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Lessons From Uncertainty Propagation Using Tabular, Multiphase Equations of State

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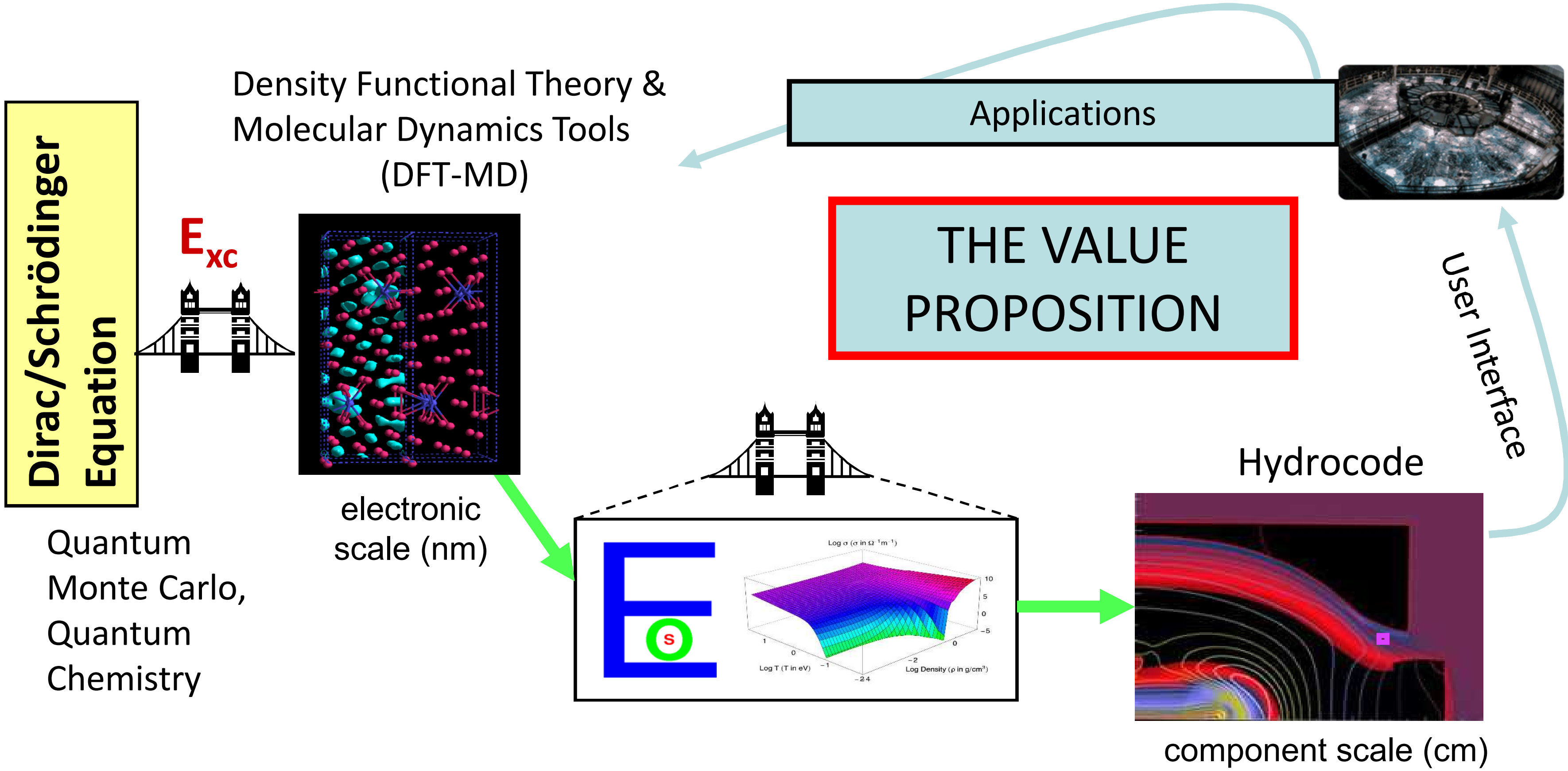
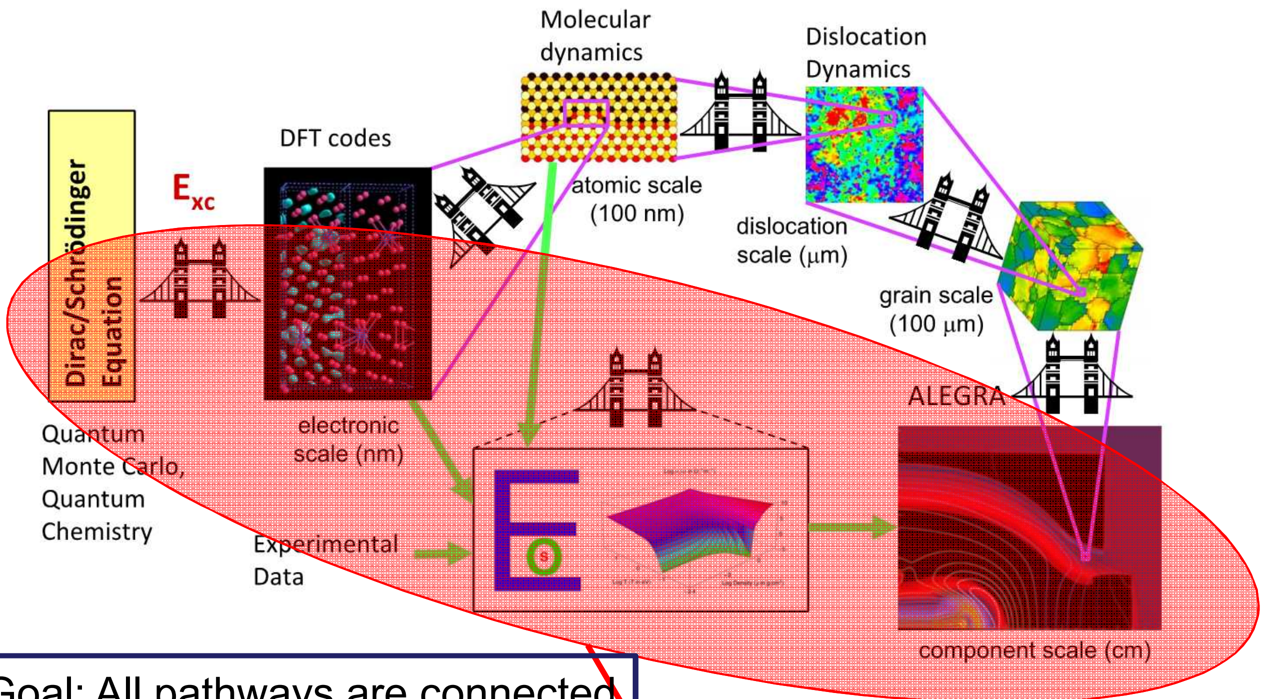
Science based engineering is a multi-scale, multi-physics, multi-parameter enterprise



