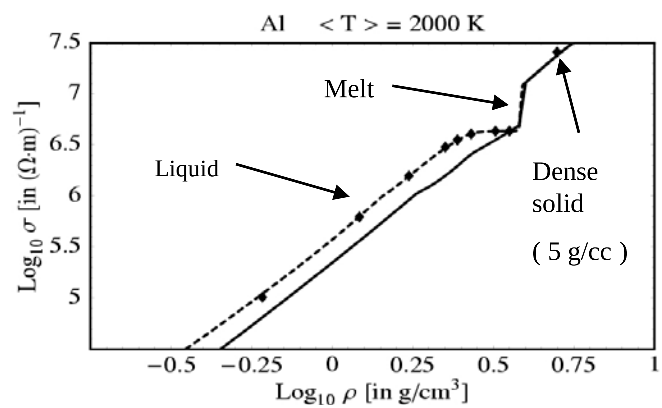
Two-sided Strip-line Flyer Plate Experiment



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.**



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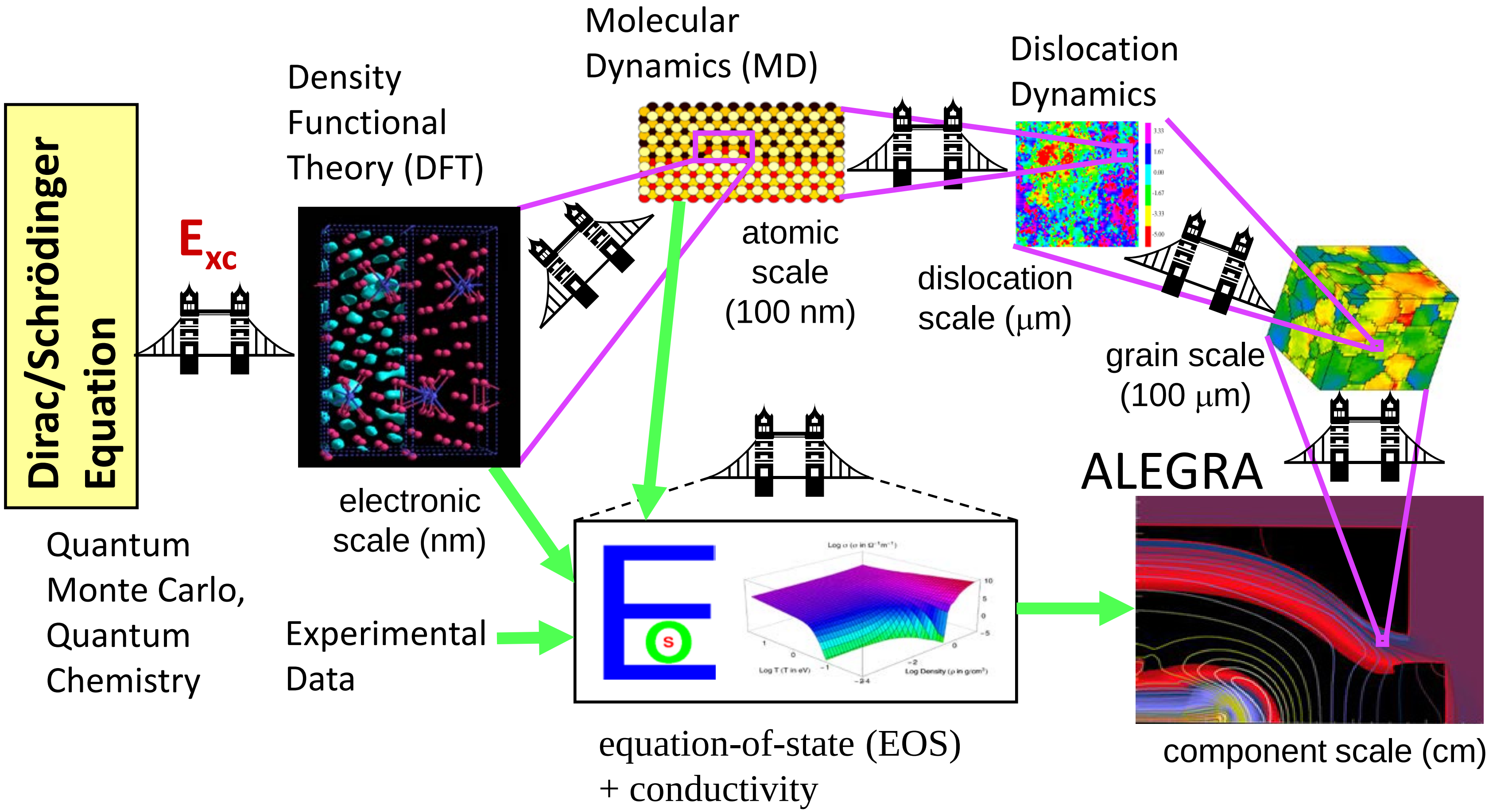
The Upscaling Promise



