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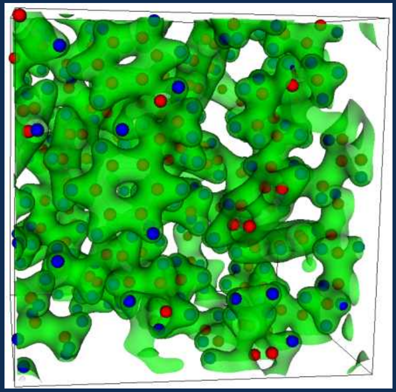

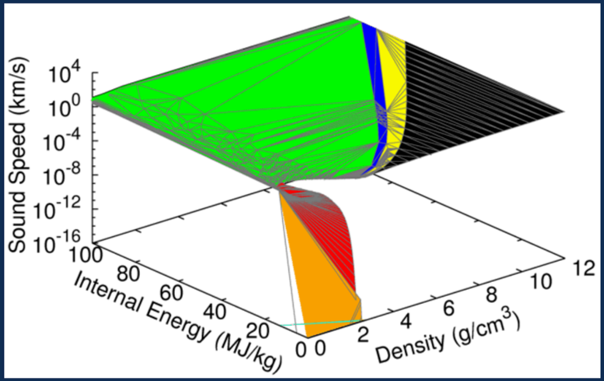

A UQ Enabled Aluminum Tabular Multiphase Equation-of-State Model

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Sandia National Laboratories

MultiMat 2015
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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Material models determine the outcome of radiation-magneto-hydrodynamic simulations

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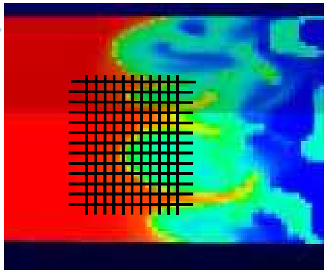
Hydrodynamics

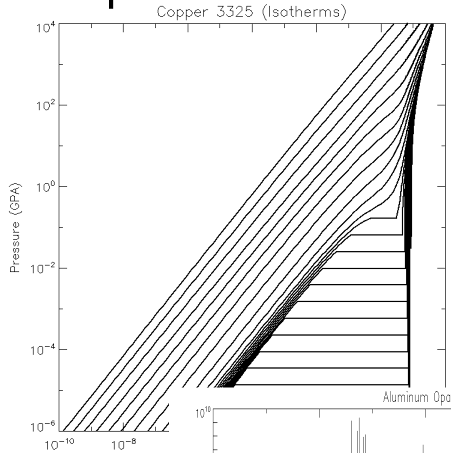
The hydrodynamics moves material based on the material properties.



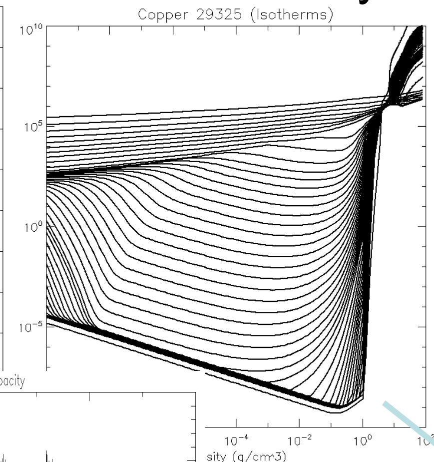
Tom Haill, SNL

Most simulation codes will tally the total energy in each cell and, based on that energy and the density, compute a new pressure and temperature in preparation for the next hydrodynamic step.

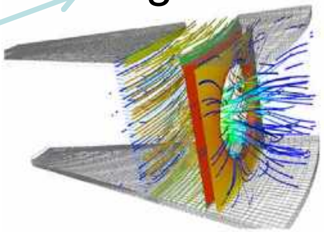
Equation of State



Conductivity

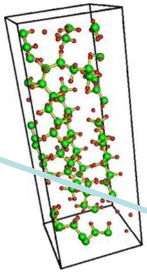


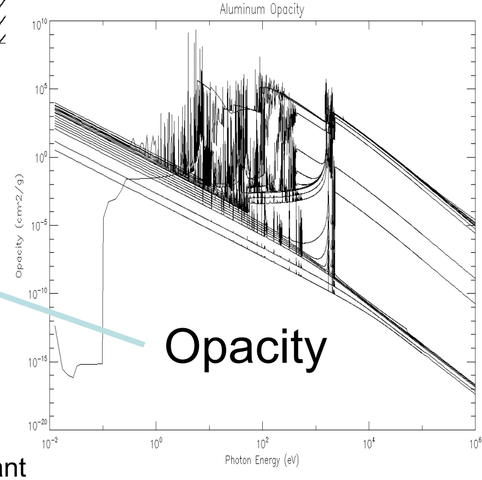
Magnetics



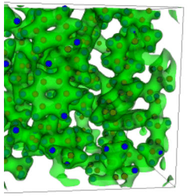
Chris Garasi, SNL

Conductivity determines magnetic field diffusion.

