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

Uncertainty Quantification and Multiscale Materials Modeling

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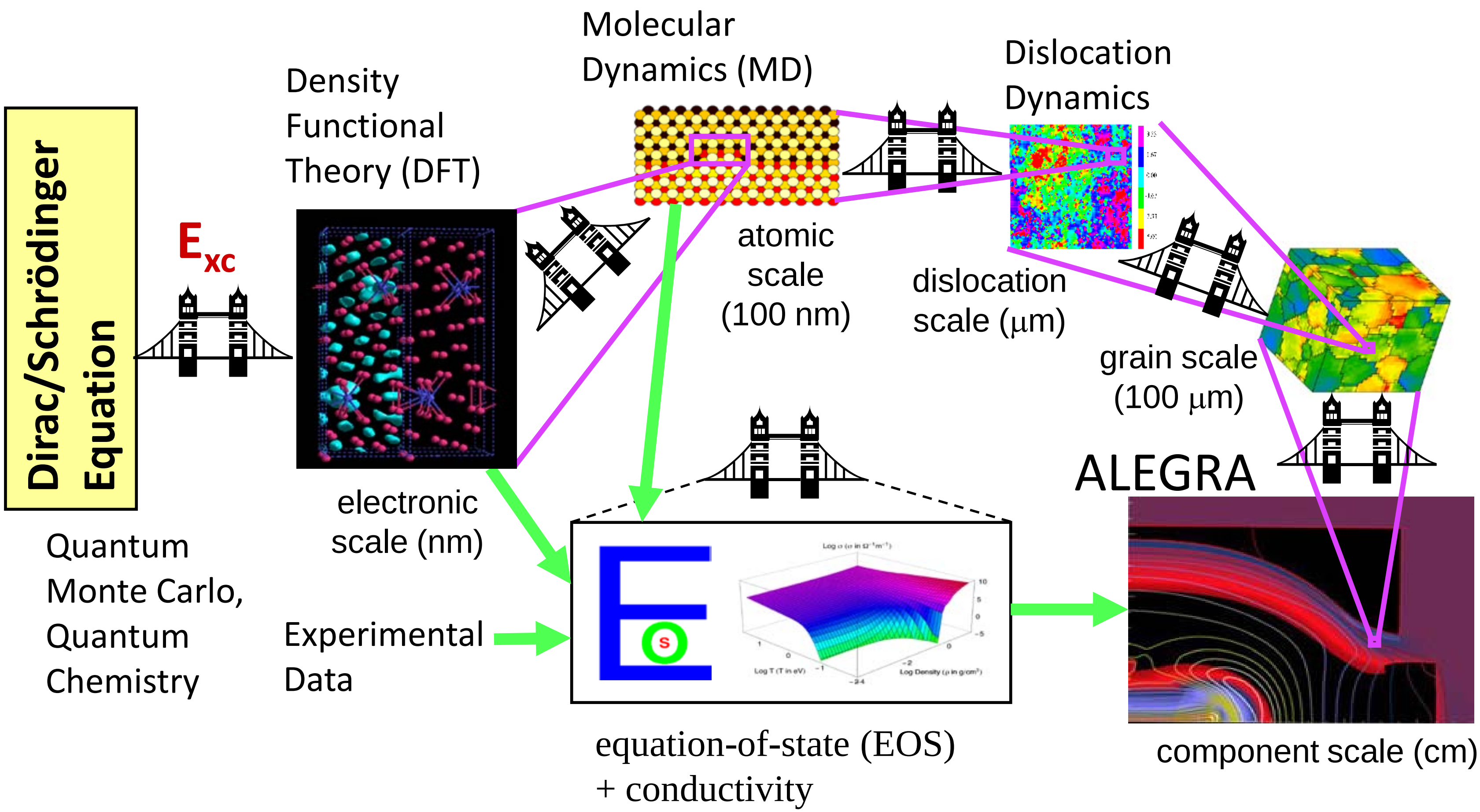
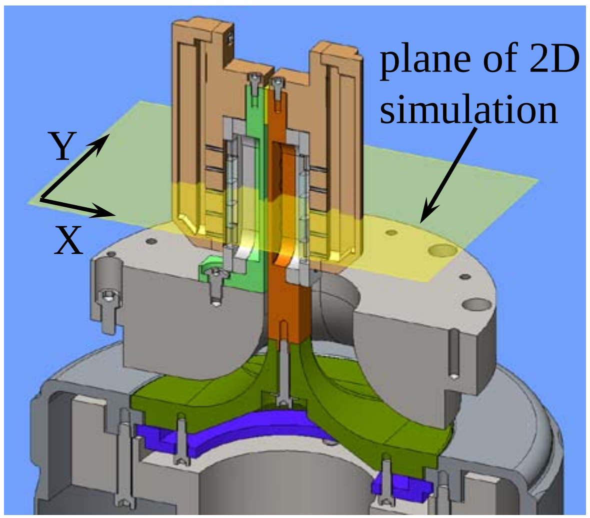
The Upscaling Promise

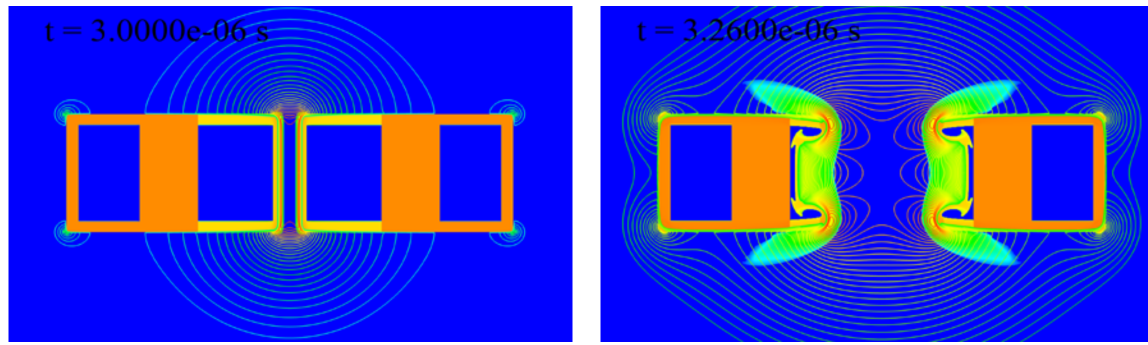


Predictive design of Z Experiments (Lemke)