Current Upscaling Practice and Our Goals

- ***Experimental data and DFT-MD are important to develop accurate EOS and conductivity models.***
- ***Various uncertainties are managed by expert users using their 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 an upscaling UQ technology for shock physics?**
  - **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,

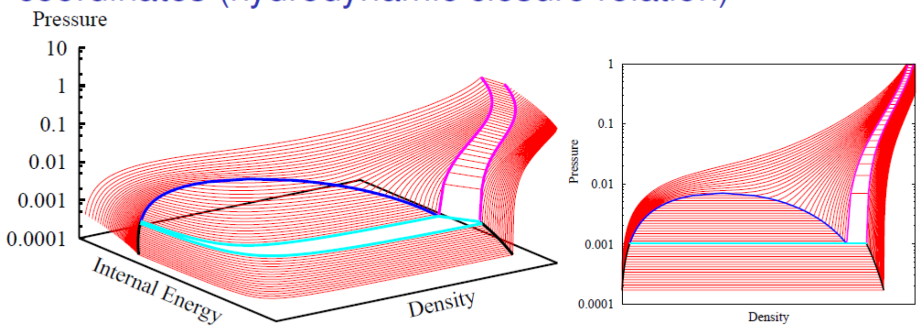
$$\rho \dot{e} + p \nabla \cdot \mathbf{u} = 0,$$

- 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)

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The Predictive Analysis Cycle

Hydro Calculations

Down scaling

Determine how and where in phase space the uncertainty in the EOS representation is affecting the uncertainty in continuum output.

Feedback requirements to DFT-MD modelers and validation data sources

DFT-MD computations + experimental data + associated error estimates

Up scaling

Formally represent an uncertain EOS

Current focus of our efforts is in blue

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Uncertainty in the EOS Bridge

The representation of the uncertainty in the EOS bridge has emerged as a critical issue to production delivery of uncertainty information.

- Uncertain parametric EOS
  - Model forms 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

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.

Direct Parametric EOS Representation

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

- The vector of parameters λ is inferred from 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 the dimension of λ becomes large.

Tabular Option 1

- 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.

- Can be used as a baseline for evaluating compressed formats.

Tabular Option 2

- If we have an ensemble of EOS tables which are a representative sample of the uncertain EOS space we try to generate an optimal representation:
  - Provide maximum flexibility to the user.
  - Achieve significant compression.
  - Must deal with phase boundaries
  - Be efficient.
- Only this option seems to have a potential production future.

Karhunen-Loève or PCA Representation

- Given a (vector valued) process, find an optimal separated representation $F(x,\xi) = F_0(x) + \sum_{i=1} \sigma_i \, \varphi_i(\xi) \, F_i(x)$
  - $\left(\sigma_i^2, F_i(x)\right)$ 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)

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

Tabular Option 2 – PCA method

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

- Collect a representative sample of tables (e.g. PCE points or Monte Carlo).

- Perform Principal Component Analysis (PCA)

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

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

- H represents sample weights (e.g Gauss-Hermite) and G represents user specified weights for the sample entries.

- Choose a truncated set of modes to export in tabular form.

- In the hydrocode, generate EOS tables on-the-fly, given a sample of the random variables associated with each mode.