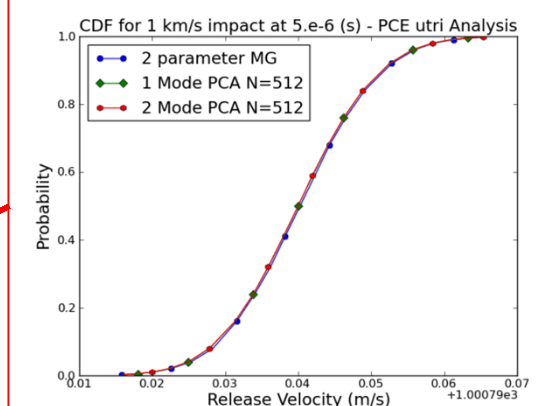
How does one enable this cycle to be more effective?

Propagation of uncertain EOS information



Goal: The analyst running the continuum code should easily get results that can be transformed into the equivalent of "50% chance of rain" to give to the decision maker.

Goal: All pathways are connected in a unified engineering process and iteratively improved. Upscaling bridges must be built with embedded UQ information.



Example: Propagate uncertainty due to statistically equivalent possible EOS fits to the same data, to the analyst.

Our proposed solution

Robinson, Berry, Carpenter, Debusschere, Drake, Mattsson, Rider, "Fundamental issues in the representation and propagation of uncertain equation of state information in shock hydrodynamics", Computers and Fluids, 83, (2013) p. 187–193.

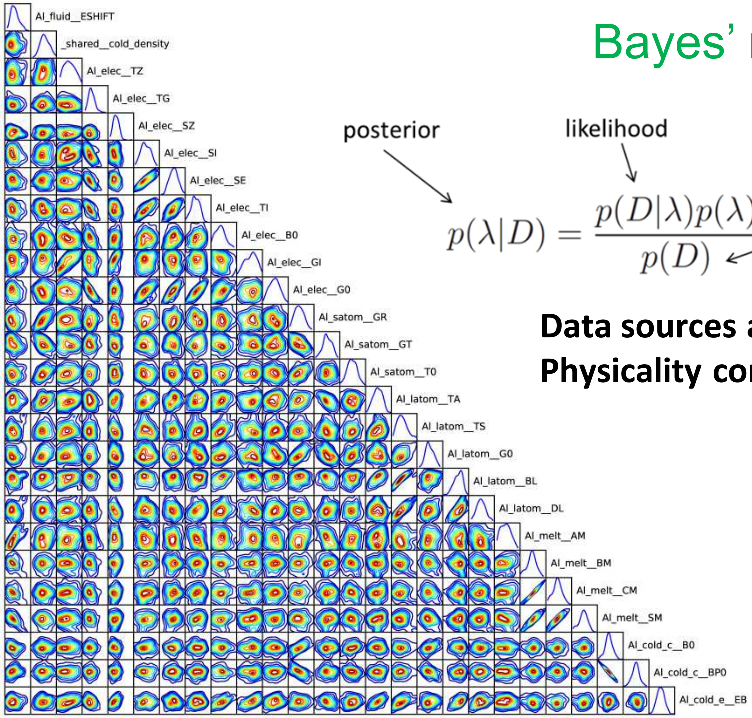
Software Package	Output
EOS model library and data	Proposal Model (XML input deck)
Bayesian Inference using Markov Chain Monte Carlo	Extensive sampling of the posterior distribution function (PDF)
EOS Table Building	Topologically equivalent tables for each sample
PCA Analysis	Mean EOS table + most significant perturbations
Hydrocode + Dakota	Cumulative Distribution Function (CDF) for quantities of interest

History: This work has been supported at Sandia since FY11 under ASC P&EM and V&V.

