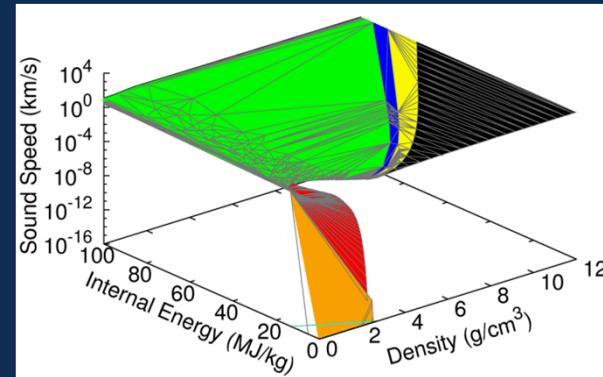
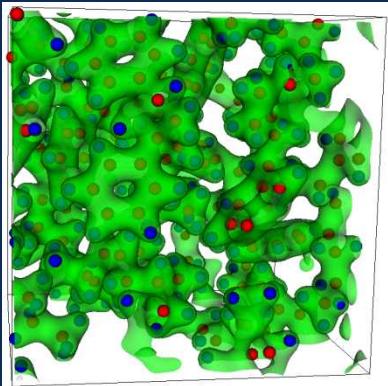


*Exceptional service in the national interest*



# Building and Using Tabular Equations of State with Uncertainty Information

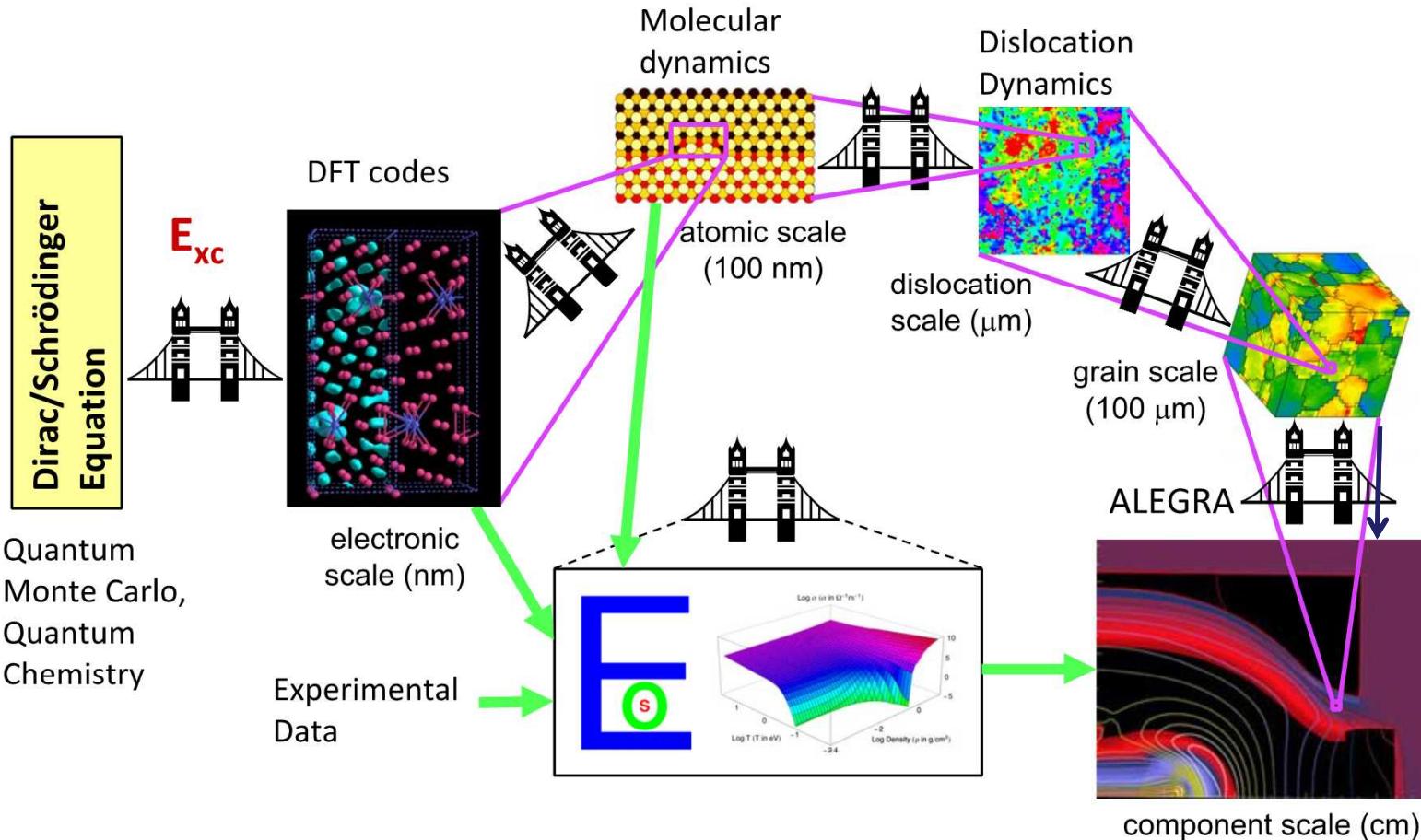
**J. H. Carpenter, A. C. Robinson, B. J. Debusschere, A. E. Mattsson**  
**Sandia National Laboratories**