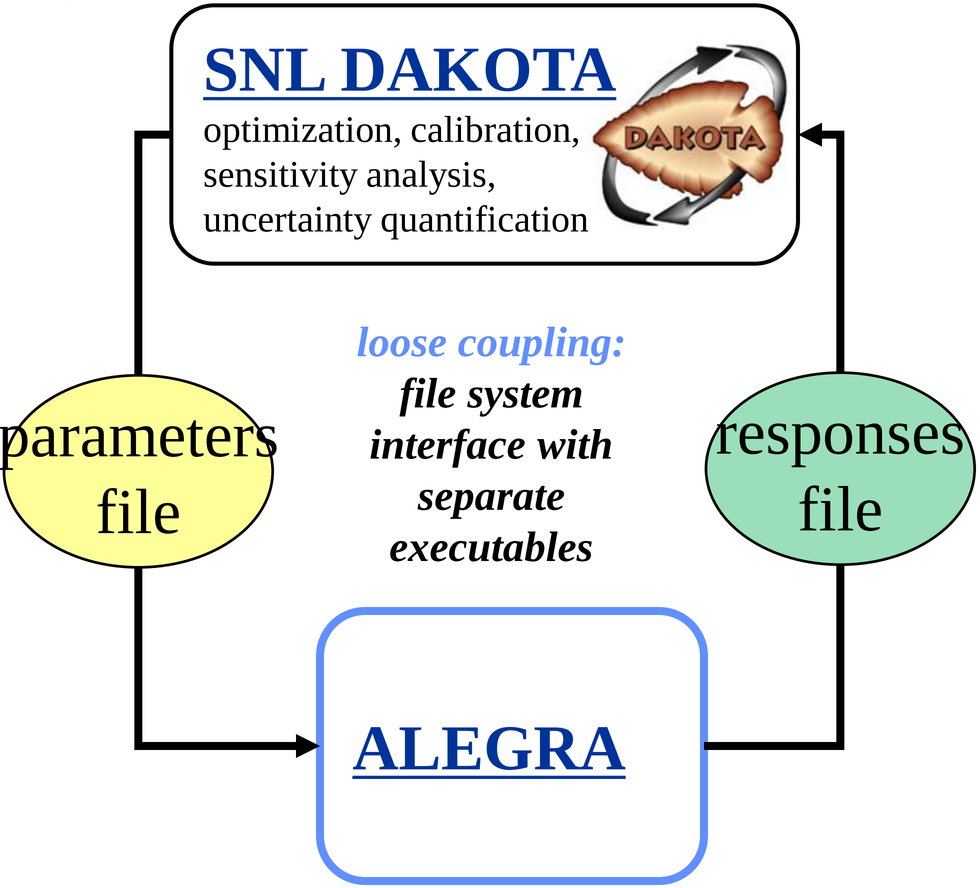
DAKOTA UQ Toolbox

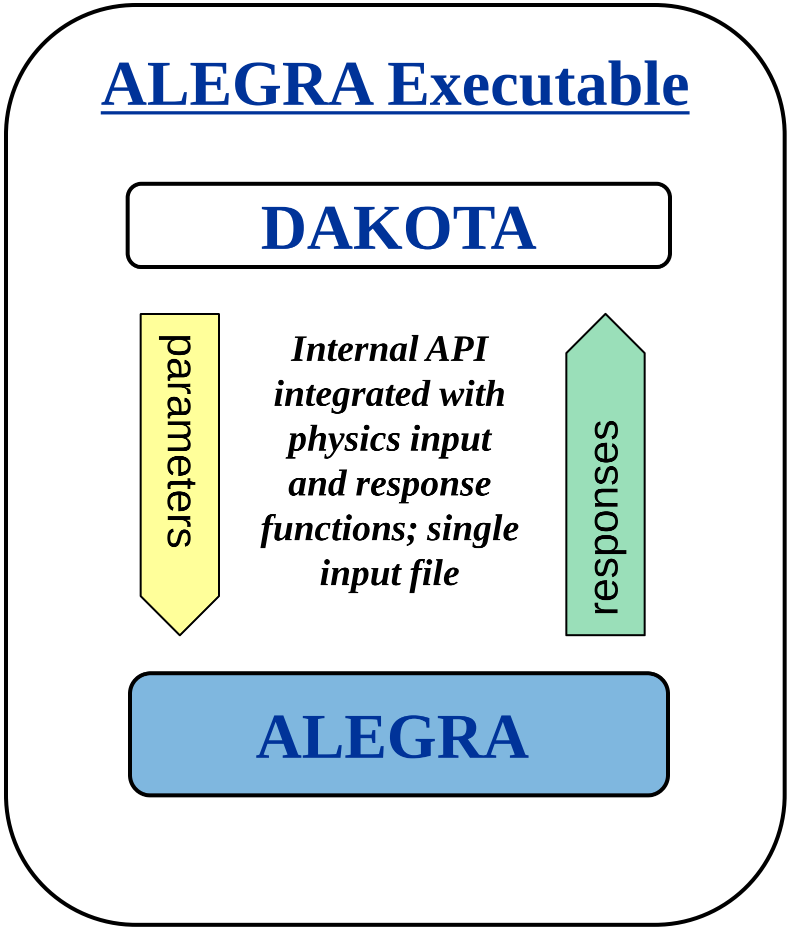
- DAKOTA is a well-known toolkit for black box large scale engineering optimization and uncertainty analysis.

- 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 Dakota Interface in ALEGRA