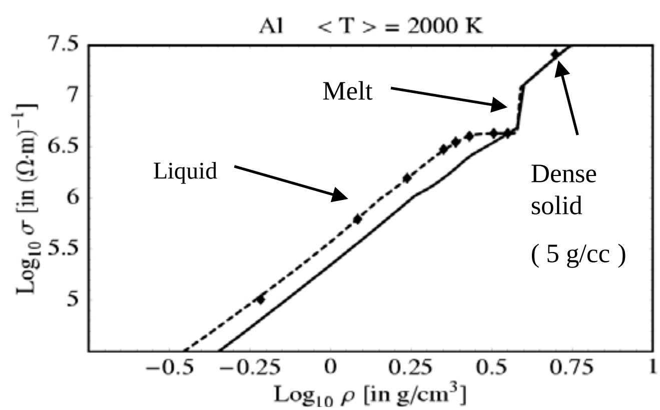
Two-sided Strip-line Flyer Plate Experiment



2D Simulation Plane of Two-sided Strip-line



- **Resistive MHD.**
- **Accurate electrical conductivities.**
- **Accurate EOS.**
- **Circuit model for self-consistent coupling.**
- **Dakota optimization loops.**
- **DFT-MD computations needed to accurately characterize material response.**



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Characteristics of current successful upscaling practice

- *Uncertainties are managed by the expert user.*
- *Careful management of continuum computations is required.*
- *DFT-MD is important to develop accurate EOS and conductivity models.*
- *No particularly ubiquitous formal processes to deal with uncertainties.*
- *The engineering job does tend to get done by a sophisticated scientific community.*
- *This community would welcome better support for what they do.*

Motivation and research target for our group

- Can we learn to communicate with each other?
- What are the practical requirements for getting into the business of commonplace and fully integrated UQ for shock physics with UQ informed upscaling?
- Can we demonstrate such a system and how it might work?
- How does DFT-MD scale UQ information flow to the continuum?
- How do continuum results transfer back down to additional requirements on DFT-MD accuracy?

Hydrodynamics

- **Euler's Equation**
  - 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, $p = P(\rho, e)$
- **The upscaling mechanism or bridge is the equation of state closure. This closure is independent of the conservation equations.**

The Predictive Analysis Delta Cycle

Hydro Calculations

Up scaling

Down scaling

Formally represent an uncertain EOS

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

DFT-MD computations + experimental data + associated error estimates

Feedback precision requirements to DFT-MD modelers and validation data sources

Current focus of our efforts is in blue

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Requirements for a Practical Solution

- Evolutionary – Start from where we are today.
- Well grounded – Acceptable practice from various expert points of view.
- Useful, understandable and accessible

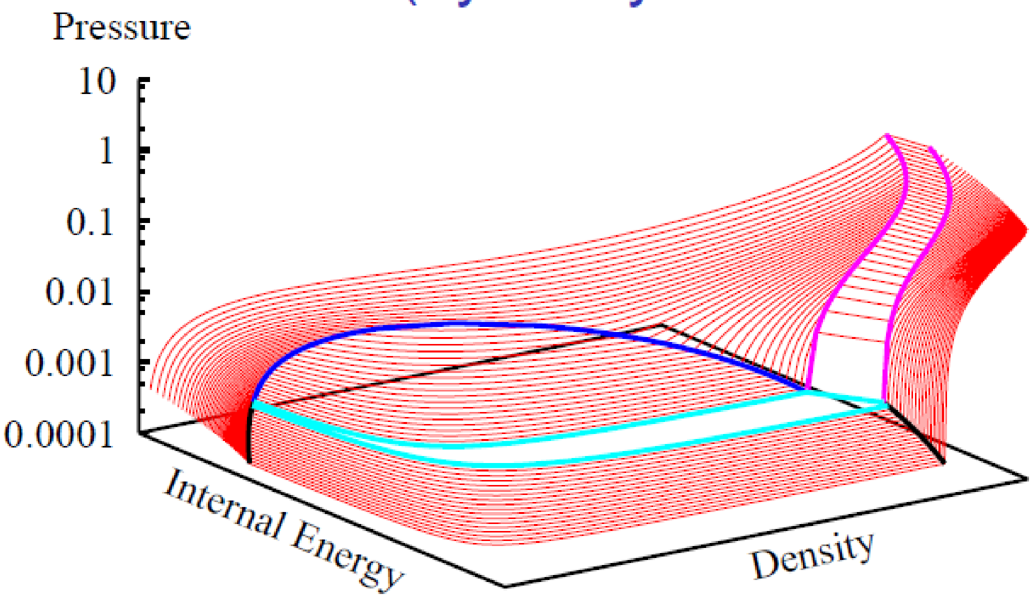
  "The purpose of computing is insight, not numbers"

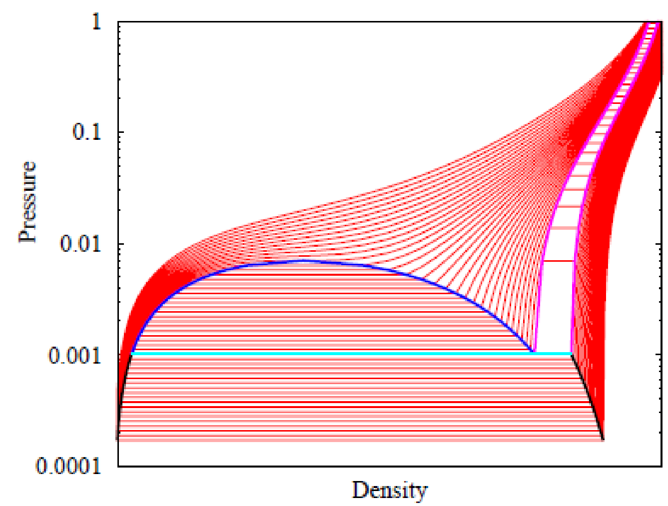
  and

  "Probability is too important to be left to the experts."
  – Richard Hamming
- Backward compatible with decades of methodology, models and data.

Equation of State Surface

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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Uncertainty in the EOS Bridge

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

We must figure out how to build this bridge.

- Full model form (Strategy I)
  - Several to tens of parameters.
  - One can build an uncertain EOS with the parameters as random variables.
  - Not a practical hydrocode solution.

- Tabular EOS (Strategy II and III)
  - Tabular forms are built for computational efficiency
  - To be practically useful we must build uncertainty into the tabular forms.
  - How much error the tabulation is allowed to introduce is an important issue to address.

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

From the product rule for probabilities $P(A,B) = P(A\,|\,B)\,P(B)$
is derived Bayes' Theorem (continuous version)

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

which expresses the density on the model parameters given data in terms a likelihood density $p(d\,|\,\beta)$ describing the data (usually a composite of fit and noise models) and a prior density $\pi(\beta)$. The denominator $p(d)$ is a normalizing factor.

