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Effective Representation and Propagation of Uncertainty Through Tabular Multiphase Equation-of-State Models

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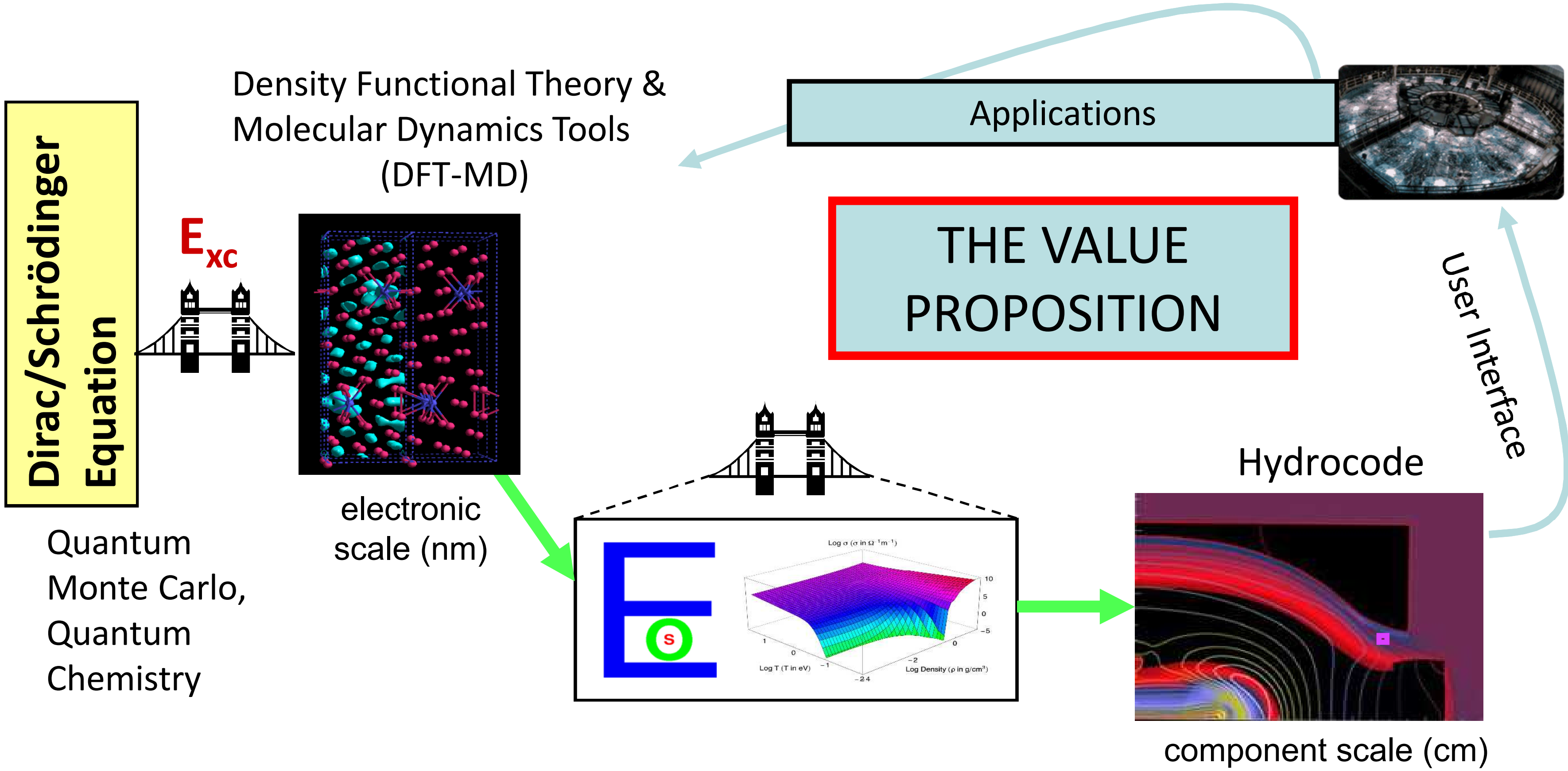
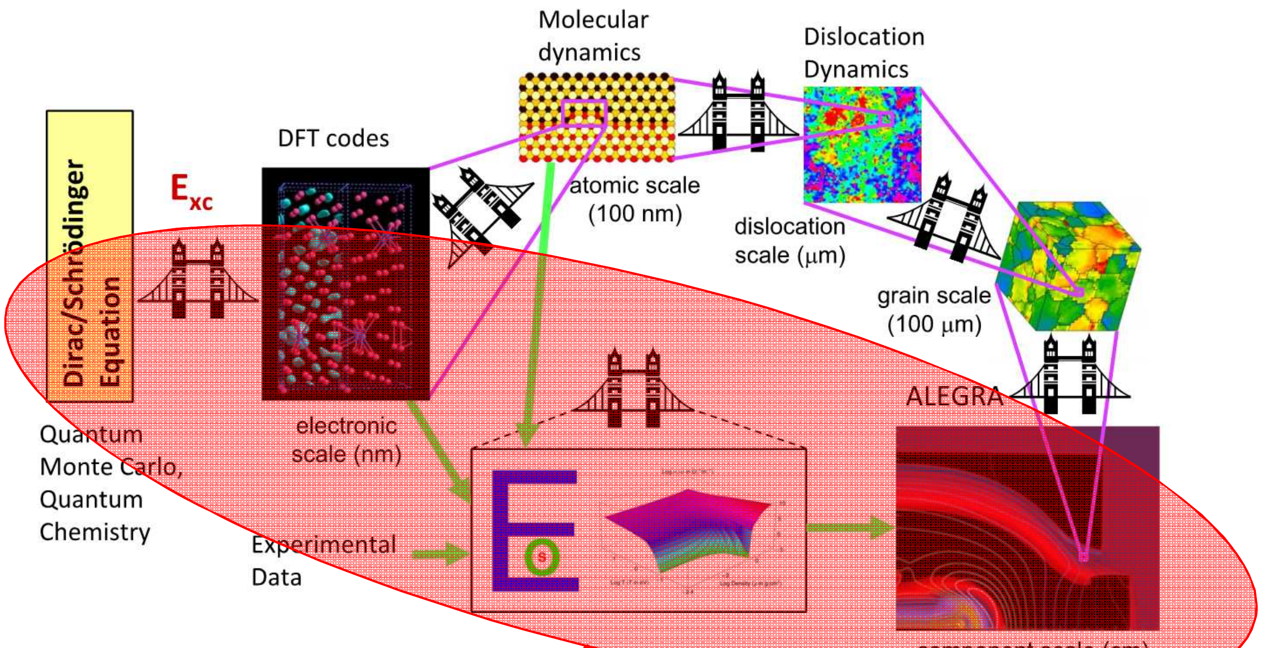
Science based engineering is a multi-scale, multi-physics, multi-parameter enterprise