**NEDPC 2015**  
**October 19-23, 2015, LANL**



Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

# Goals for EOS Upscaling Paradigm



- Provide quantitative uncertainty estimates to the analyst based upon fundamental measurements and calculations used to build the EOS.
- Preserve model providence throughout the process.
- Produce a usable system for generation and use of the EOS.

# 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.

# The Process Glue: a Common XML Input Deck

## XML Input Deck is really the “EOS Model”:

<EOSModel> -- Traditional EOS model definition

<EOSData> -- EOS data and uncertainties used for model calibration

<Inference> -- Controls for the inference

<Tabulation> -- Controls for the tabulation

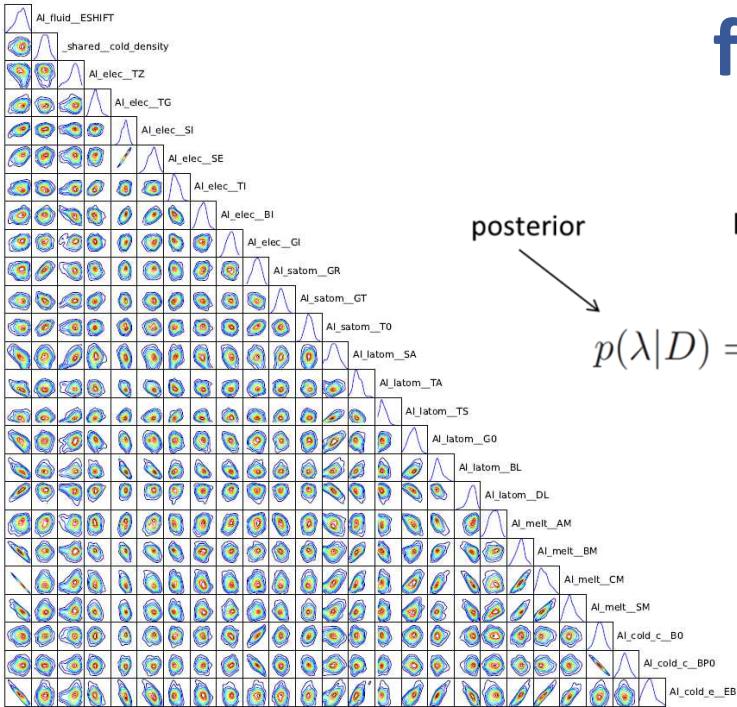
## Key Requirement:

- 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.

## Aluminum as an example case:

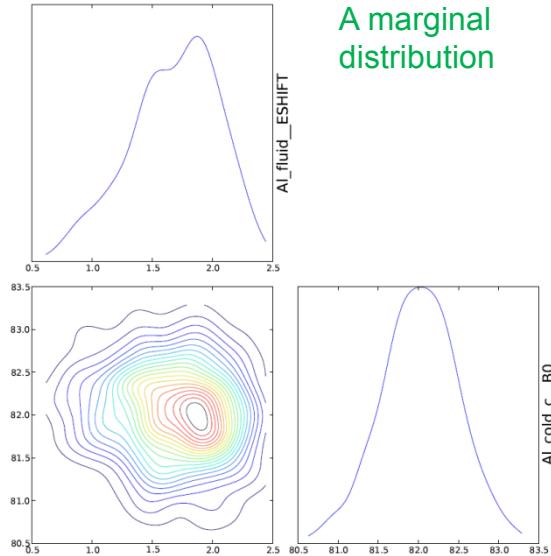
- Wide range Al EOS is built from semi-empirical models, with solid and liquid phases including melt/vaporization/sublimation.
- 37 total parameters, 25 constrained well enough by data for inferring UQ information.
- 16 standard data sources: Isobaric enthalpy and density for solid and liquid, Shock data for solid and liquid, Isothermal compression data for solid, QMD calculations of critical point plus melt and vaporization data.
- Constraints on physicality: smoothness and convexity change limitations along phase boundaries; thermodynamic stability checks across range of interest.