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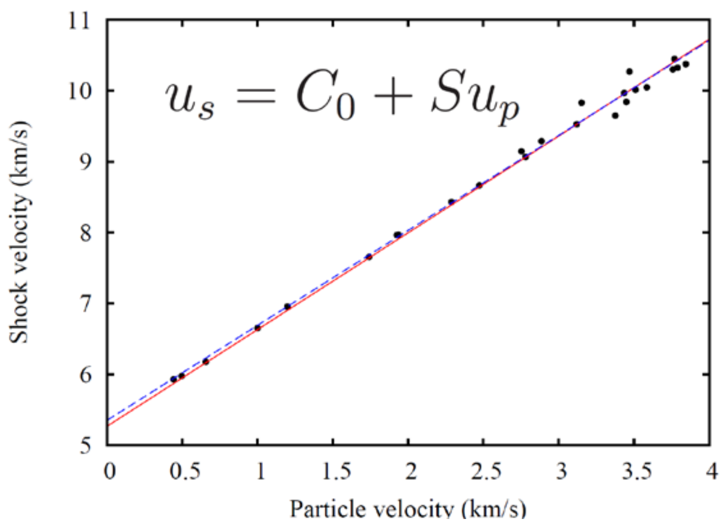
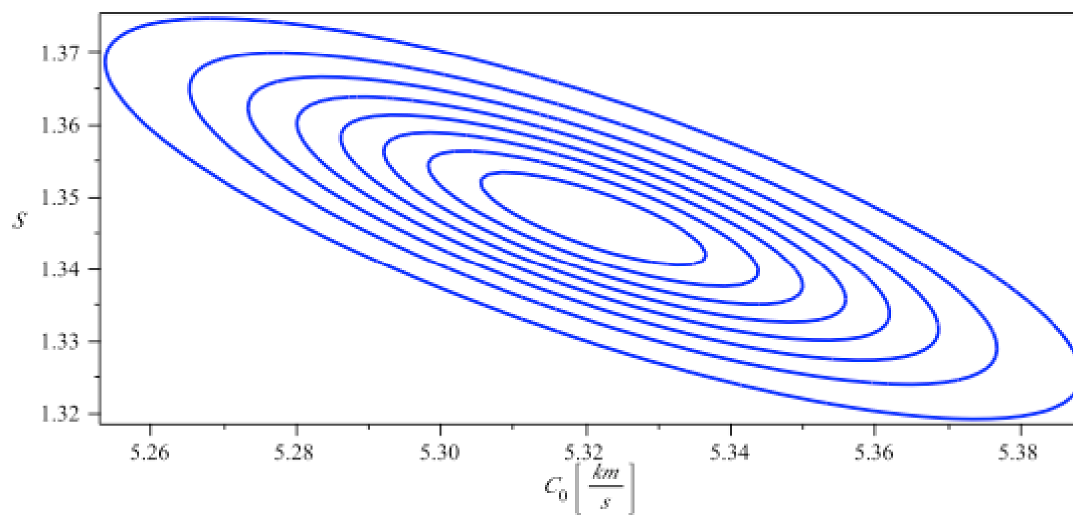
Strategy I – Parametric representation

Consider an EOS

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

- 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
- Pressure and temperature become random variables (for fixed density and internal energy)





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Strategy II – Table Perturbations

•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.

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Karhunen-Loève Representation

- Given a (vector valued) process, find 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 = PCA (subtract mean, calculate SVD for data array)

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

Strategy III – PCE Table Library

- 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.

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

The Hydrocode Interface

- **Dakota is a well-known general toolkit for black box large scale engineering optimization and uncertainty analysis developed and distributed by Sandia.**

- **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.**

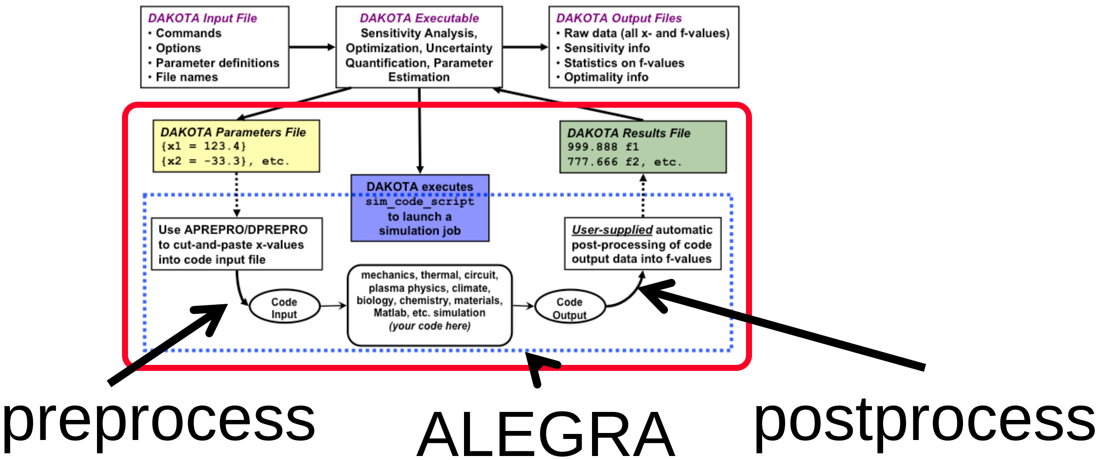
- **Making the UQ enabled upscaling/downscaling process an engineering reality requires a much smaller "user energy barrier" at multiple points.**

Simplifying ALEGRA/Dakota Usage

- **Can we make usage of Dakota as easy as building an ALEGRA input deck with a Dakota input section?**
- **What response functions (or quantities of interest (QOI) or figures of merit) should be provided as easy-to-use production features?**
- **Can specialized response function scripts be easily implemented?**
- **Does overall robustness and ease of use improve evidenced by more ubiquitous UQ enabled results?**

Embedding DAKOTA in ALEGRA

File interface:



Embedded interface:

```
DAKOTA INPUT "
    method, nond_sampling, samples = 10
    variables, normal_uncertain = 2
        means           =   1.076e+12  0.355
        std_deviations  =   0.01e+12   0.1
        descriptors         '_YMOD_'   '_POIS_'
    responses, num_response_functions = 1
        no_gradients, no_hessians
    interface,direct,
       analysis driver='alegra'
       processors_per_analysis=2
"
termination time 3.5e-05

... (normal ALEGRA input) ...

model 100 elastic plastic
  youngs modulus     _YMOD_
  poissons ratio     _POIS_
  yield stress       6.0e+9
  hardening modulus  2.0e+9
  beta               0.5
end
```

samples

```
transient magnetics

  ... (physics input) ...

  tracer points
    lagrangian tracer 20, x=0.0 y=0.0 z=4.0
  end

  response functions
    tracer 20, variable = COORDINATES, z, end
  end

end
```