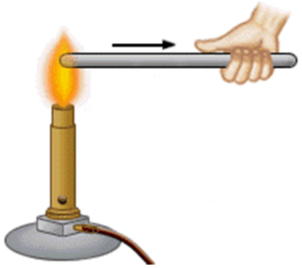




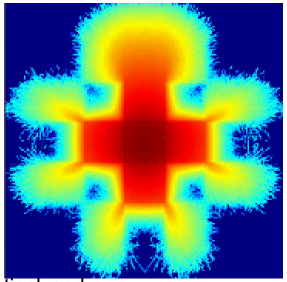
Opacity



Conduction



Radiation



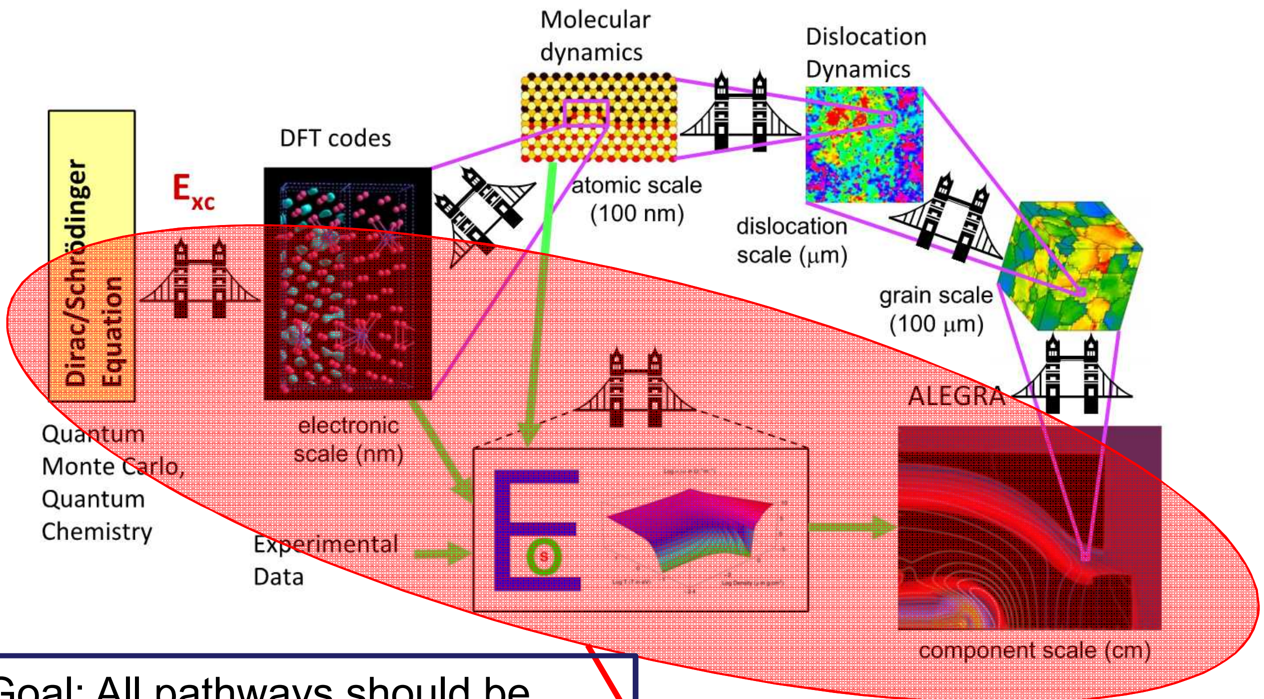
Tom Brunner, LLNL

Nuclear Mathematical and Computational Sciences: A Century in Review, A Century anew

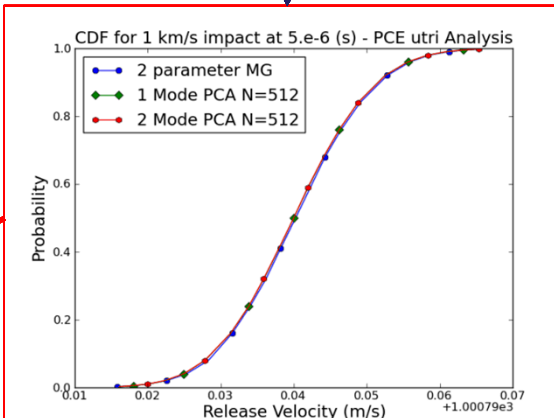
Radiation is an important energy transfer mechanism for hot systems

Thermal conduction is used to augment the movement of energy in a simulation.

During modeling process, information on closure property uncertainty must be captured and propagated.



Goal: The analyst running the continuum code should easily get distributionally based information on any chosen Quantity of Interest (QOI).



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

We wish to propagate uncertainty due to statistically equivalent possible EOS fits to the same data, to the analyst.

Our approach to solving this problem

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.

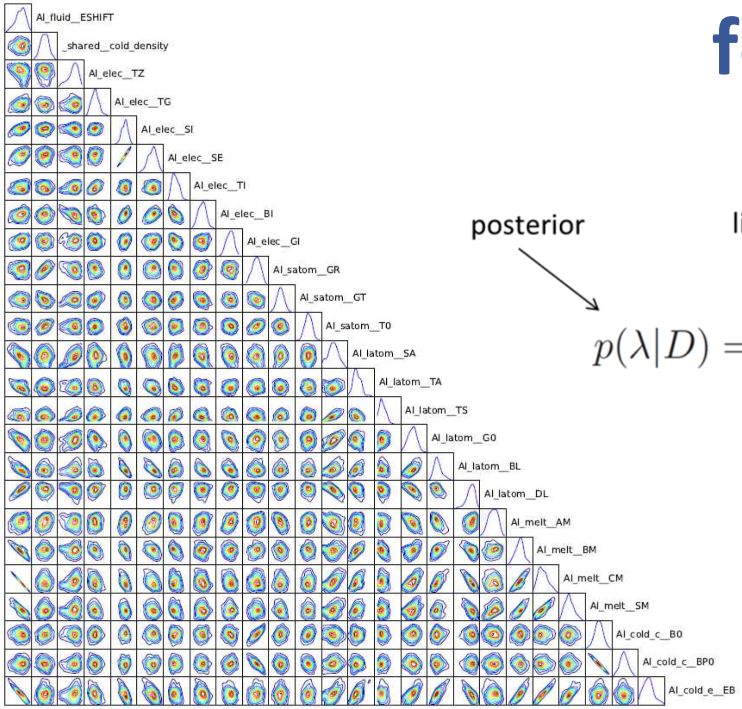
Software Package	Output
EOS model library and data	Proposal Model (XML input deck)
Bayesian Inference using Markov Chain Monte Carlo	Extensive sampling of the posterior distribution function (PDF)
EOS Table Building	Topologically equivalent tables for each sample
PCA Analysis	Mean EOS table + most significant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

History and Context: This work has been supported at Sandia since FY11 and the basic ideas have not changed much from the beginning but working out the **operational , production quality details** for multiphase EOS has been very challenging.