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

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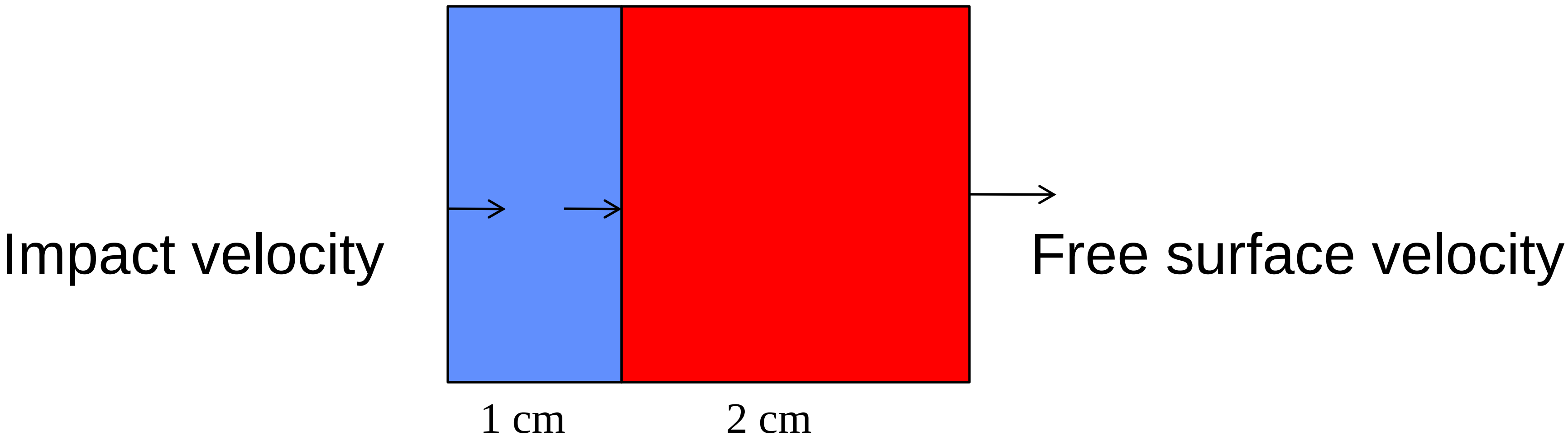
AL Flyer/Target Impact Test Case

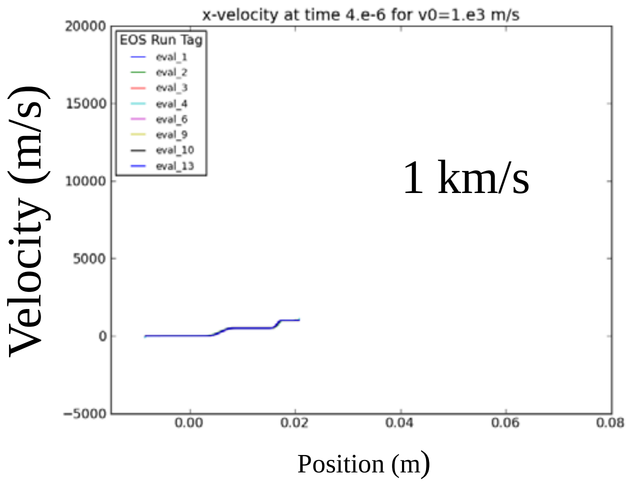
We are using the new embedded interface for the results presented here.

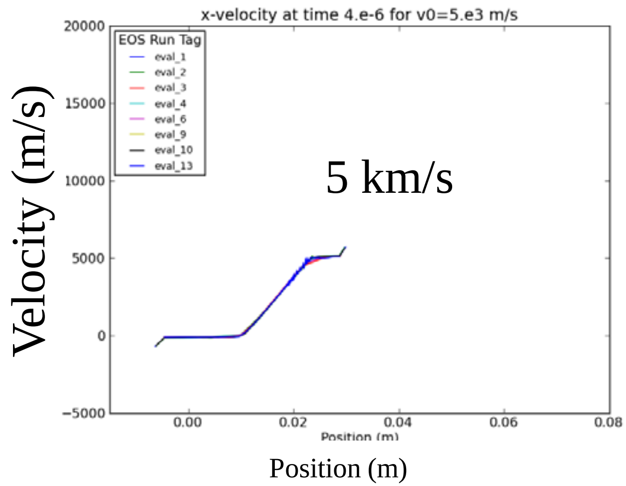


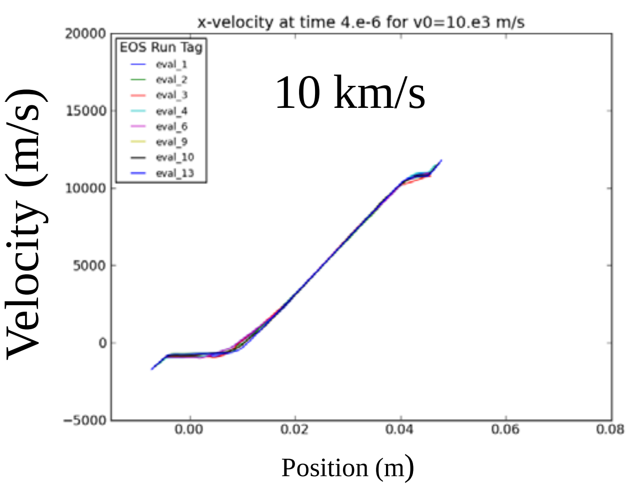
Simple shock analysis says that the free surface velocity should be slightly larger than the impact velocity for convex Hugoniots and release isentropes.