Multiphase EOS model for Aluminum

- **Key Requirement:**
  - All expert knowledge of EOS construction and proper behavior must be encoded into the xml input file and associated software.
  - This enables later steps to complete since these assume correct EOS behavior
  - XML input files serves as documentation on how to generate the EOS
  - The strategy is similar to hydrocode software build/run environment requiring a reproducible methology except that the output is an EOS table.
- The EOS is built from semi-empirical models, with solid and liquid phases including melt/vaporization/sublimation.
- 37 total parameters, 26 constrained well enough by data for inferring UQ information.
- 16 Data Sources from: Hugoniot expt./calc., IEX/thermophysical expansion data, QMD isotherms near critical point, DAC compression, DFT cold curve, melt and vaporization expt./calc.
- Constraints on physicality: smoothness and convexity change limitations along phase boundaries; thermodynamic stability checks across full range of interest

Al EOS model calibration and inference



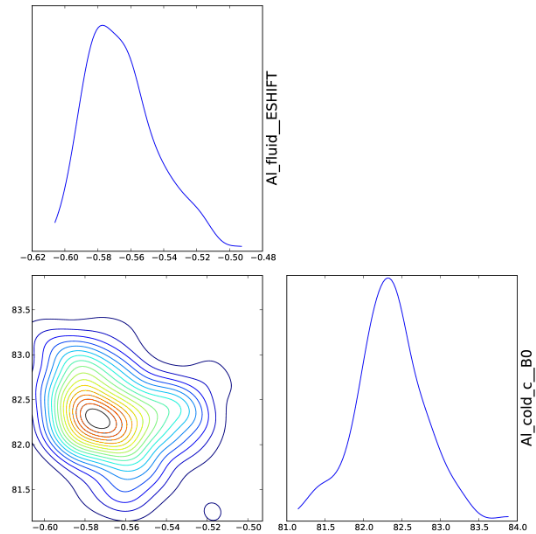
Al model EOS inference

Bayes' rule

posterior — likelihood — prior — normalization

$$p(\lambda|D) = \frac{p(D|\lambda)p(\lambda)}{p(D)}$$

Data sources appear in <u>likelihood</u>
Physicality constraints appear in <u>prior</u>



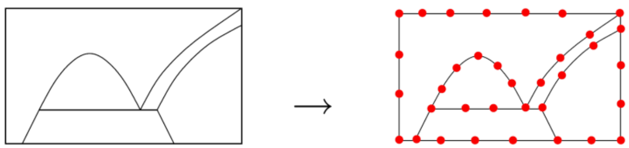
A marginal distribution

Bayesian inference to determine posterior distribution function of parameters is costly:

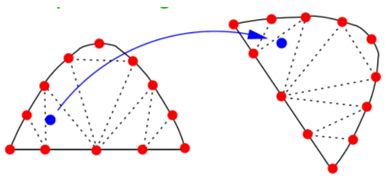
- Use adaptive Markov Chain Monte Carlo (MCMC) scheme to reduce number of steps
- Use optimization to find Maximum A Posteriori (MAP) parameters from which to start chain
- <u>Each posterior evaluation is roughly equivalent to generating an entire EOS table and having an expert check it for correct behavior!</u>
- PDF evaluations may be parallelized to enable long chains (~3M steps for this EOS, one serial evaluation is approximately 3 sec.)

Tabular EOS generation

- UTRI tabular format
  - Triangular mesh e.g. (density, energy) or (density,temperature) with all other thermodynamic quantities and their derivatives tabulated at the mesh nodes.
  - Mesh nodes added to reduce error below tolerance with respect to model.
- Must build N UTri tables which are topologically equivalent and of similar accuracy:
  - Adaptively mesh boundaries:



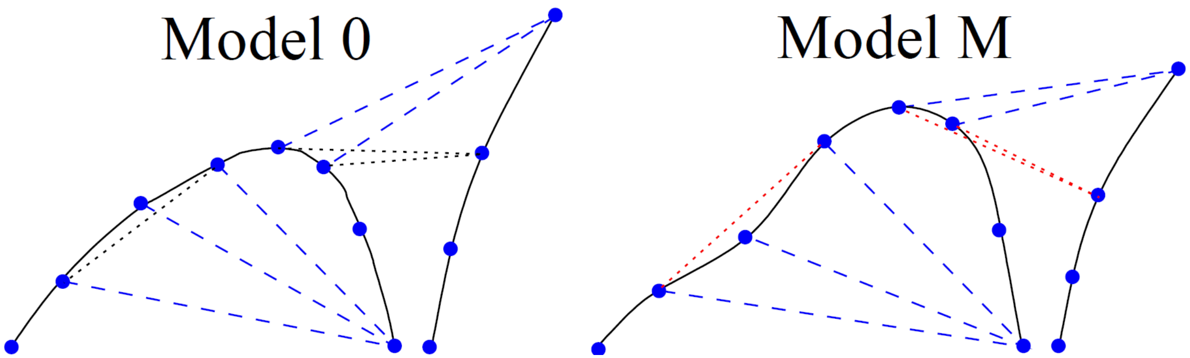
  - Adaptively mesh phase regions:



- Complexities:
  - Constrained Delaunay triangulation used as transfer function
  - Extreme non-convexity in individual phase regions
  - Computational chain must be parallelized for large numbers of tables
- Lesson Learned: Great care must be taken with non-convexity issues associated with phase regions.