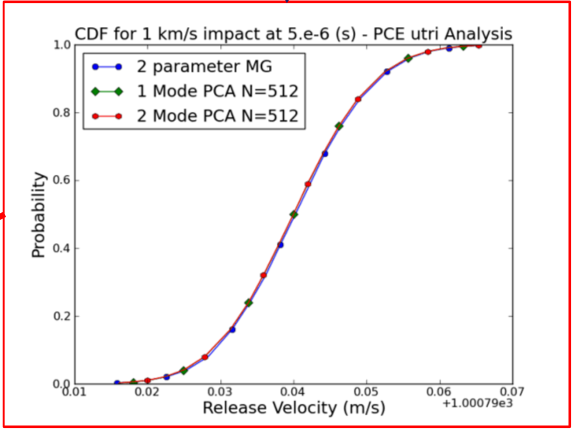
How does one enable this cycle to be more effective?

Propagation of uncertain EOS information



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



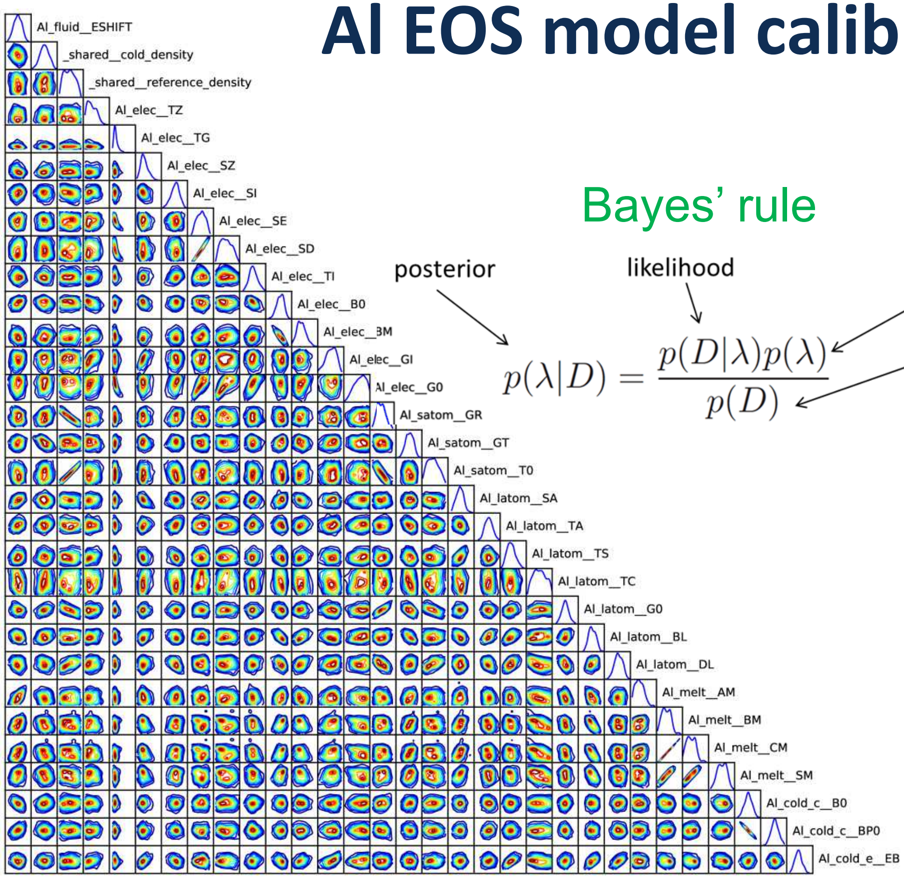
Example: Propagate uncertainty due to statistically equivalent possible EOS fits to the same data, to the analyst.