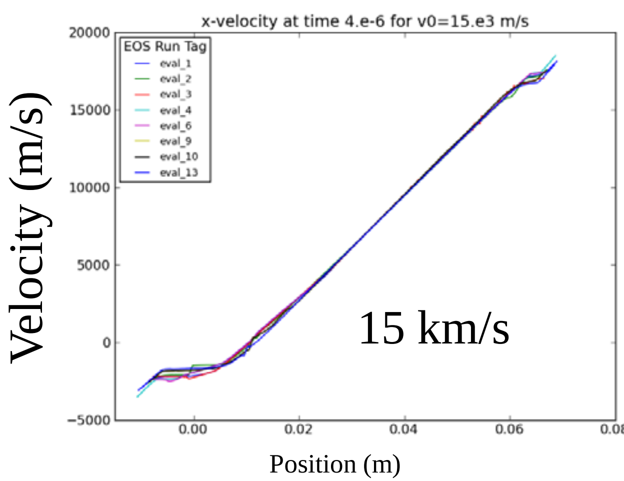
A Computational Experiment

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.

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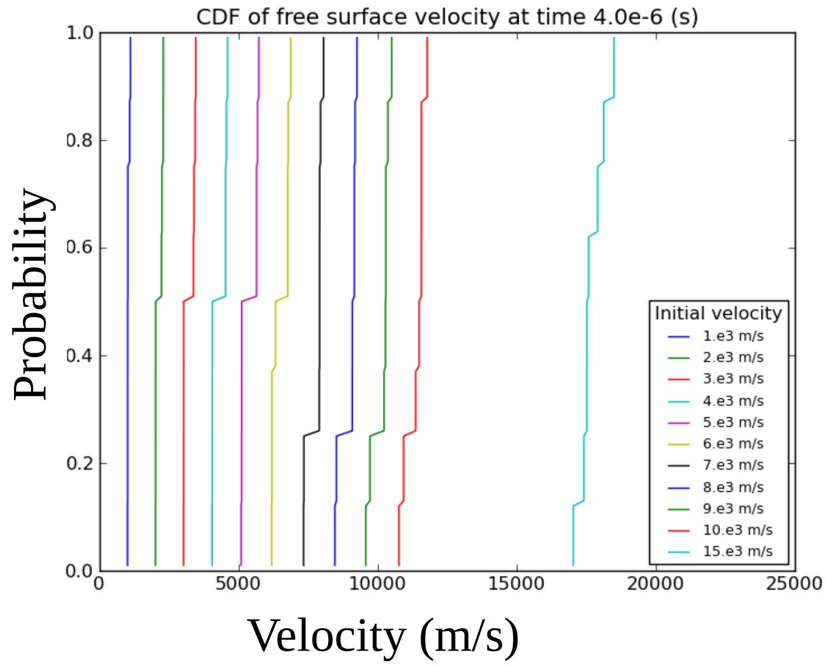
A UQ View of the Experiment

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.
- Such a simplistic distribution assumption is, however, unacceptable.

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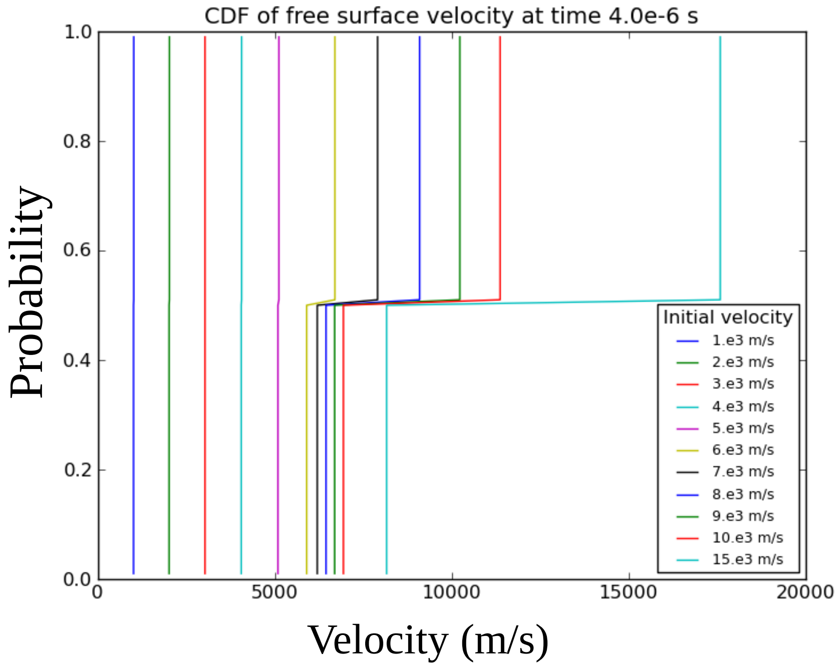
Another UQ Experiment to Emphasize the Point

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.