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. (Reproducible!)
  - This enables later steps to complete since these assume correct EOS behavior
- Wide range AL EOS is built from semi-empirical models, with solid and liquid phases including melt/vaporization/sublimation.
- 37 total parameters, 25 constrained well enough by data for inferring UQ information.
- 16 Data Sources from:
  - Hugoniot experiments and calculations
  - Isobaric and thermophysical expansion data
  - DFT-MD isotherms near critical point
  - Diamond Anvil Cell compression data
  - DFT cold curve
  - Melt and vaporization experiments and calculations
- Constraints on physicality: smoothness and convexity change limitations along phase boundaries; thermodynamic stability checks across range of interest

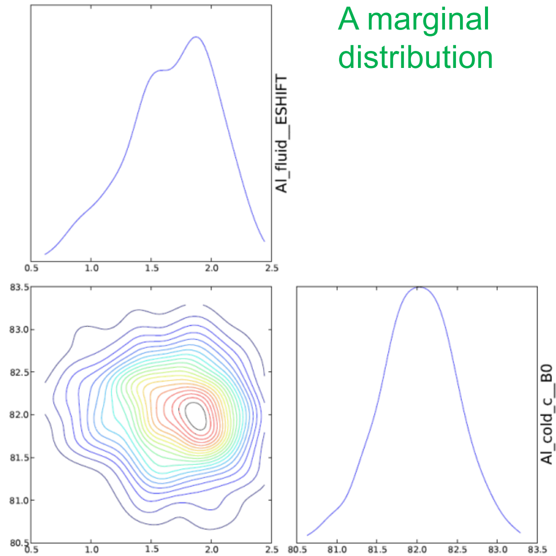
Al EOS Model Parameter Bayesian Inference for Posterior



posterior — likelihood — prior — normalization

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

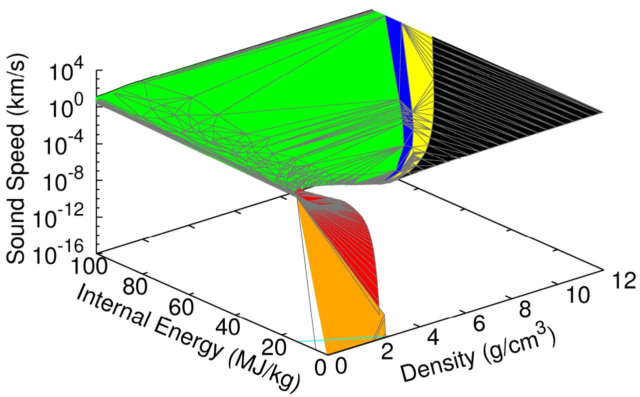
A marginal distribution



- Data sources appear in likelihood with a noise model.
- Use adaptive Markov Chain Monte Carlo (MCMC) scheme to reduce the 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 and having an expert check it for correct behavior!
- PDF evaluations may be parallelized to enable long chains (~4.5M steps for this EOS, one serial evaluation is approximately 2 sec.)
- Bottom Line: The inference process is costly.

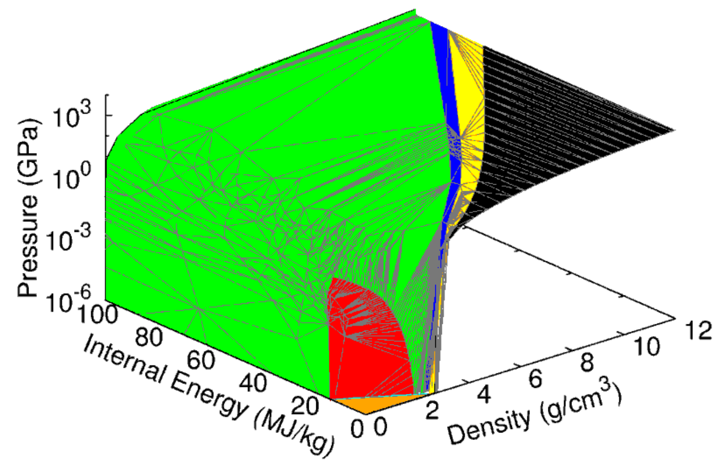
UTri EOS tables accurately match the model

- UTRI tabular format
- Triangular mesh e.g. (density, energy) 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.
- Accurate EOS tables correctly represent the thermodynamic sound speed as being very small in certain mixed phase regions with precise phase jumps.



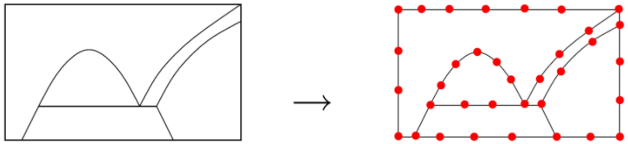
Phases:

off table
solid
fluid
melt
vaporization
sublimation



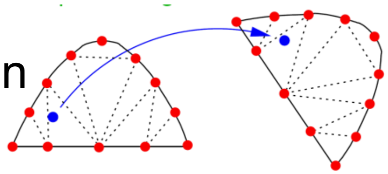
UTri Tabular EOS generation

- Must build N UTri tables which are <u>topologically equivalent</u> and of similar accuracy:
  - Adaptively mesh boundaries:



  - Adaptively mesh phase regions:

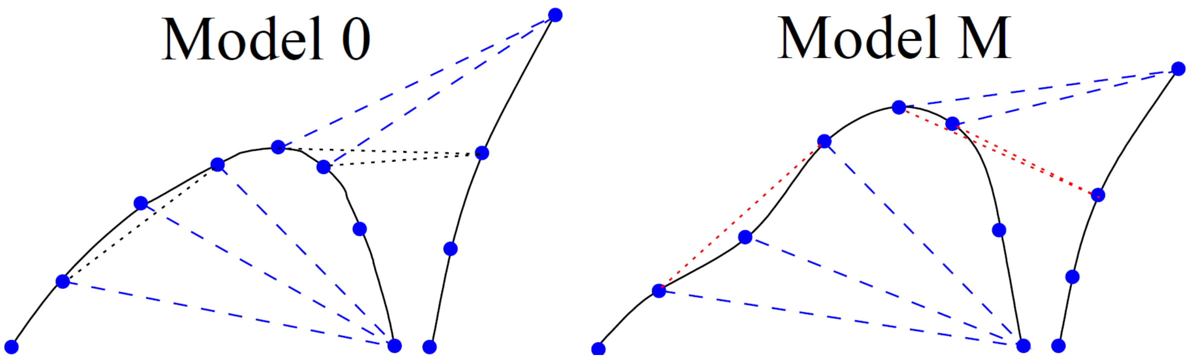
- Complexities:
  - Constrained Delaunay triangulation used as transfer function
  - Extreme non-convexity in individual phase regions
  - Computational chain must be parallelized for large numbers of tables



- Lesson Learned: Great care must be taken with non-convexity issues associated with phase regions.

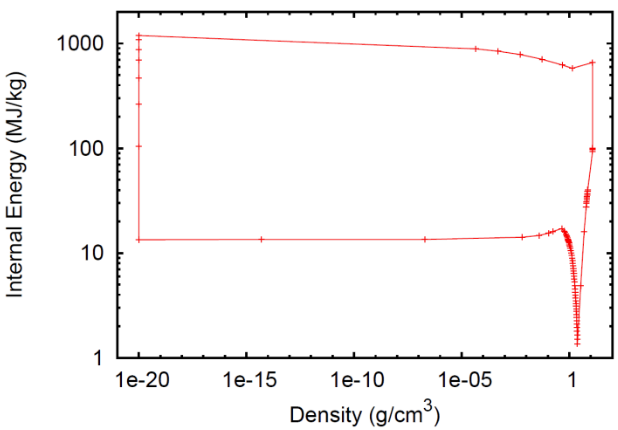
Convexity Complexity

- Non-convexity of boundaries complicates the mapping:

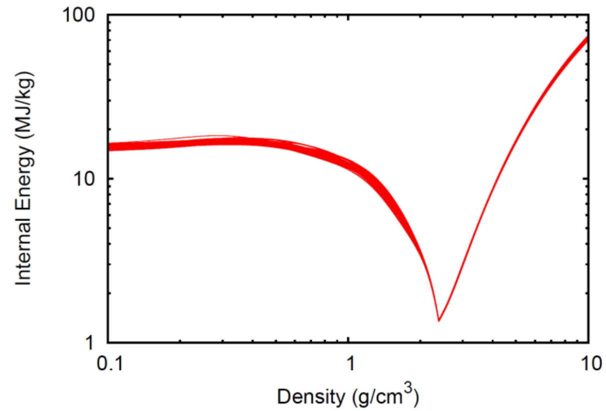


Must iteratively “fix” the bad triangles

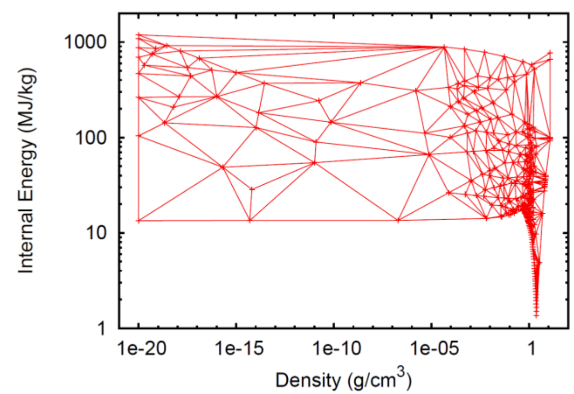
- Reality is messy:



Mesh 0 boundary (1.0 tolerance)



70 other phase boundaries



Mesh 0 grid

Tabular EOS 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
- PCA solver currently scales as MN^2 so this limits the practical number of samples.