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

Al EOS model calibration and inference



Al model EOS inference

Bayes' rule

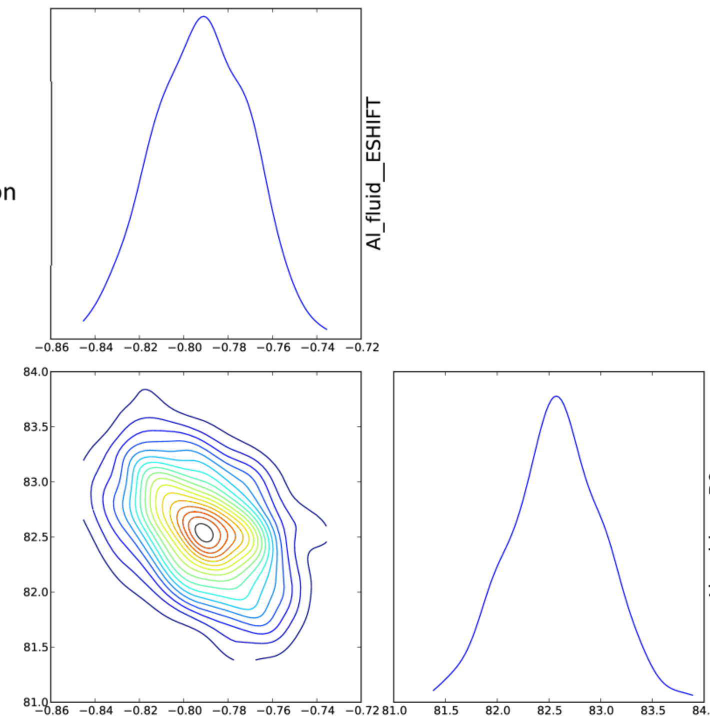
posterior

likelihood

prior

normalization

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



A marginal distribution

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

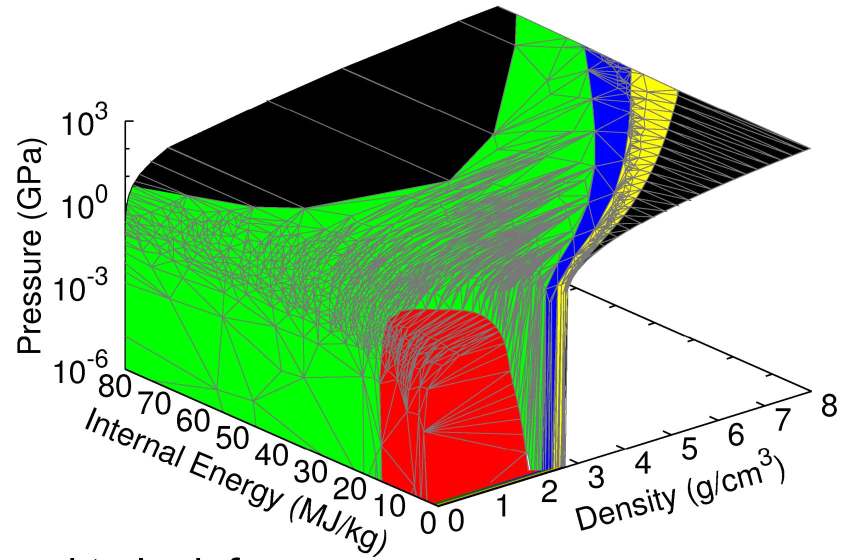
- Use adaptive Markov Chain Monte Carlo (MCMC) scheme to reduce number of steps
- Use optimization to find Maximum A Posteriori (MAP) parameters from which to start chain
- Each posterior evaluation is roughly equivalent to generating an entire EOS table

Tabular EOS generation and UQ representation

Simultaneously tabulate N parameterizations of an EOS model

- New UTri format uses linear interpolation on triangles to capture salient features
- Each tabulation is topologically equivalent (smooth mapping of nodes)
- Optimized node placement is costly but can reduce table size

Example PCA mean pressure table at 0.1 tolerance



phases:

off table
solid
fluid
melt
vaporization

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)
- Random variables ξ are uncorrelated, with zero mean and unit standard deviation, but not necessarily independent