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

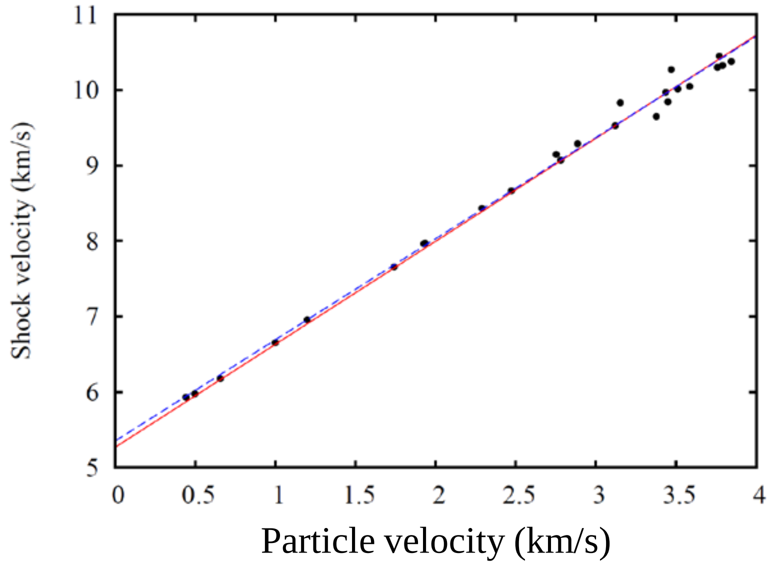
Even though we know the MG equation of state is not accurate over a wide range it does have a small number of parameters and we can use this model as a test case for a more formalized approach for a wide range EOS.

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

$$u_s = C_0 + S u_p,$$

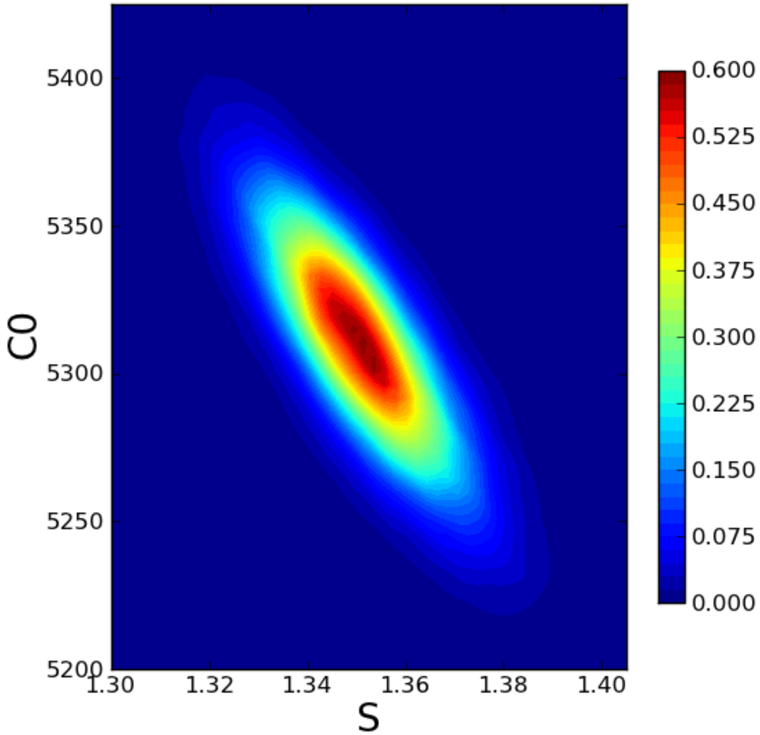
$$
\begin{aligned}
P_R(\rho) &= P_H(\rho) = P_0 + \rho_0 u_s u_p \\
E_R(\rho) &= E_H(\rho) = E_0 + (P_H + P_0)\mu / 2\rho_0 \\
T_R(\rho) &= T_H(\rho) = e^{\Gamma_0 \mu}[T_0 + C_V^{-1} \int_0^{\mu} e^{-\Gamma_0 \mu} \mu^2 u_s \frac{du_s}{d\mu} d\mu]
\end{aligned}
$$

MG "Analytic" Model
Uncertain model parameters obtained from data



$$u_s = C_0 + S u_p,$$

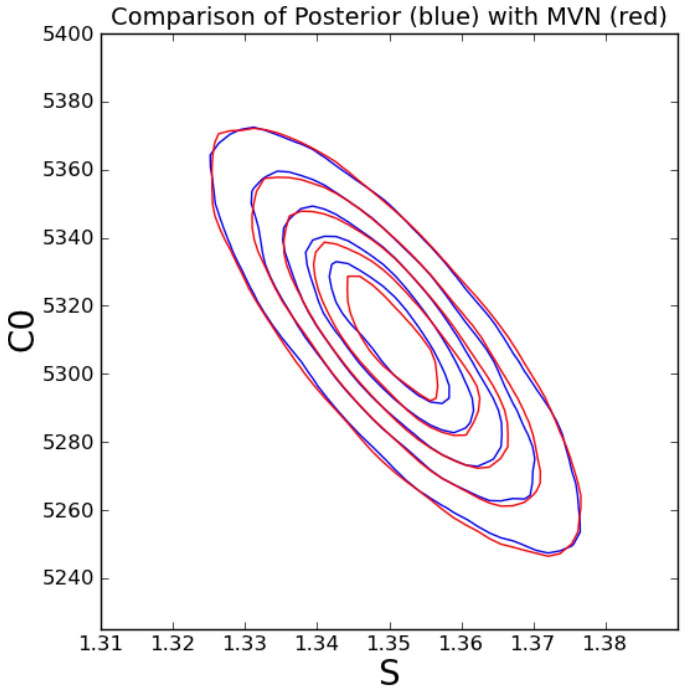
Infer parameters C_0 and S from shock data