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

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

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

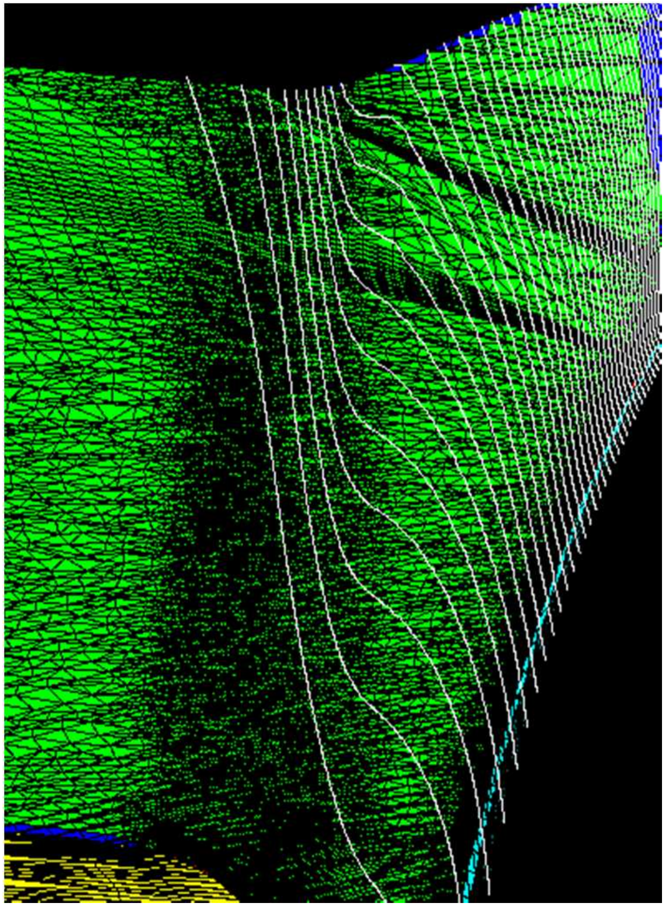
$$\Updownarrow$$

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

Multiphase Tabular Generation and Representation: 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. 12 parameters were fixed due to insufficient constraining data. The MCMC inference samples 25 parameters.
- We took 442 samples from the chain. There were 7 modes at 1e-3 cutoff in the PCA analysis.
- Accuracy of the tables is set at a relative tolerance of 0.01.



Isobars of mean table in density-energy plane

Develop surrogate random variable distributions

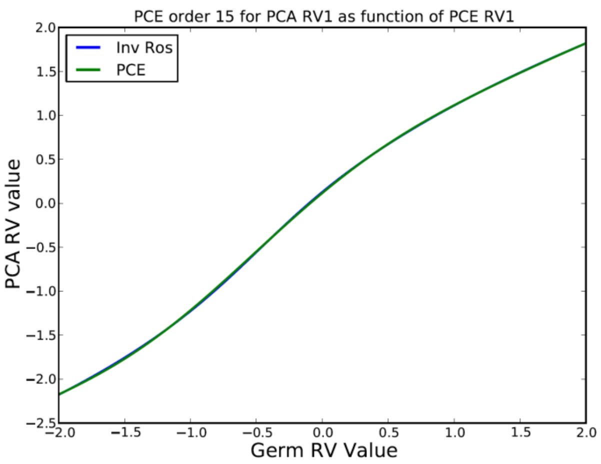
$$T = \bar{T} + \xi_1 T_1 + \xi_2 T_2 + \xi_3 T_3 + \cdots$$

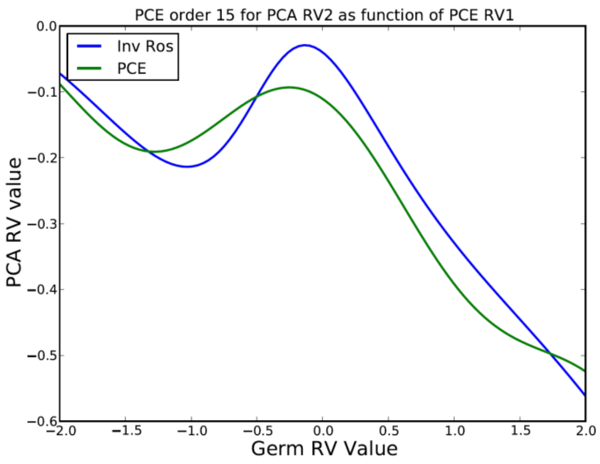
- We keep K ordered modes and expect the end user to sample K_u ($0 \leq K_u \leq K$) of them in some way at their discretion.
- The PCA provides a set of samples for the random variables ξ_i which are zero mean and unit co-variance (Not necessarily independent)
- One can <u>assume</u> independence (not justifiable) OR
- Model the distribution of these random variables using a kernel density estimator and use a Rosenblatt transformation to create a Hermite PCE representation in which the random variables are <u>independent</u> but still preserve ordered dependencies.

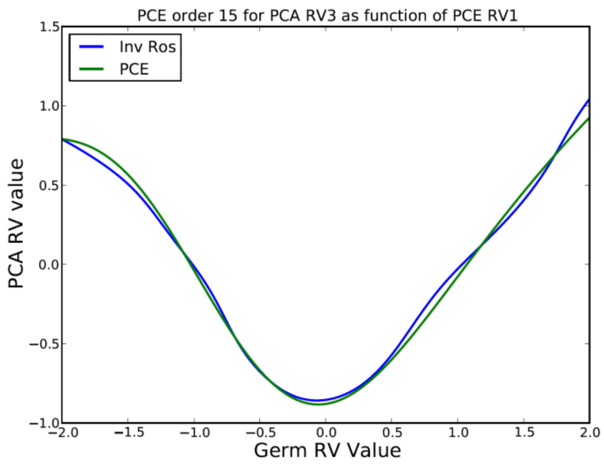
$$\xi_i(\boldsymbol{\eta}) = \sum_{j=0}^{\binom{K+r}{r}-1} a_j \psi_j(\boldsymbol{\eta})$$