- **<u>Implementation Challenges</u>:**
  - **Make ALEGRA and some Third Party Libraries(TPLs) re-entrant**
  - **MPI communicator cannot be hardcoded.**
  - **Establish a transparent Dakota interface**
  - **Place Dakota as TPL in build system.**
- **<u>Response Functions</u>:**
  - **Tracers and Globals at specified times**
  - **Future: Normed differences relative to user defined information.**

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UQ Tools for Downscaling Information Extraction

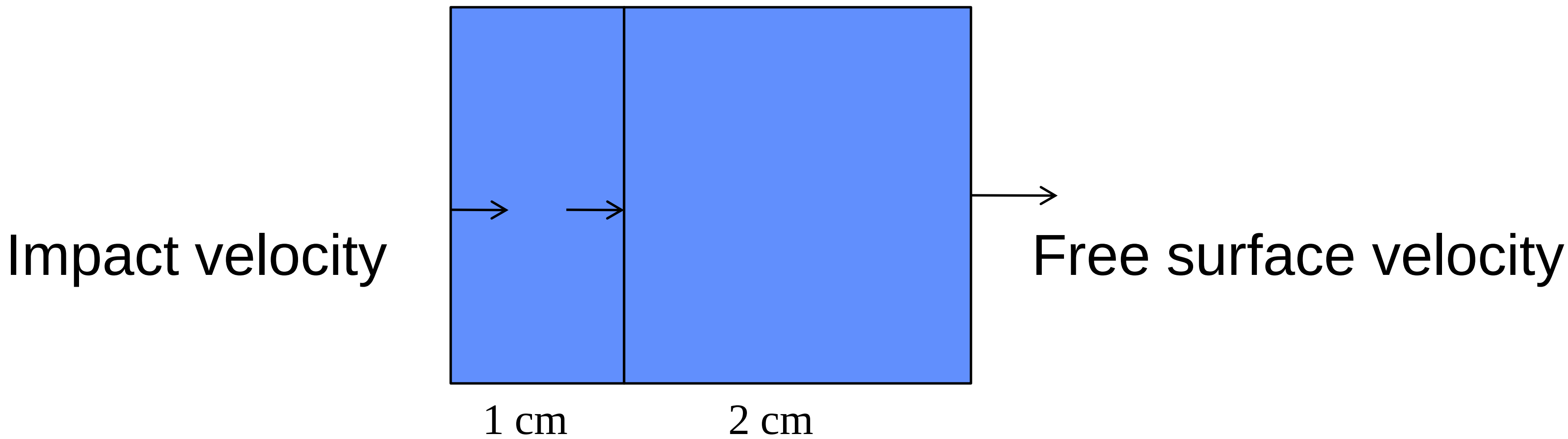
Engineering insight into how epistemic and aleatory uncertainty is affecting an engineering response function or quantity of interest should be readily accessible and visually clear to the engineering user. Part of our research entails finding delivery solutions to remove operational hitches and barriers to insight.

"Probability is too important to be left to the experts."

Dakota is still on the development curve relative to standardized output databases. We developed a python tool for reformatting Dakota text output to be useful by simple plotting tools.

This simple tool provided visual access to a probabilistic viewpoint on the output results.