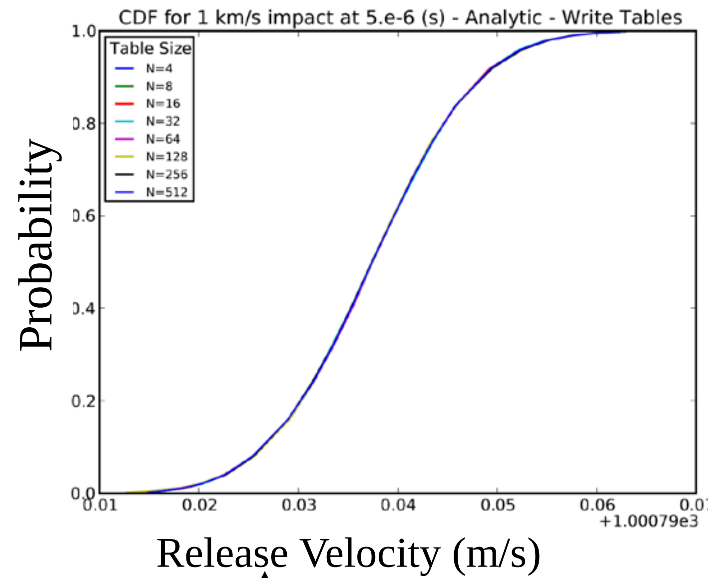


Joint posterior distribution of the two parameters

- represents uncertainty due to data noise
- sampled with Markov Chain Monte Carlo

Uncertain parameters represented with Polynomial Chaos expansions and propagated through hydrocode





$$S = a_0 + a_1\,\xi_1 + a_2\,\xi_2 \qquad S = 1.351 + 0.01367\,\xi_1$$

$$C_0 = b_0 + b_1\,\xi_1 + b_2\,\xi_2 \qquad C_0 = 5310 - 26.25\,\xi_1 + 20.25\,\xi_2$$

1st order Wiener Hermite coefficients obtained by Cholesky factorization of posterior covariance matrix (multi-variate normal (MVN) approximation)