Rosenblatt transformation needs more samples

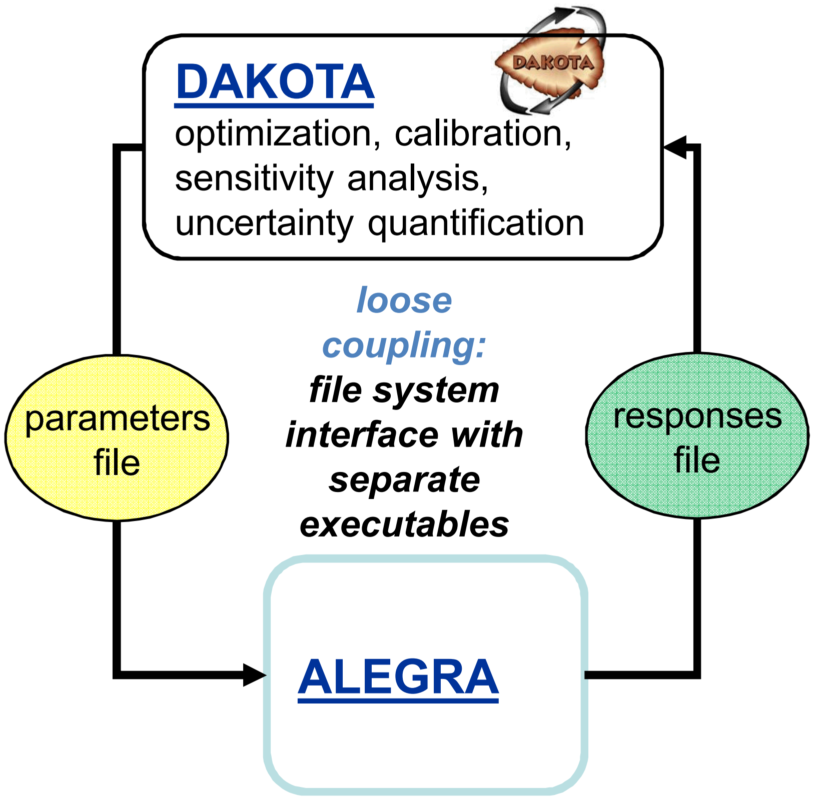
- The Rosenblatt transformation seems to do quite well in the main components. I.e. relating the first mode to the first PCE dimension.
- However, the coupling terms between the different modes are much more nonlinear, and seem a bit noisy. Even 15th order PCE does not seem to be sufficient.
- We need more samples, and higher order PCEs (or another mapping approach).
- We are now going for 10,000 sample tables! With this many tables we are now hitting conditions where the meshing near the critical point is failing. This has to do with the constraints on the model and possibly some small inconsistencies in how the critical point is computed. This is the next major item to be fixed in the automatic table generation process.

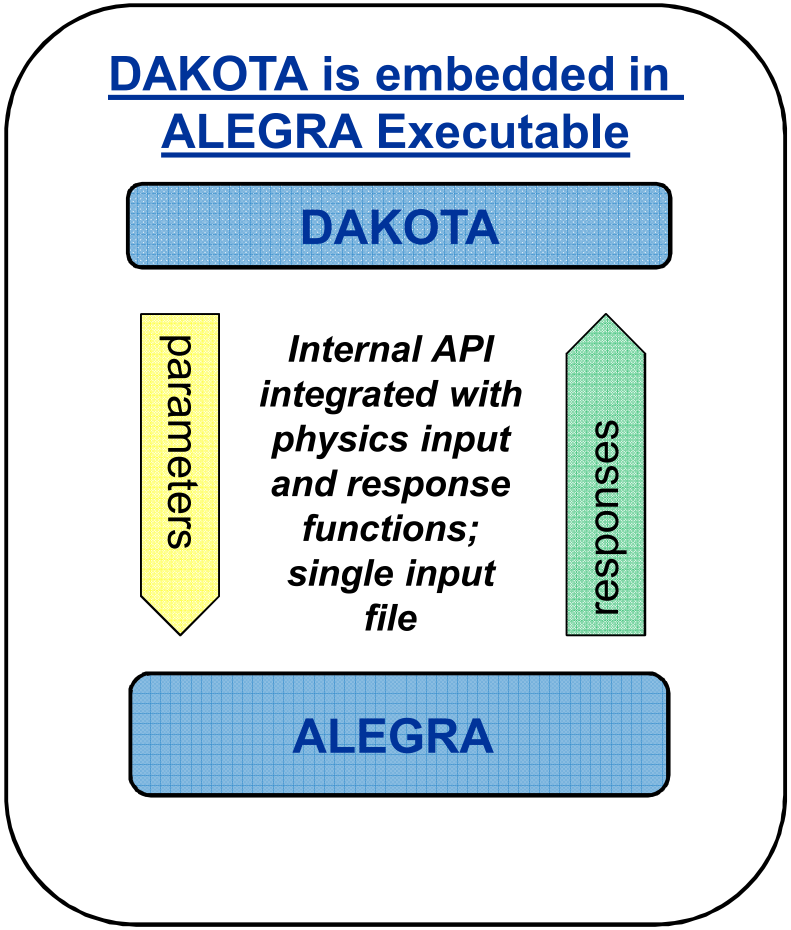






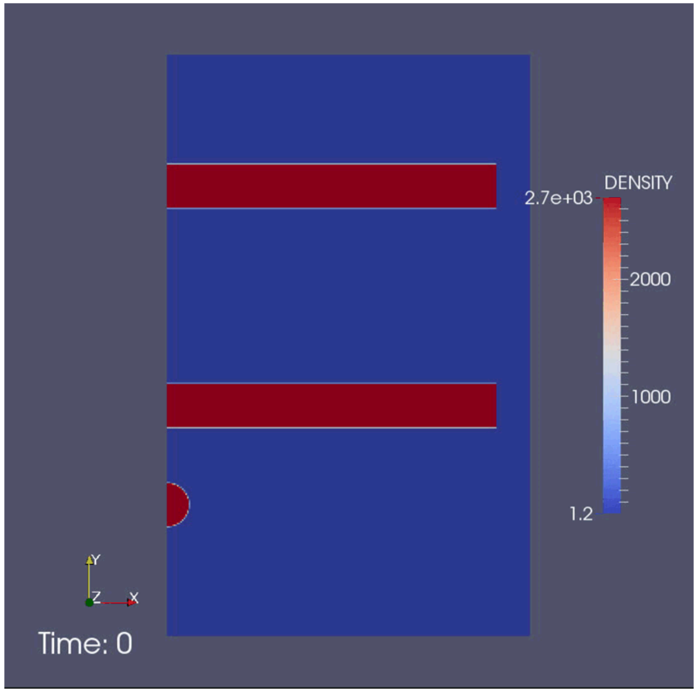
Meta-analysis approach for enabling users