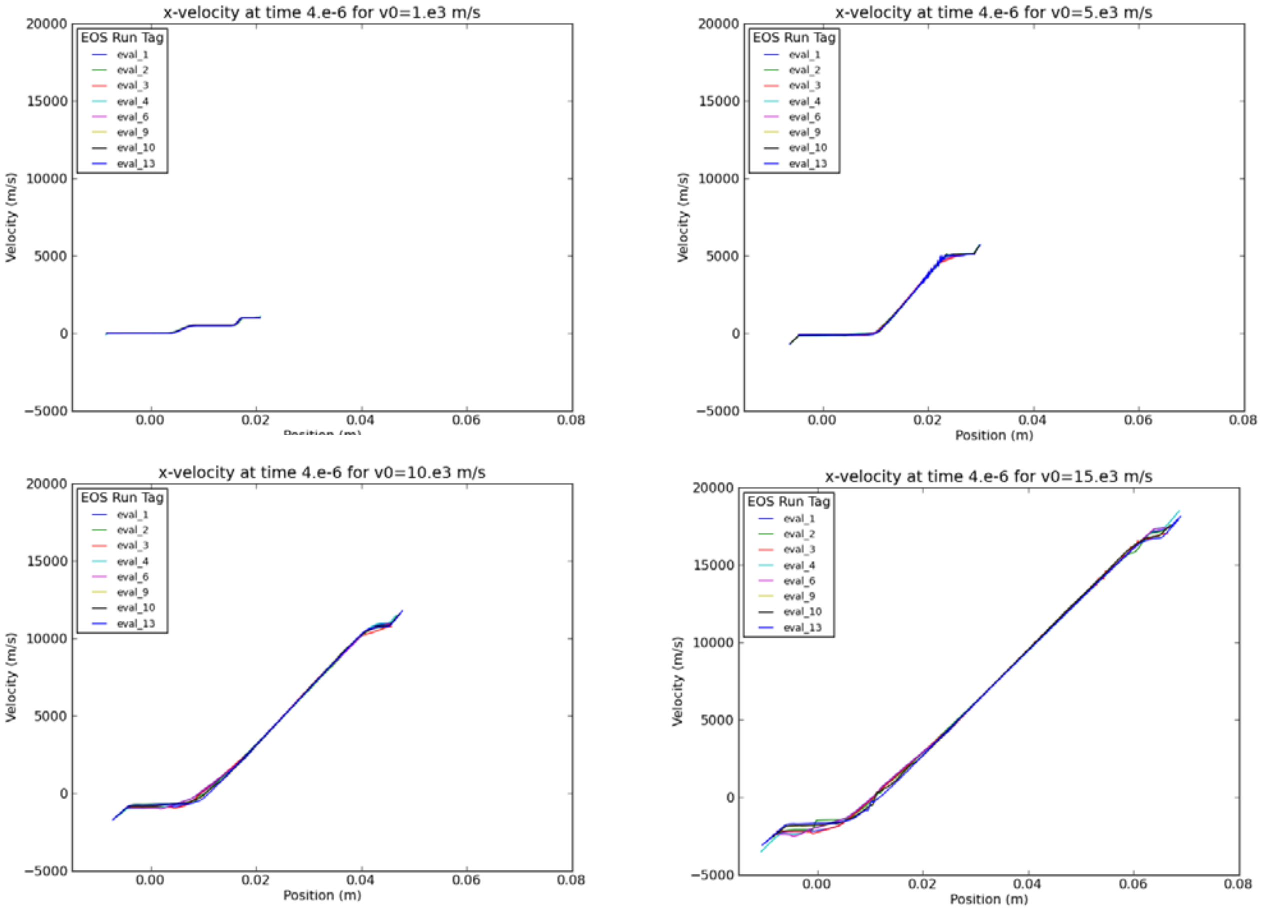
AL Flyer/Target Impact Test Case



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

An Experiment

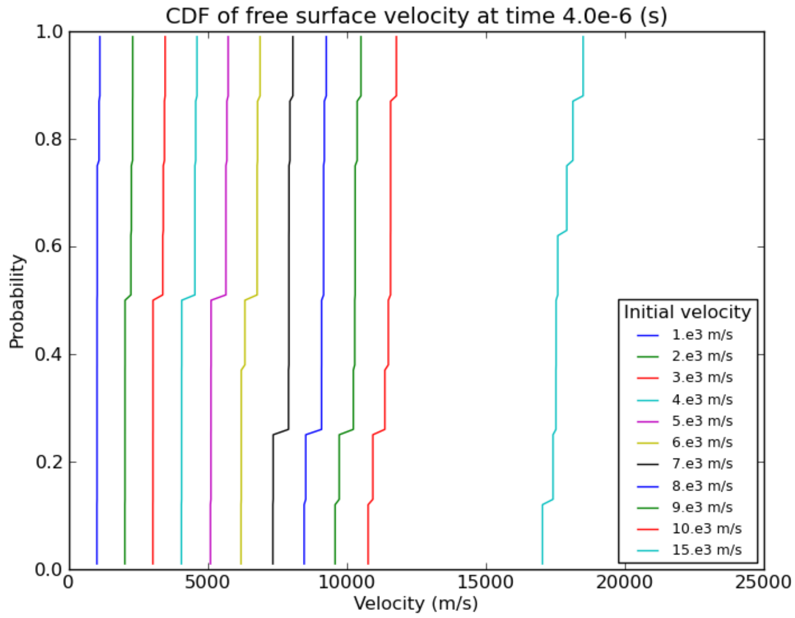
Current tabular models do not come with a UQ representation. Can we get a feel for the variation to be expected from different wide range tabular models with varying provenance, for a given interpolation scheme? 8 wide range tables were used as a surrogate for the drawing of realizations from a random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

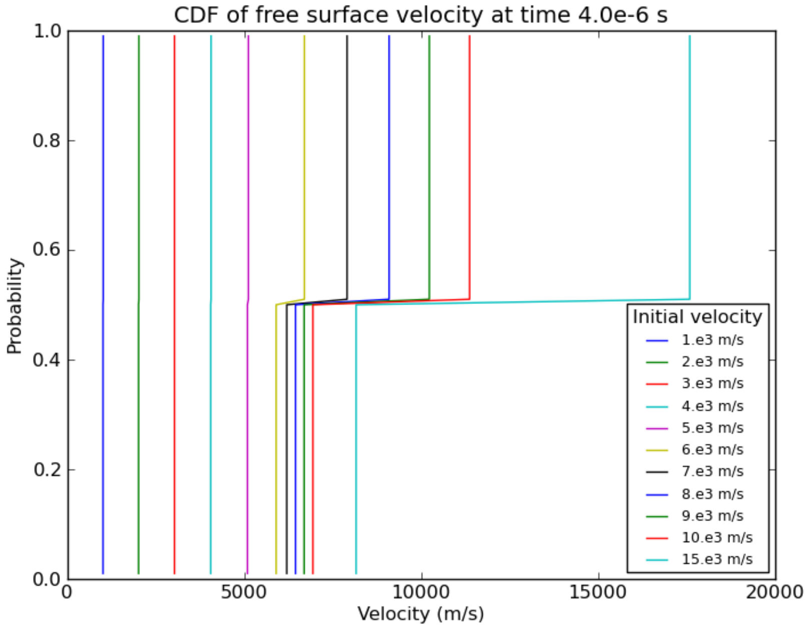
Assume that the 8 tables each occur with a .125 probability



- 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.
- Note that the physical information content is not as rich as the previous slide.
- We shall see that the simplistic distribution assumption is suspect.

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 you know nothing and give each EOS a .5 probability. The huge variation at higher velocities is indicative of severe epistemic uncertainty as expected.



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Using 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.