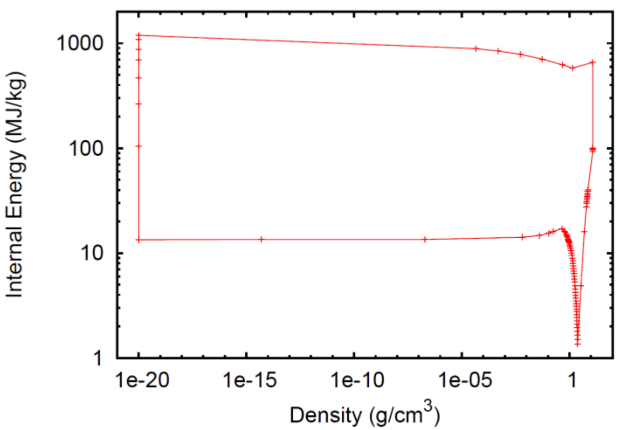
Convexity Complexity

- Non-convexity of boundaries complicates the mappping:

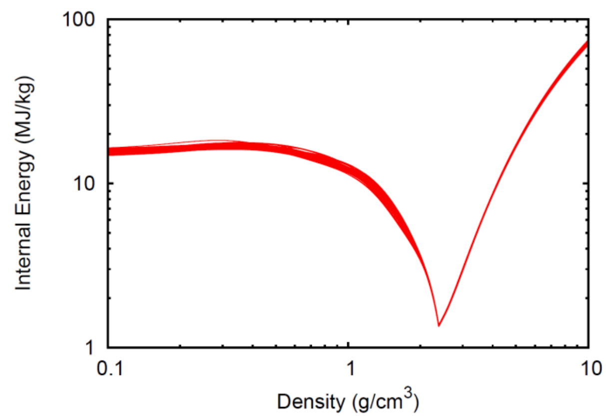


Must iteratively “fix” the bad triangles

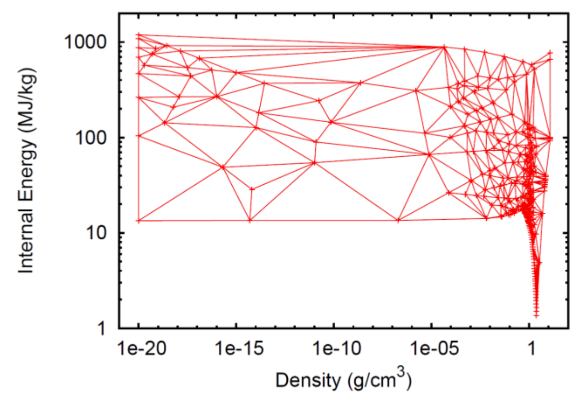
- Reality is messy:



Mesh 0 boundary (1.0 tolerance)

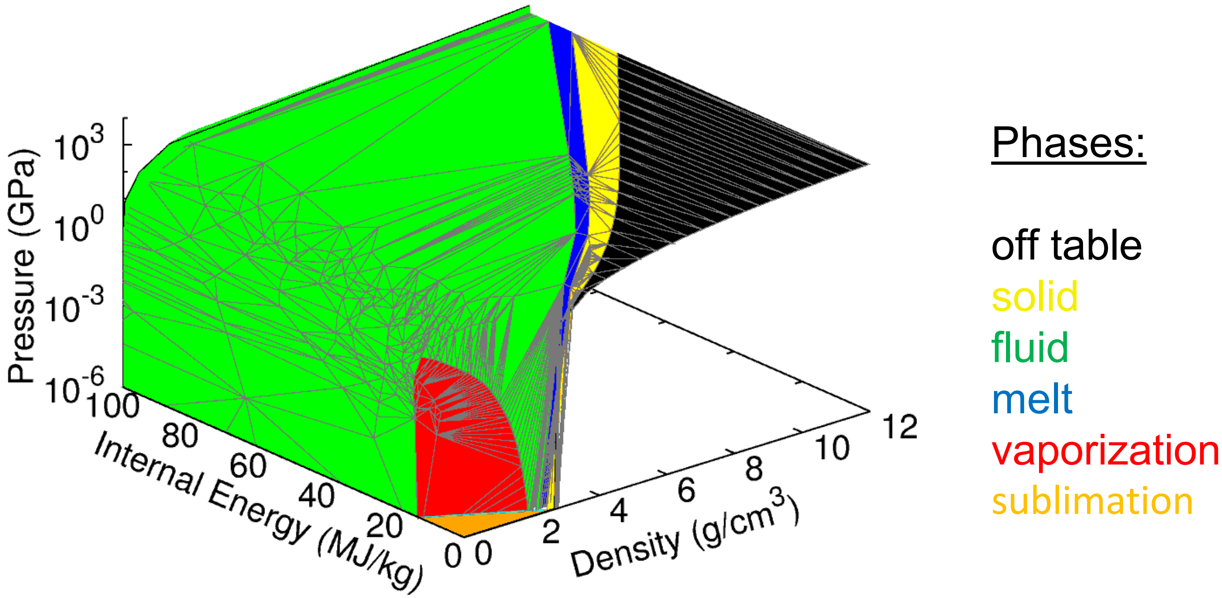


70 other phase boundaries



Mesh 0 grid

Tabular EOS generation and UQ representation



Principal Component Analysis (PCA) is used to look for a tabular representation with reduced dimensionality:

- N tables from previous meshing step are starting point
- Export a truncated set of mode tables that capture most of the details (i.e. eigenspectrum energy)
- Multi-precision floating point is necessary due to dynamic range of multi-phase tables.
- Log density and log energy used in PCA analysis (also ensures positivity)
- Parallel processing of SVD matrix creation is important.
- Random variables ξ are uncorrelated, with zero mean and unit standard deviation, but not necessarily independent

$$\bar{z} = ZH\mathbf{1}/\mathbf{1}^T H\mathbf{1}$$

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

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

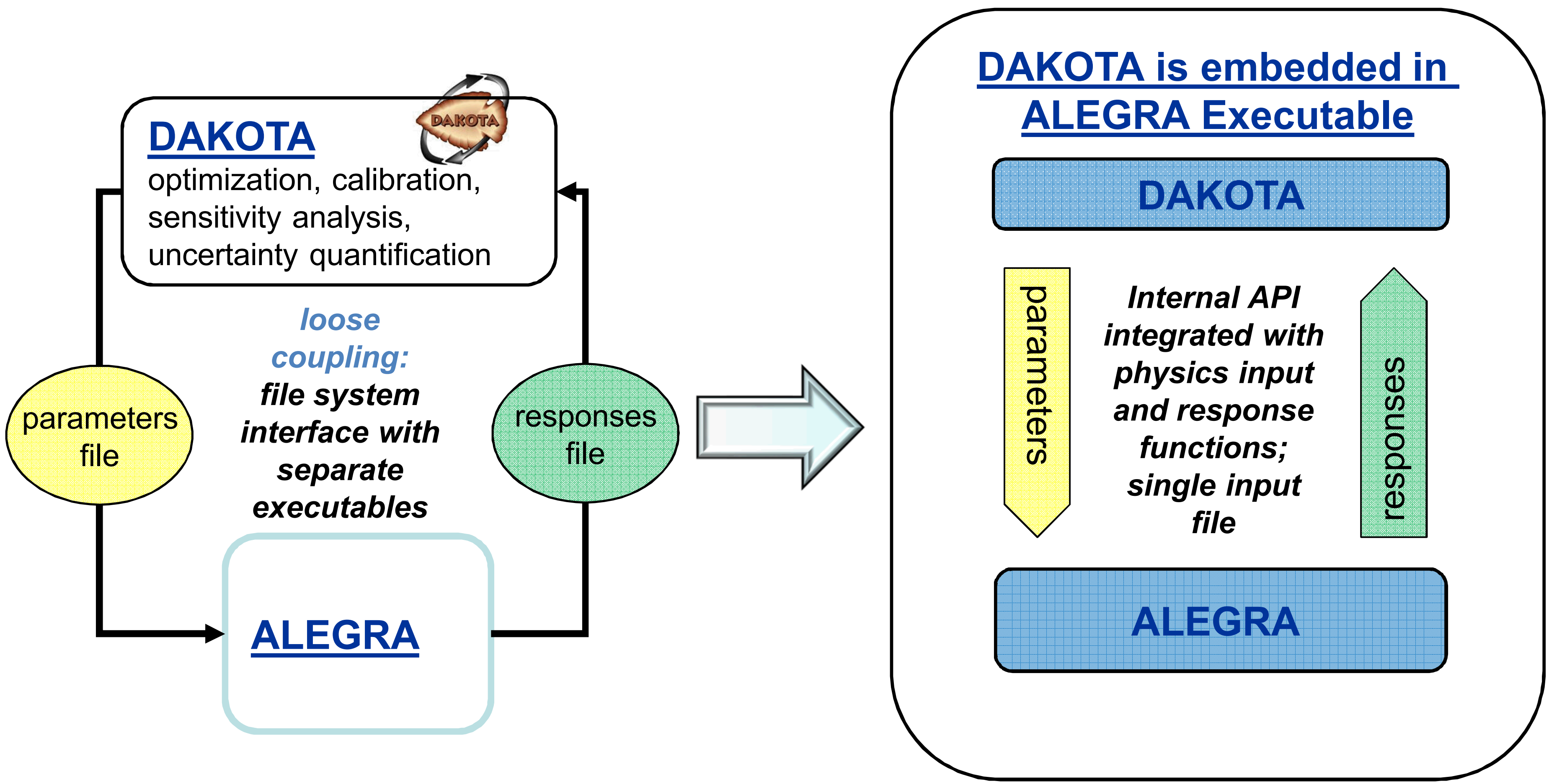
$$\mathbb{T} = \bar{\mathbb{T}} + \sum_k \xi_k \mathbb{T}_k$$