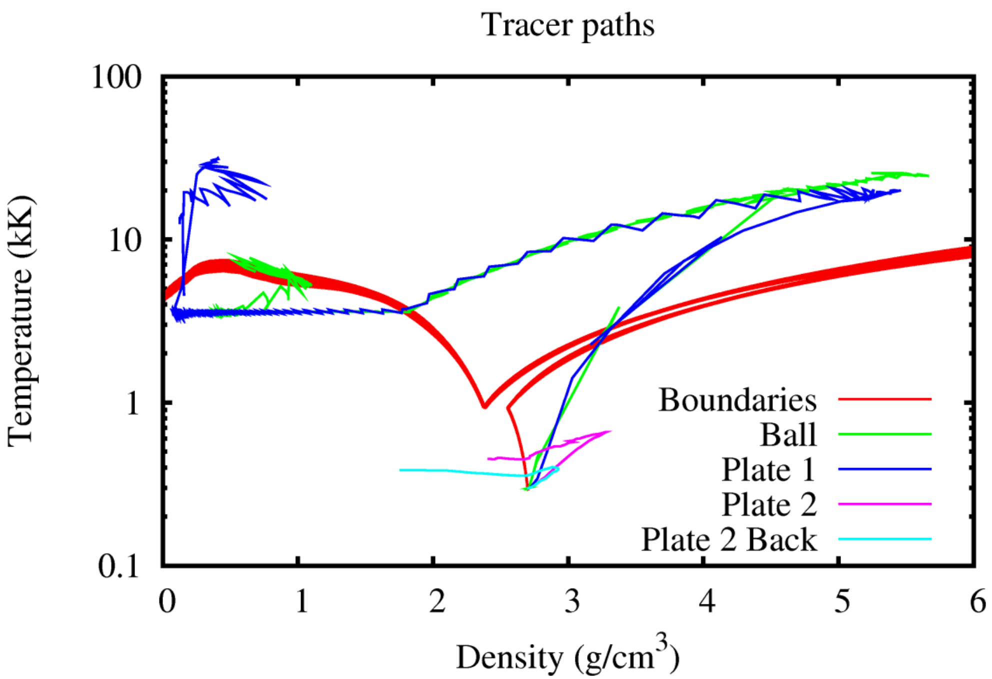




It helps users to have a unified, user-friendly and regularly tested capability

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

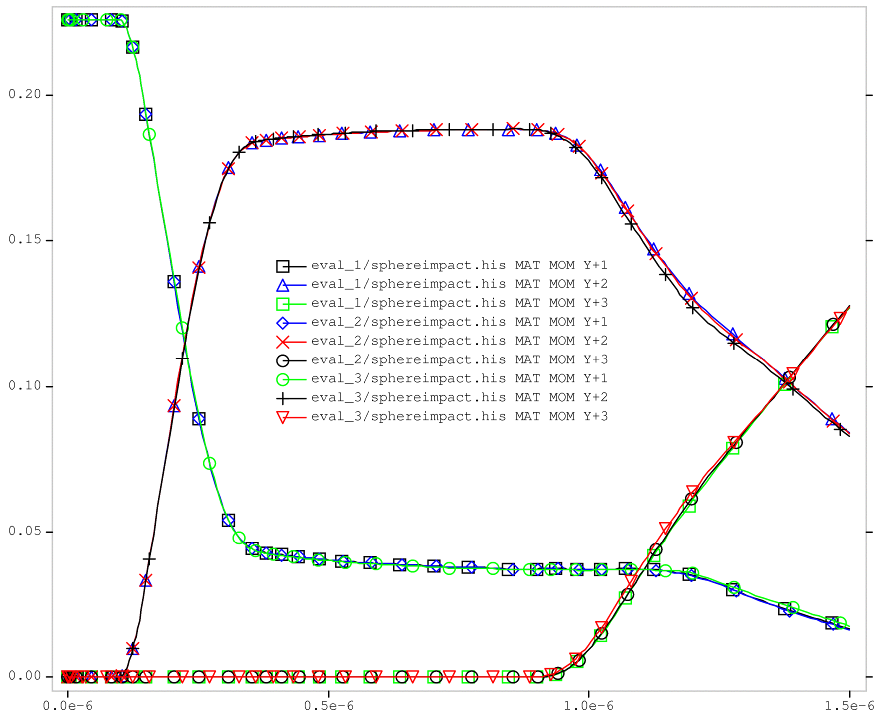




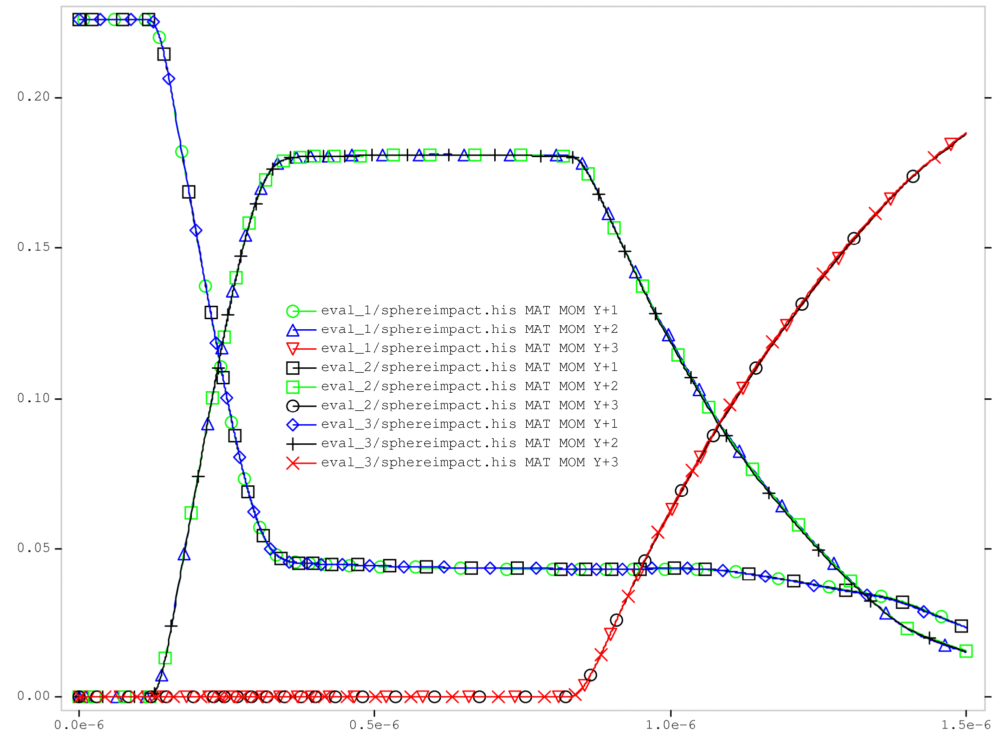
Phase boundary lines of PCA source EOS files are shown along with phase space trajectory of tracers (mean table, csmin=0, mfac=4). (The results on this slide are from the Aluminum EOS as of Fall 2014)