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

$$u_s = C_0 + S u_p,$$

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

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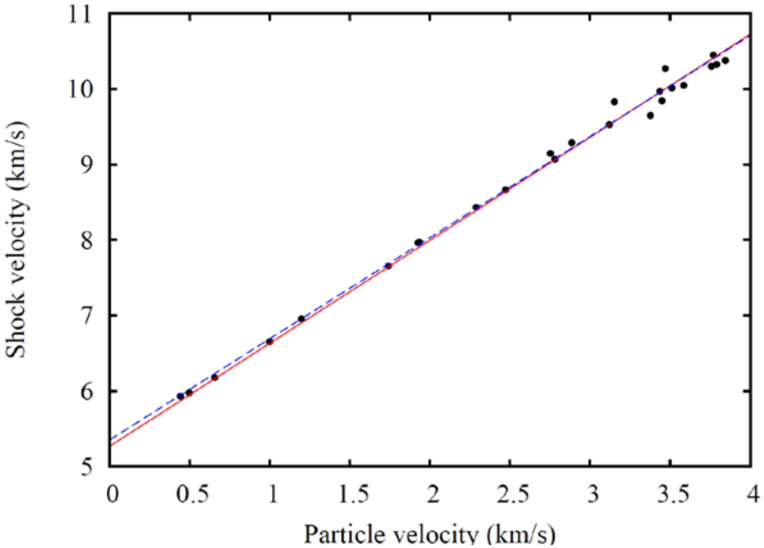
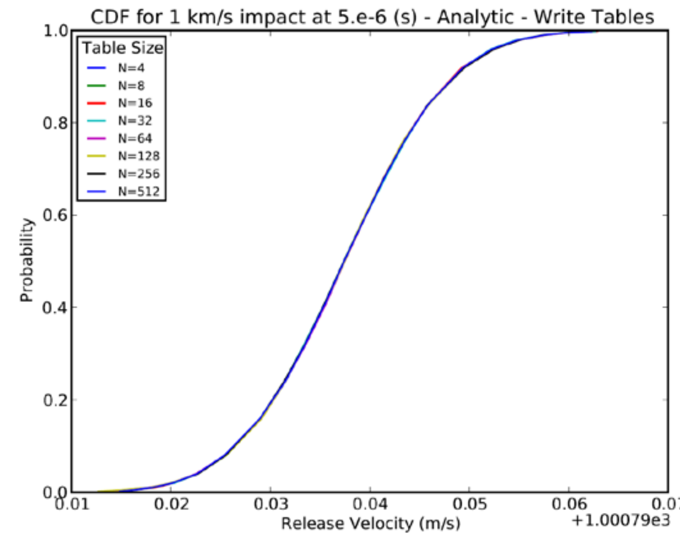
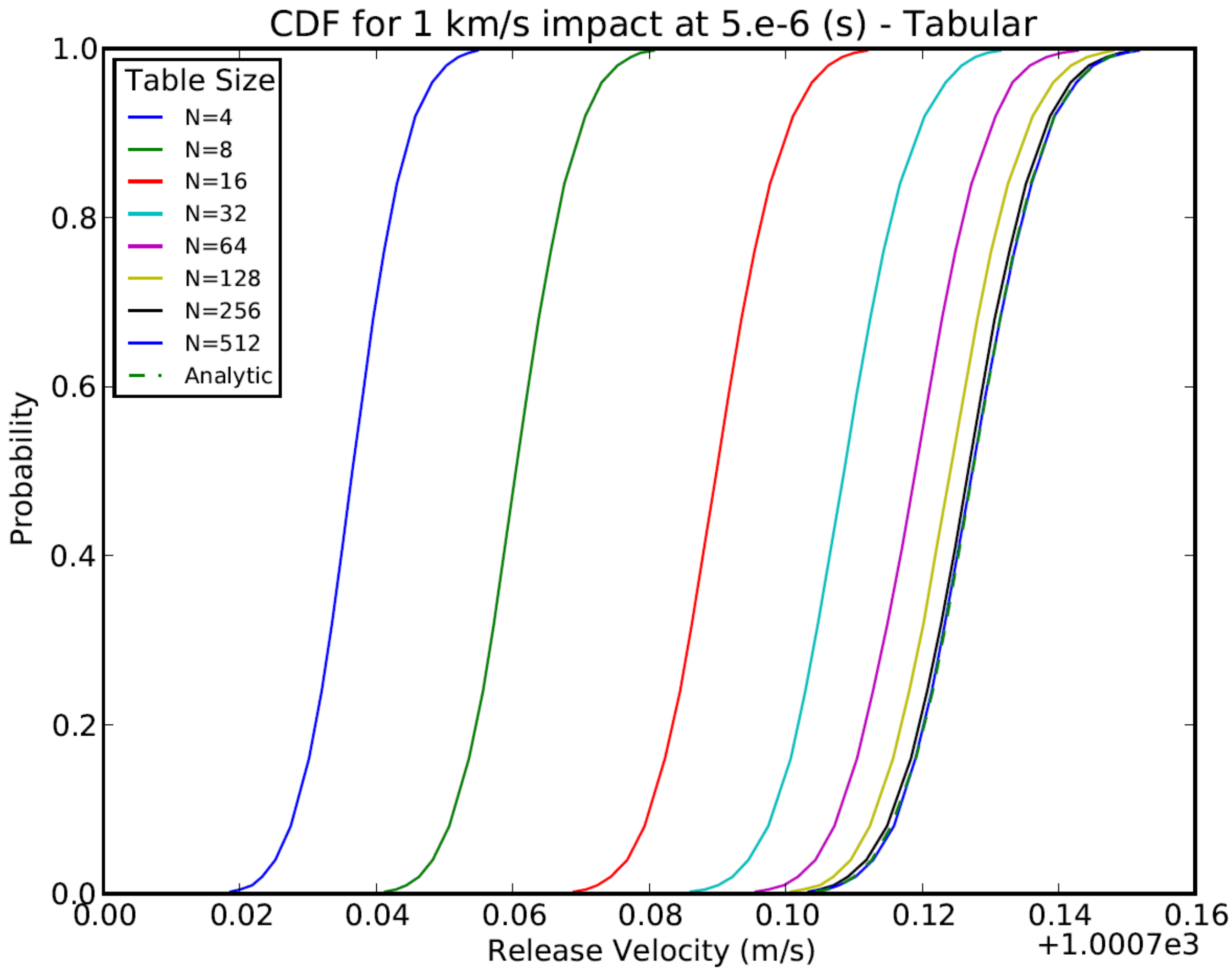
MG "Analytic" Model
3x3 Polynomial Chaos Expansion (PCE) UQ





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

Parametric UQ with 9 PCE Tables



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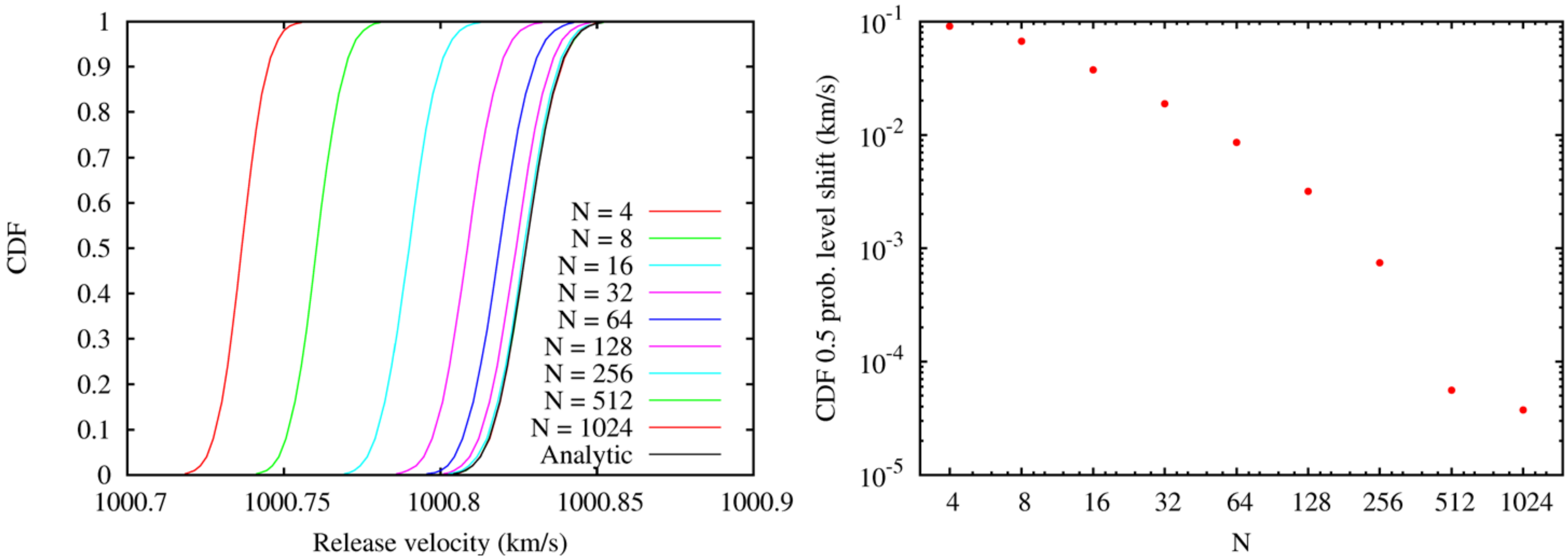
Sorting out the effect of Tabular interpolation