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

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

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

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

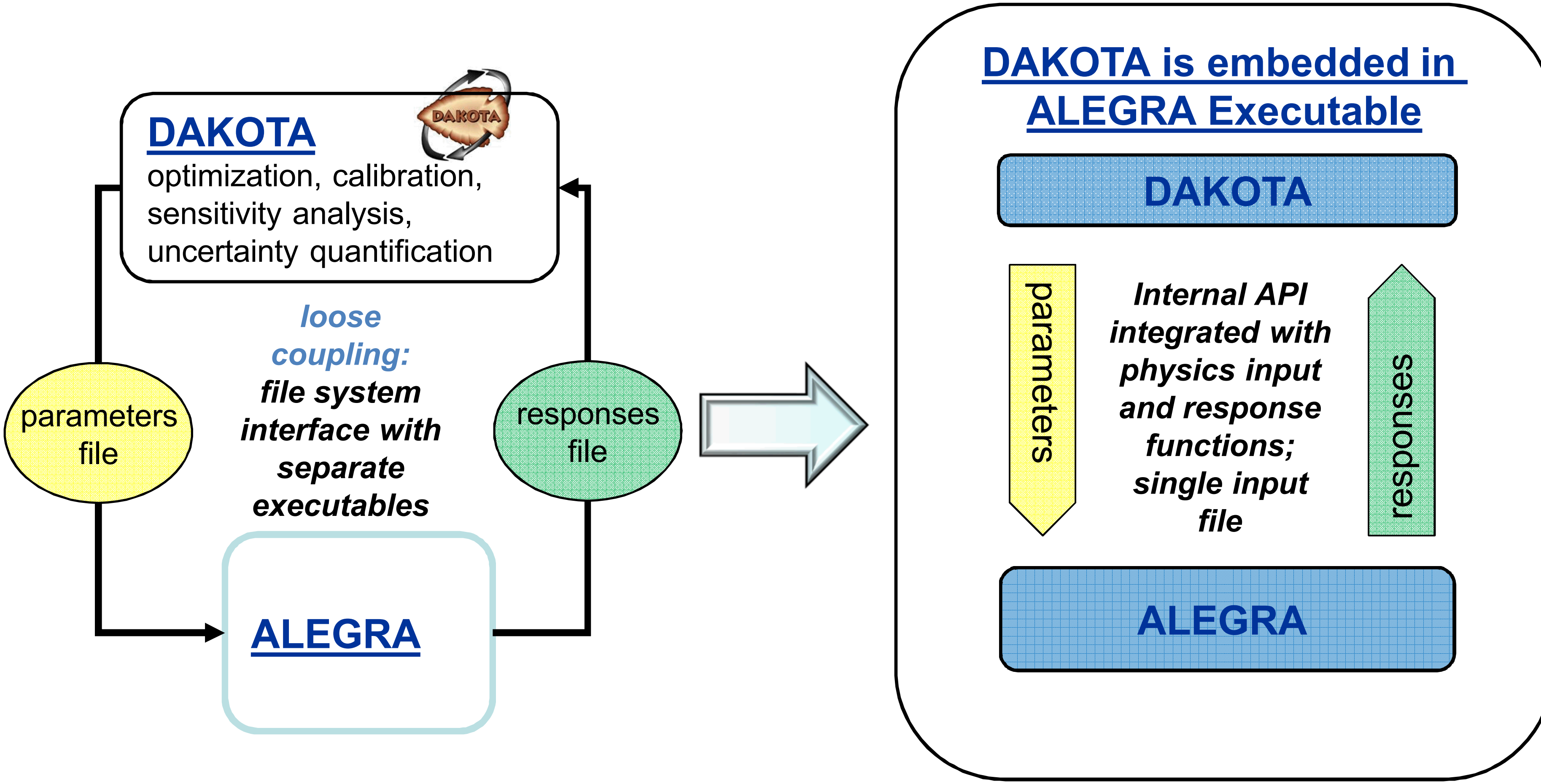
Robinson

Multiphase Tabular Generation and Representation: Initial AL UQ enabled table

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

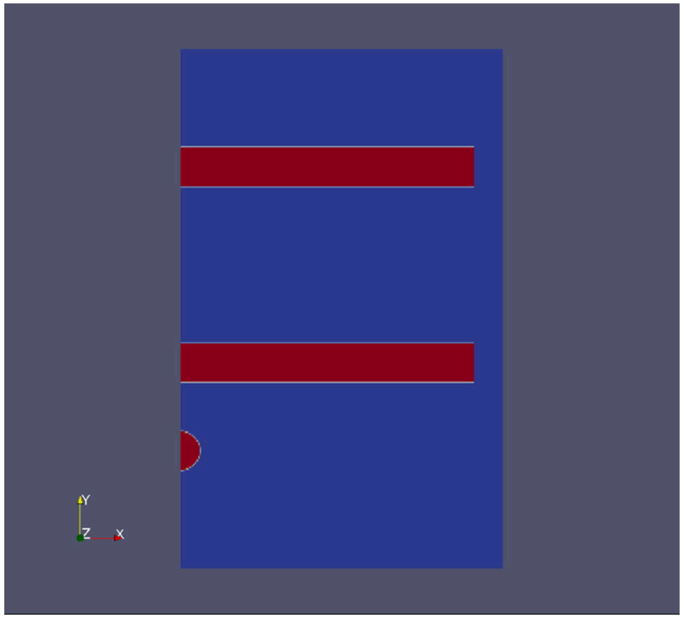
- Current wide range UQ AL EOS with 6 phase regions in the density-energy table.
- With the current multi-phase model there are 37 free parameters.
- 6 parameters were fixed due to insufficient constraining data.
- The MCMC inference samples 31 parameters
- We took 400 samples from the chain. Due to unresolved topology issues in the table generation process, only 6 of those were successfully tabulated simultaneously. There were 3 significant modes at 1e-6 cutoff in the PCA analysis. Work still in progress.
- Accuracy of the tables is set at a relative tolerance of 0.1.
- PCA solver currently scales as N^2 so this limits practical number of samples.