Looking at UQ Results via ALEGRA-DAKOTA

- 3 PCE (polynomial chaos expansion) quadrature points and 1 tabular mode with K=3 and r=6 Rosenblatt transformation. (eval_2 centered quadrature point)
- Showing here material momentums plots at factor of 1 and 4 times resolution.
- Sample output time histories are a good way to gain perspective on what might be important.



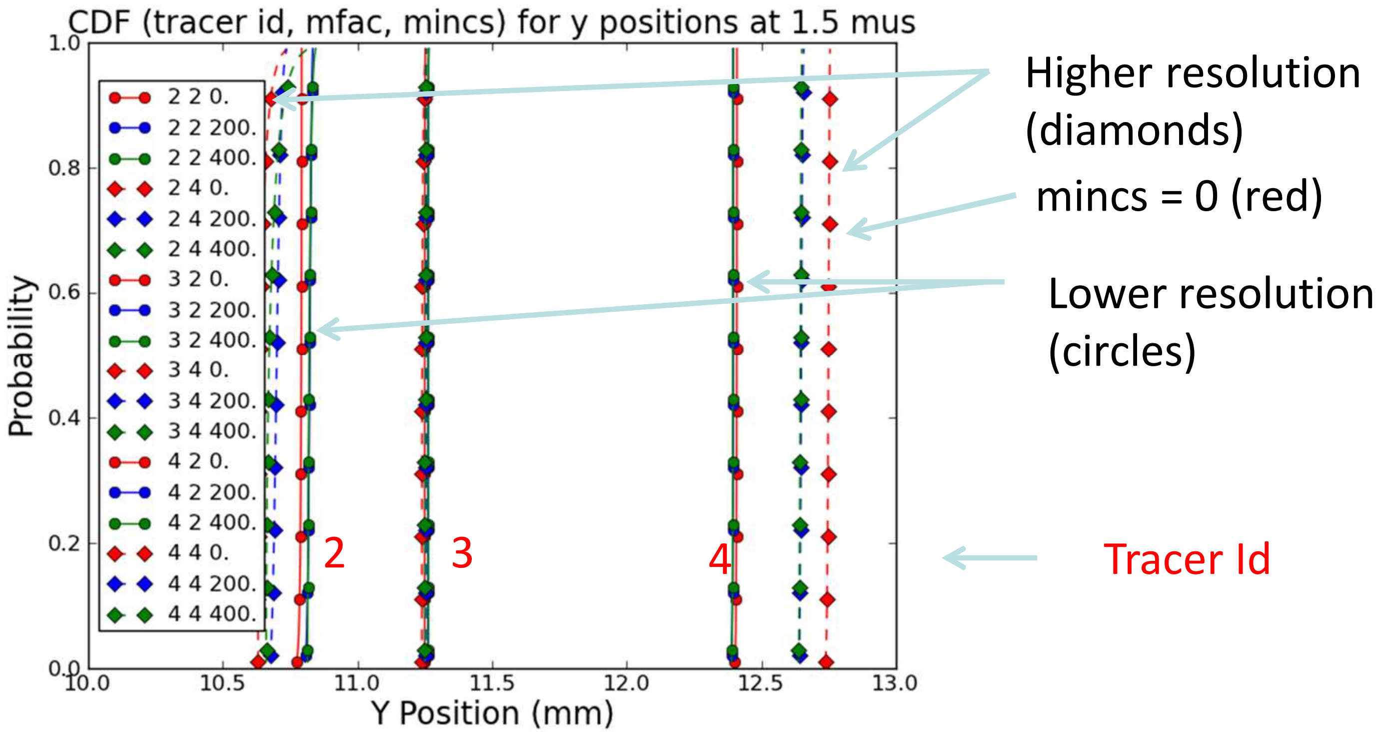
Low resolution



4 times resolution

Uncertainty analysis using UQ enabled AL EOS

3 PCE (polynomial chaos expansion) quadrature points and 1 tabular mode with 3 mode (K=3,r=6) Rosenblatt transformation.



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 UQ material model approach encourages a UQ viewpoint on the whole modeling process.
4) UQ enabled table capability tends to drive useful verification and numerical work

Conclusion

A multiphase EOS table approach with embedded UQ provides the following value:

- More precise EOS surface representation including phase boundaries
- Embedded UQ information in EOS
- Usable EOS representation for UQ enabled continuum analysis
- Quantitatively improves clarity for the end user on issues of model and model data uncertainty relative to other V&V issues.

What is next:

- Build a representation based on 10,000 sample tables to provide a satisfactory usable representation.
- Implement other closure models (i.e. conductivity) into the same consistent framework.
- Eventually, work toward providing UQ enabled strength modeling.