A tabulated EOS is an imperfect representation of an "analytical" EOS. One expects that for an accurate enough tabulation the uncertainty due to tabulation may be safely ignored in the UQ analysis. The following tabular convergence study tests this hypothesis.

Convergence study details:

- MG model described previously is analytic baseline
- Tabulate MG model on NxN density/temperature grid
    - N=4,8,16,32,64,128,256,512,1024
    - Reference density/temperature included in grid
    - Large enough ranges ensures no extrapolation
    - Uses rational interpolation on a Coon's patch
- Perform prior UQ analysis for each N
- Test convergence of CDF to analytic result
- Correlate convergence with accuracy of tabulation

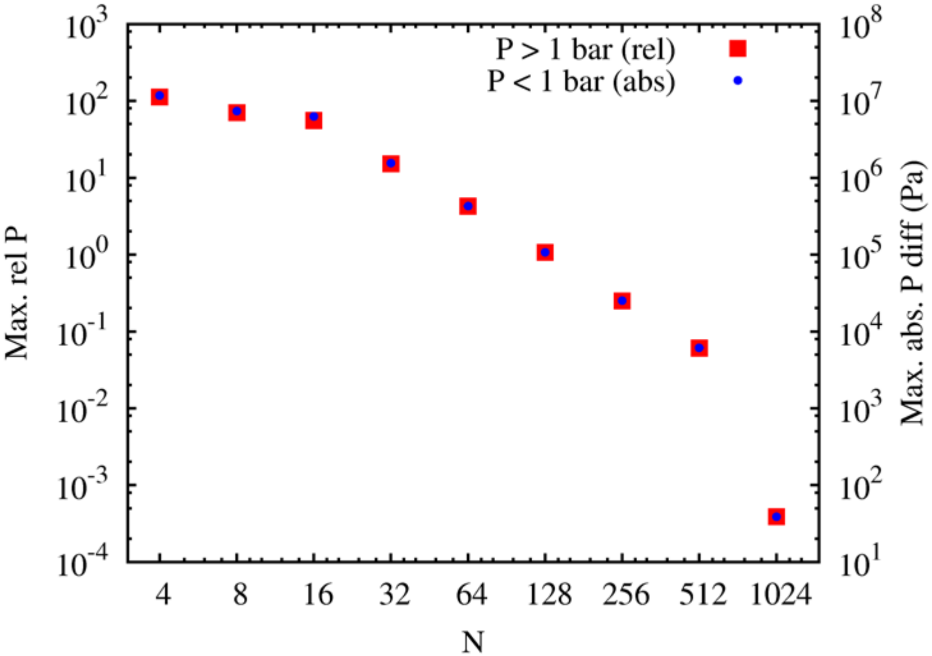
CDF convergence under table refinement

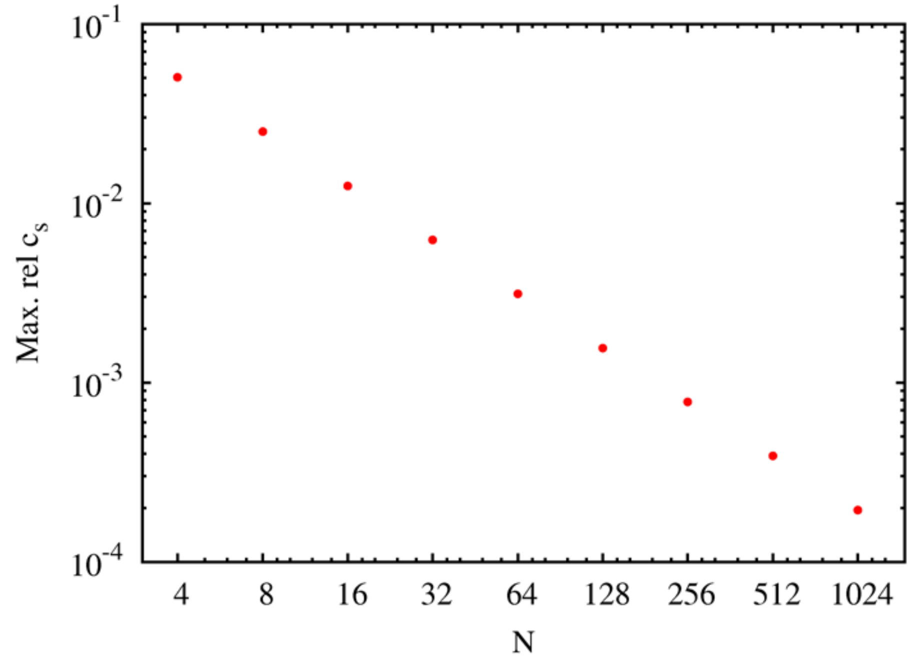


- CDF converges to analytic result, as expected
  - Shift is converged within sampling error at N=512
  - Convergence appears faster than a power law
- Problem: the converged N=512 produces a very large table for a simple, limited range EOS. Wide range EOS models typically have N~128. Improved tabulation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

Tabular interpolation verification

Maximum relative difference to analytic EOS over all state evaluations for pressure and sound speed:





- Power law scaling in relative error: $P \sim N^{-2}$, $c_s \sim N^{-1}$
- Absolute pressure difference scales identically to relative pressure
- Max relative errors at convergence: P = 6% and c_s = 0.04%
- Implication: improved tabulation schemes need only reproduce the analytic pressure to ~ 6% to obtain a converged result

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Is there a better tabular approach?