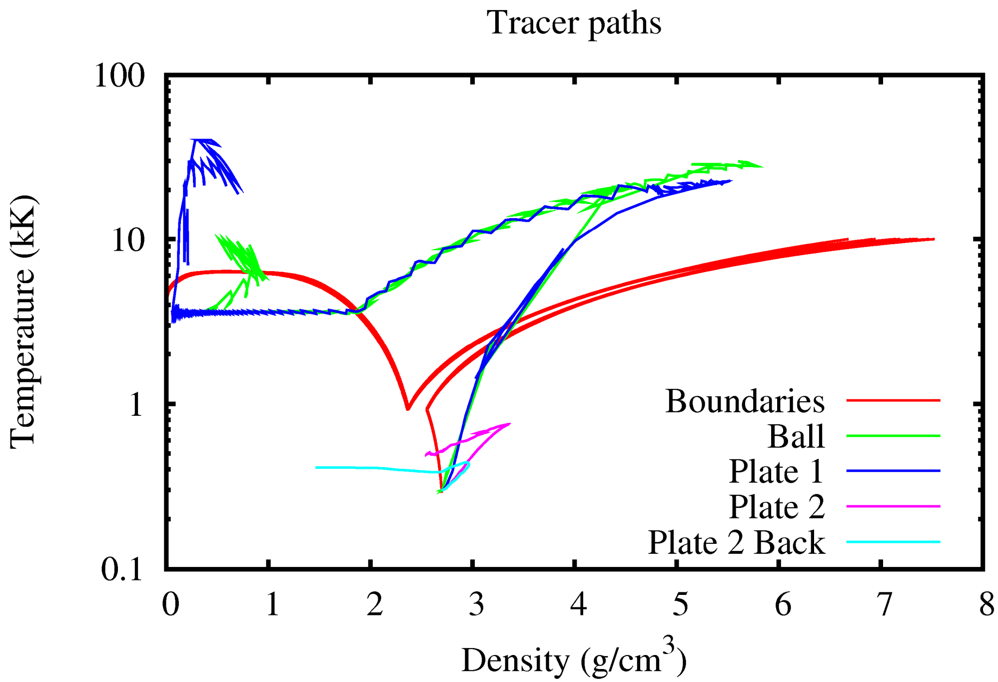
Meta-analysis approach for enabling users



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

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

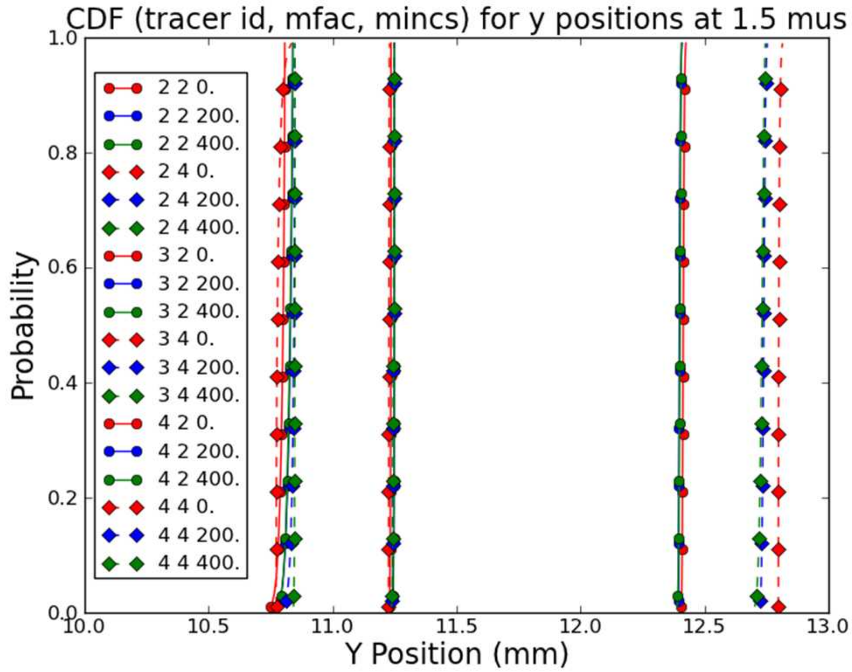




Phase boundary lines of PCA source EOS files are shown along with phase space trajectory of tracers (mean table, csmin=0)

Example uncertainty analysis using UQ enabled AL EOS

3 PCE (polynomial chaos expansion) quadrature points and 1 tabular mode



Lessons Learned:

1) UQ EOS information can be comparable to other model uncertainty (e.g. mesh resolution (mfac), numerical or modeling constants (mincs))
2) UQ enabled table capability tends to drive useful verification and numerical work
3) Formal approach leads to more precise and detailed thinking.

Summary

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

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

Diving into the meta-analysis world tends to efficiently bring out quality issues. This serves to help the whole joint 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 magnetohydrodynamics code see above references and following link (download PDF file):
  - http://arc.aiaa.org/doi/abs/10.2514/6.2008-1235