Multiphase Tabular Generation and Representation: Initial AL UQ enabled table

$$T = \bar{T} + \xi_1 T_1 + \xi_2 T_2 + \xi_3 T_3 + \cdots$$

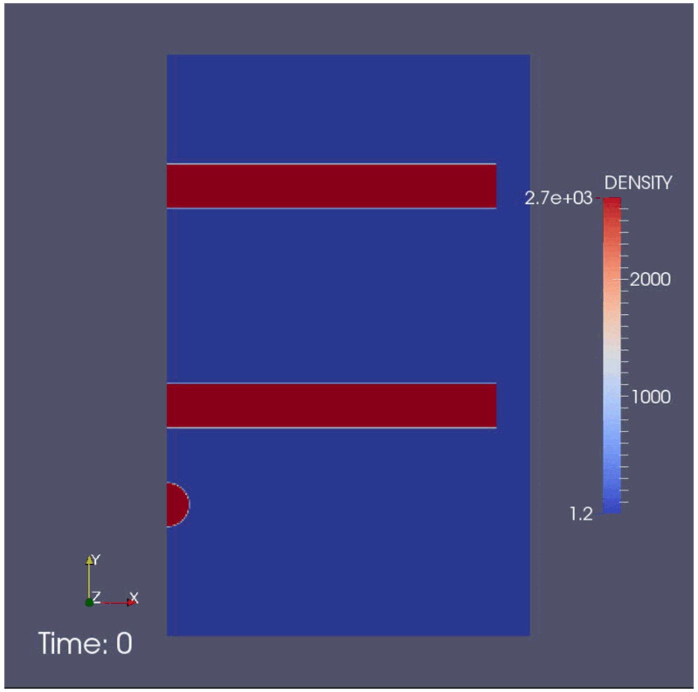
- Current wide range UQ AL EOS with 6 phase regions in the density-energy table.
- With the current multi-phase model there are 37 free parameters.
- 11 parameters were fixed due to insufficient constraining data.
- The MCMC inference samples 26 parameters.
- We took 300 samples from the chain. Due to unresolved topology issues in the table generation process, only 135 of those were successfully used due to insufficient constraints on liquid-vapor phase boundary shapes that caused failure in tabulation. There were 8 significant modes at 1e-3 cutoff in the PCA analysis.
- Accuracy of the tables is set at a relative tolerance of 0.1. Vapor dome issues still occurring at 0.01 tolerance.
- PCA solver currently scales as N^2 so this will limit the practical number of samples.

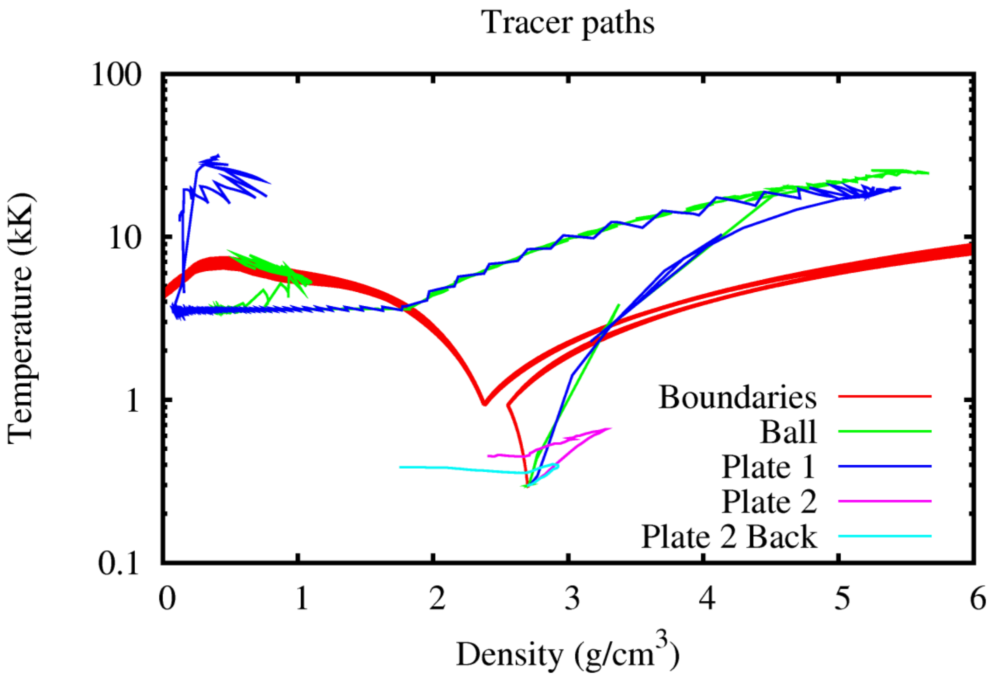
Meta-analysis approach for enabling users



Move users from a potentially fragile, study-specific script interfaces to a unified, user-friendly capability

2mm diameter Al ball impacting spaced Al plates at 20 km/s in air background. Termination at 1.5 microsec