Use Principal Component Analysis to look for a reduced tabular representation with the hope that most of the uncertainty can be represented in a few modes and therefore reduce the overall size of the delivered tables.

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

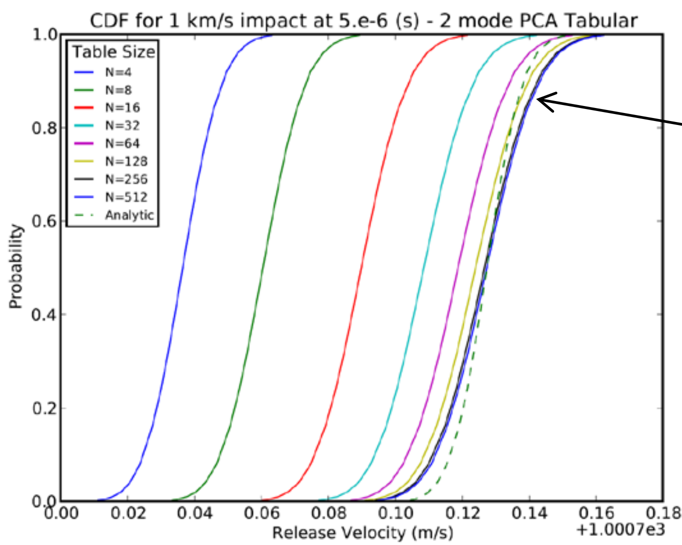
Perform Principal Component Analysis (PCA)

Choose a truncated set of modes.

Compare with previous results.

Parametric UQ with Principal Component Tables from PCE

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



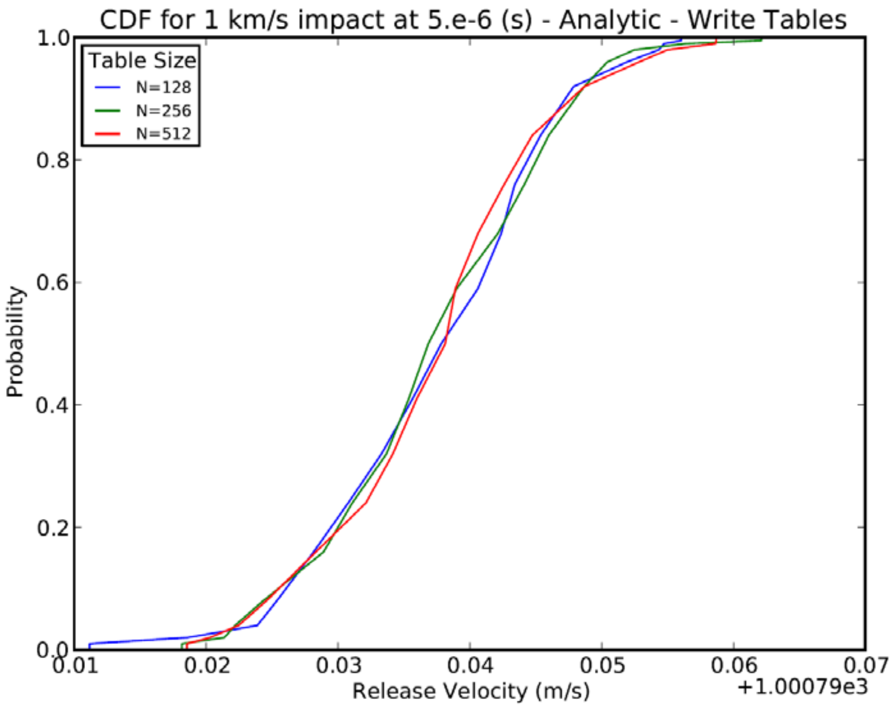
Output distribution is too broad.

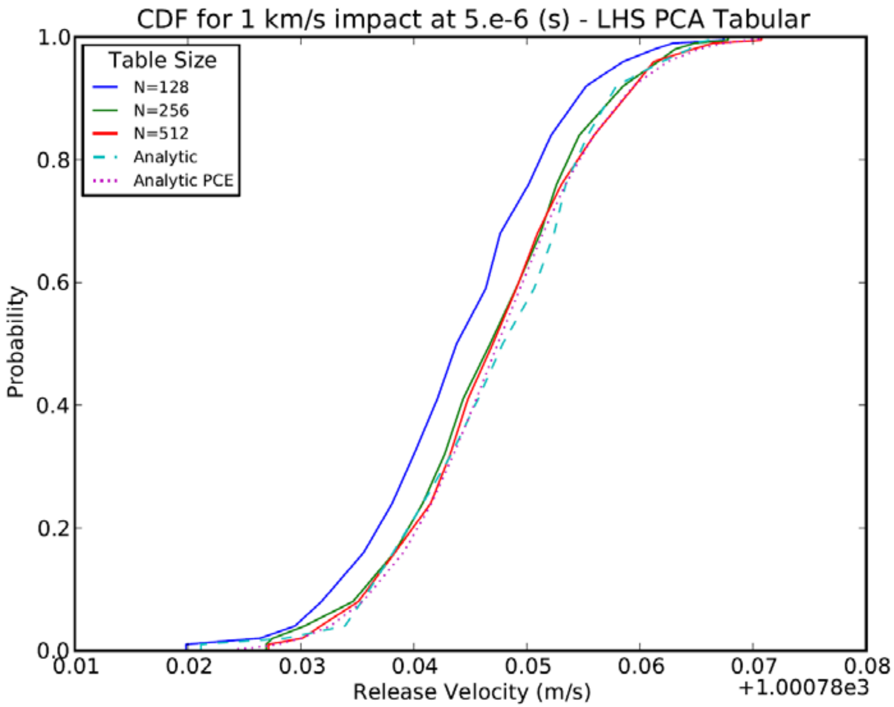
Why?

We need a weighted PCA which accounts for PCE weights.

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.

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Wide Range EOS – The real problem

- The basic PCA approach clearly works for Mie-Gruneisen EOS.

- What about wide range EOS?
  - Will we still get useful compression from PCA?
  - What about phase boundaries?
  - How does uncertainty information from experiment/DFT-MD get characterized and feed into the complex model forms?
  - What about EOS stability?
  - How much control on the mean field can or should be given to the wide range EOS modeler?

- How to enable downscale information transfer returning along the bottom of the delta cycle?

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Summary

- We have outlined a general way of thinking about the upscaling 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 sustainable going forward.