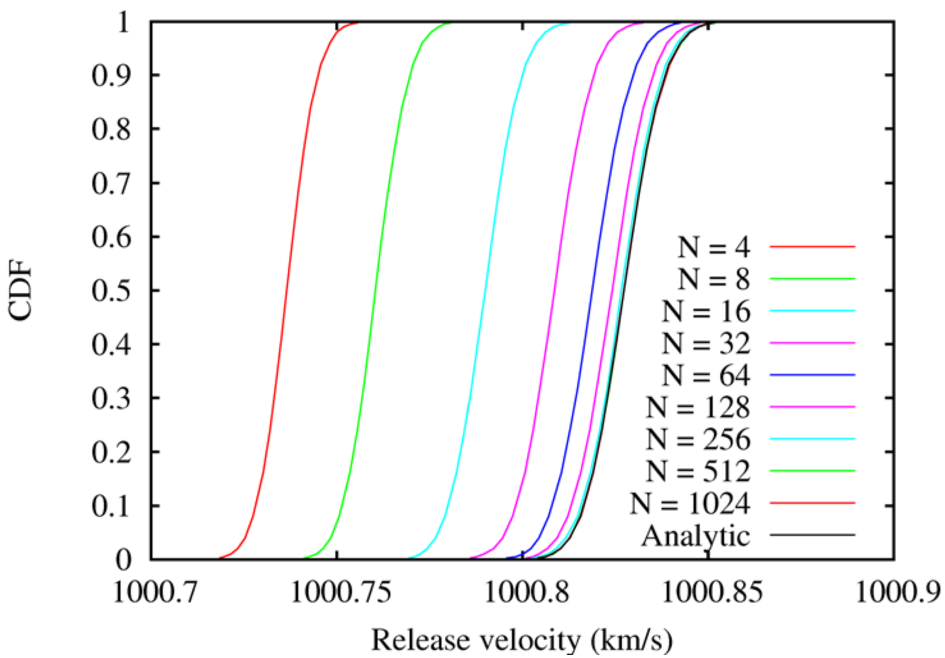
$$\updownarrow$$

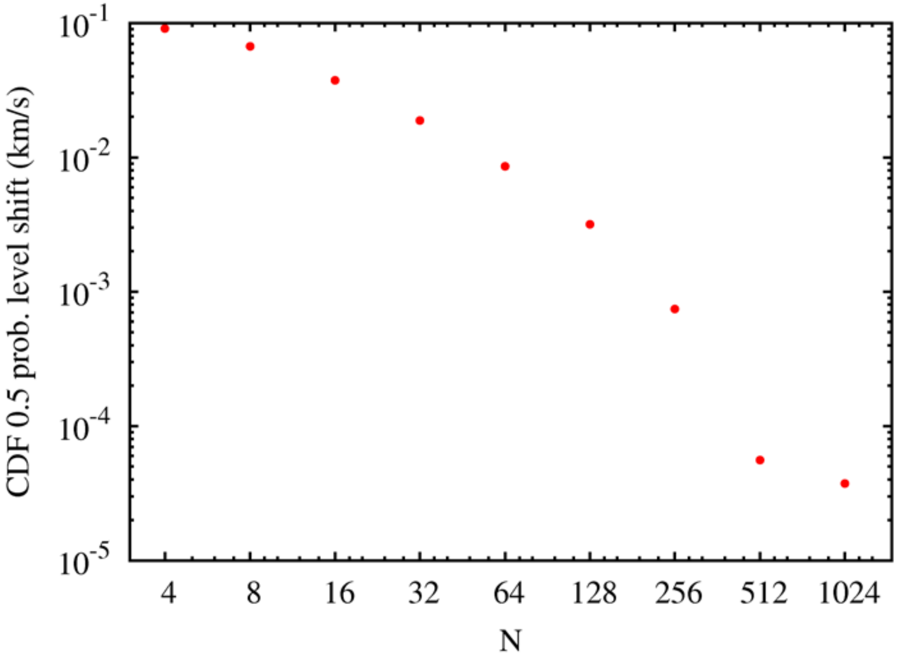
$$R = \sum_{n=0}^{N} \alpha_n \psi_n(\xi)$$

$$\alpha_n = \frac{\langle R\,\psi_n(\xi)\rangle}{\langle \psi_n(\xi)^2 \rangle}$$

Use 3 x 3 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.

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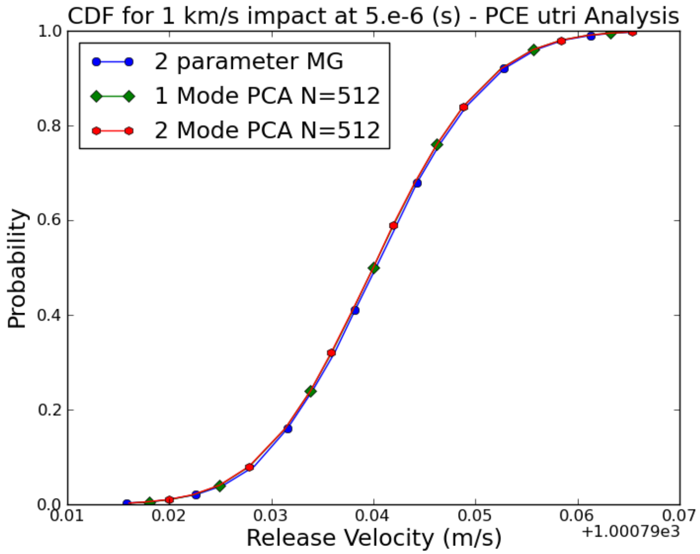
Improved Tabular Representation

EOS tables built using unstructured triangular grids:

- **Wide-range EOS features, such as phase boundaries, easily followed.**
- **Grid adaptation allows reduction of table size.**
- **Using triangulated grid points identical to the rectangular tables, the PCA approach has been verified on the MG EOS example case.**



Some issues remain for a fully unstructured capability:

- **Grid adaptation for EOS representation error reduction can induce significant noise in the PCA analysis.**
- **Boundary grid locations may be carefully chosen to eliminate this noise, but interior points of the mesh are a much more difficult optimization problem.**

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Wide Range EOS UQ Infrastructure

- We are developing a wide range EOS UQ modeling infrastructure that will allow significant automation of the modeling process and enable broader access for the engineering community to these capabilities.
- The developed infrastructure includes:
  - User input:
    - EOS models and inference parameters
    - Experimental and calculation data
    - Choice of noise model
  - Bayesian inference of posterior distributions using MCMC techniques.
  - Automated extraction of multi-variate Gaussian PDF for inferred parameters.
  - Sampling of the inferred model parameters using Dakota.
  - Coordinated table generation at each sample point.
  - Condensed PCA representation of the ensemble of tables.
  - Unstructured triangular table read/write utilities for hydrocodes.

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Summary

- We have outlined a general way of thinking about the upscaling UQ problem for shock hydrodynamics.
- The basic PCA tabular 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 have pulled together an initial set of required technologies which are compatible with a sustainable UQ enabled EOS modeling technology.