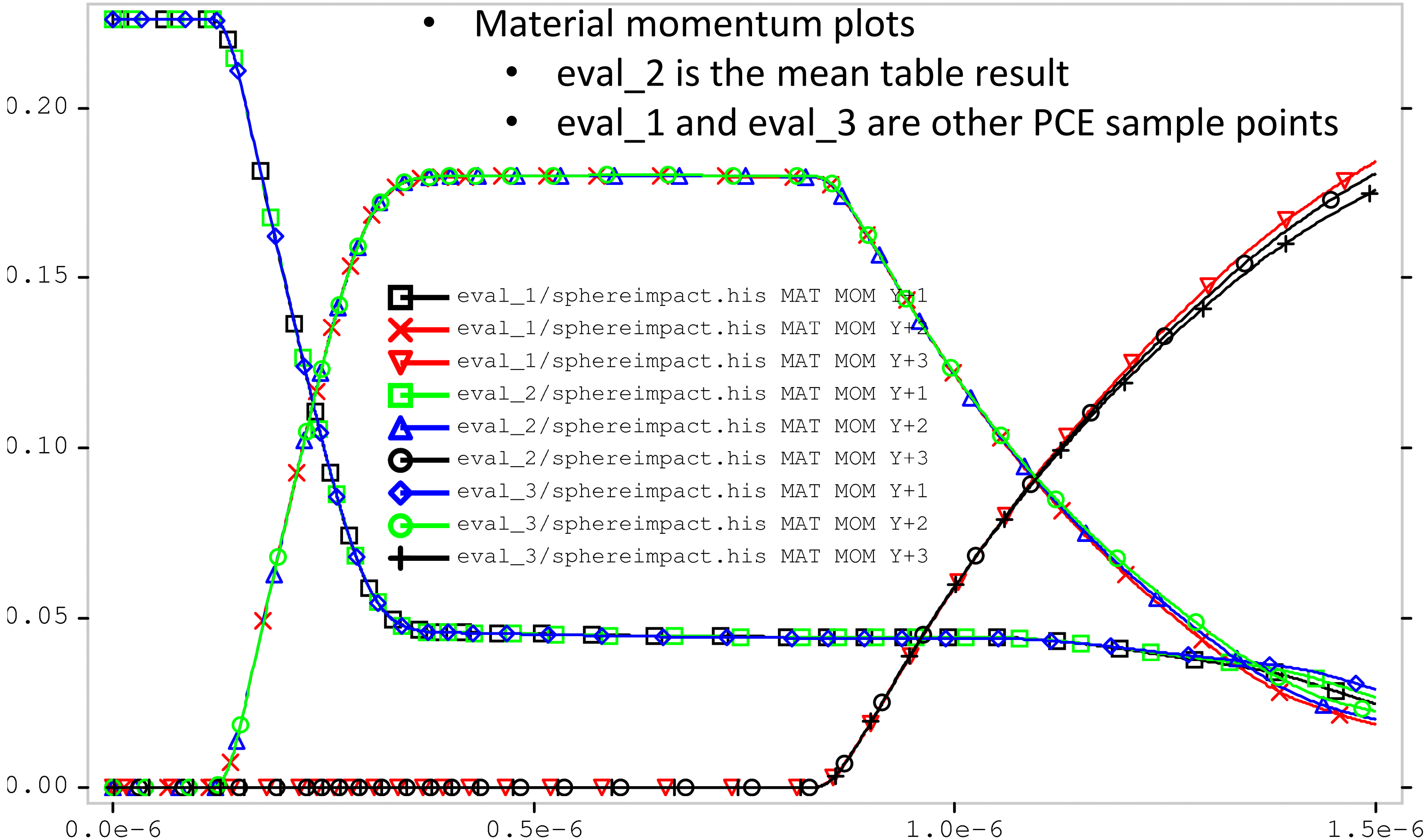




Phase boundary lines of PCA source EOS files are shown along with phase space trajectory of tracers (mean table, csmin=0, mfac=4)

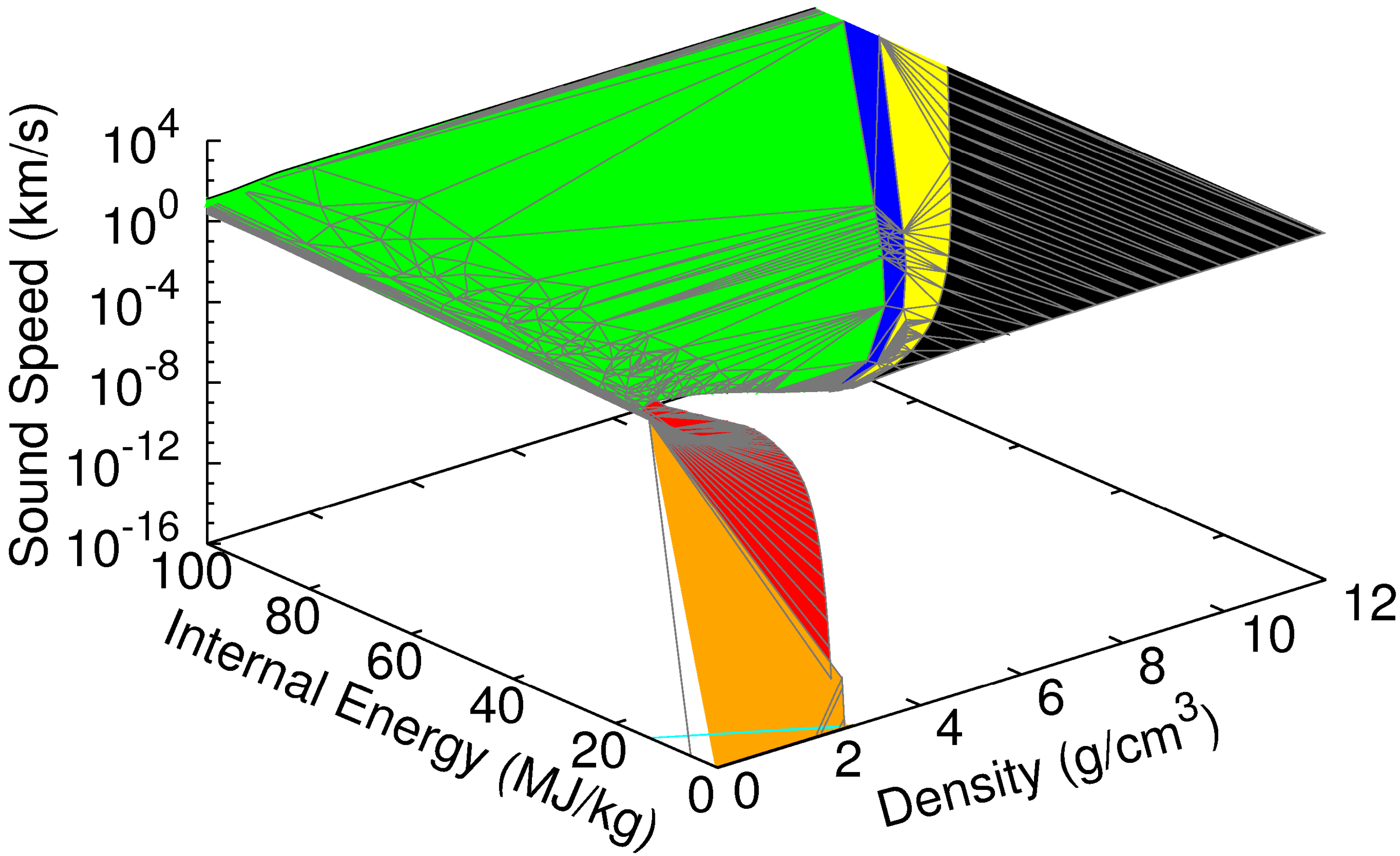
Looking at UQ Results via ALEGRA-DAKOTA

- 3 PCE (polynomial chaos expansion) quadrature points and 1 tabular mode
- Sample output time histories are a good way to gain perspective.



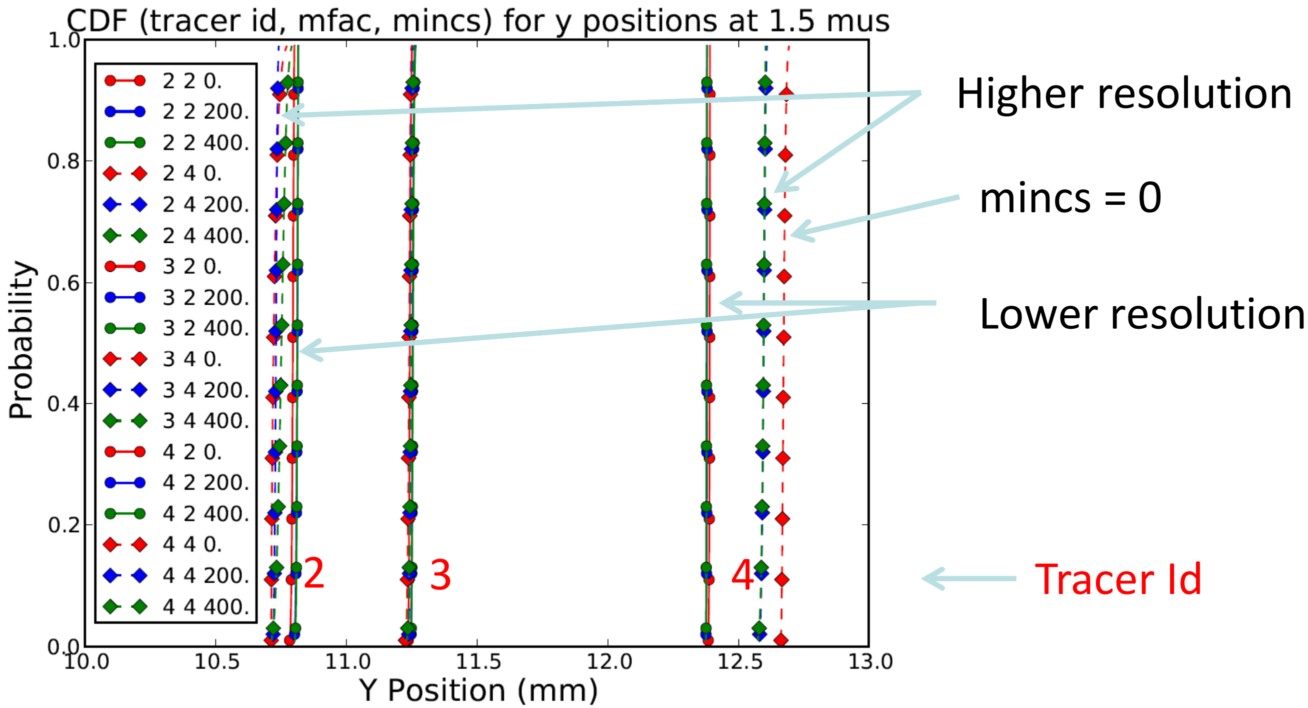
UTri EOS tables accurately match the model

- Accurate EOS tables correctly represent the thermodynamic sound speed as being very small in certain mixed phase regions with precise phase jumps.



Uncertainty analysis using UQ enabled AL EOS

3 PCE (polynomial chaos expansion) quadrature points and 1 tabular mode out of 8.



Lessons Learned:

1) Effects of EOS uncertainty can be comparable or smaller than other model uncertainty (e.g. mesh resolution (mfac), numerical or modeling constants (mincs))
2) Conclusions will depends on where you look! QOI is fundamental.
3) Availability of the formal approach encourages a UQ viewpoint.
4) UQ enabled table capability tends to drive useful verification and numerical work

Summary

A multiphase EOS table approach with embedded UQ has been developed providing the following value:

1) More precise EOS surface representation
2) Embedded scalable UQ upscaling approach
3) Usable representation for downstream UQ continuum analysis

Diving into the meta-analysis world tends to efficiently bring out quality issues. This serves to enable and support the scientific and engineering enterprise.

References

- Robinson, A. C., et. al., “Fundamental issues in the representation and propagation of uncertain equation of state information in shock hydrodynamics”, Computers and Fluids, 83, (2013) p. 187–193.
- For the ALEGRA MHD code follow below link (download PDF file):
  - http://arc.aiaa.org/doi/abs/10.2514/6.2008-1235