# AI EOS Model Parameter Bayesian Inference for Posterior



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

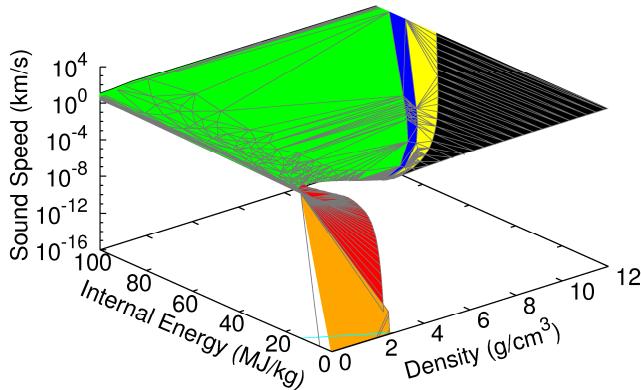
posterior      likelihood      prior  
 normalization



- 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.

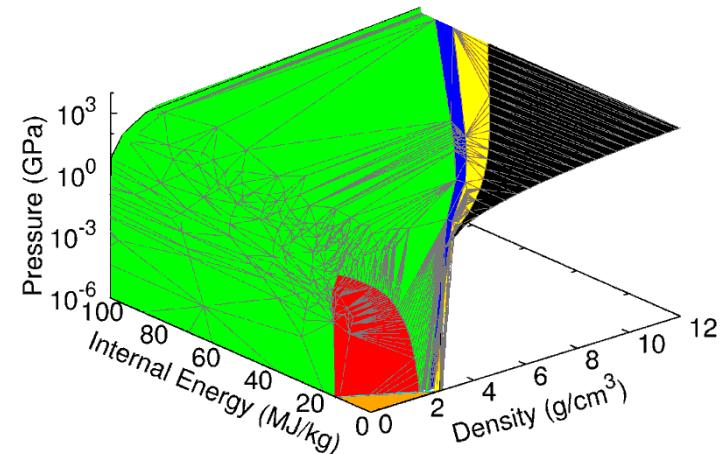
# UTri EOS tables accurately match the model

- 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.
- Prescribed accuracy means tabulation error may be quantified and/or eliminated from uncertainty considerations.



Phases:

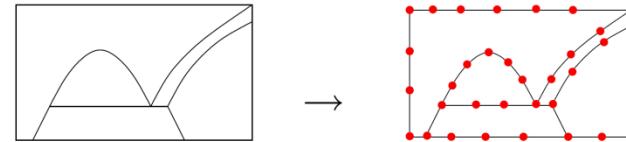
off table  
solid  
fluid  
melt  
vaporization  
sublimation



# UTri Tabular EOS generation

- Must build  $N$  ( $\sim 10,000$ ) UTri tables which are topologically equivalent and of similar accuracy:

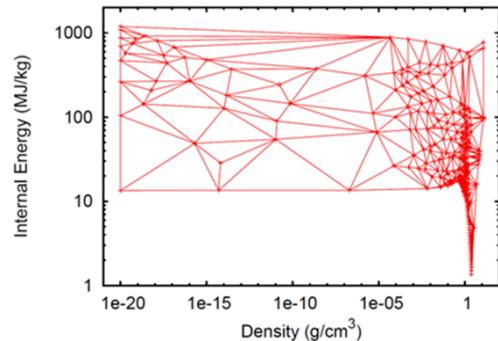
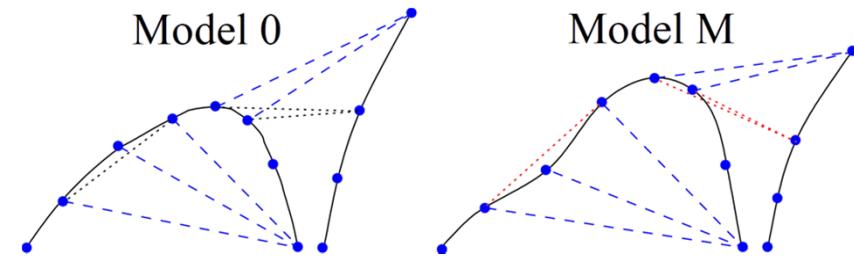
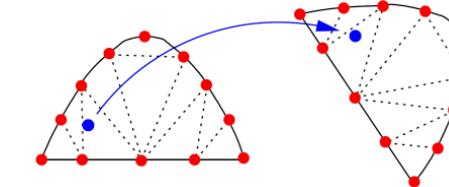
- Adaptively mesh boundaries:



- Adaptively mesh phase regions:

## Phase region 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
- Mesh 0 for AI fluid region



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

# 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  $\xi$  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.

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

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

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

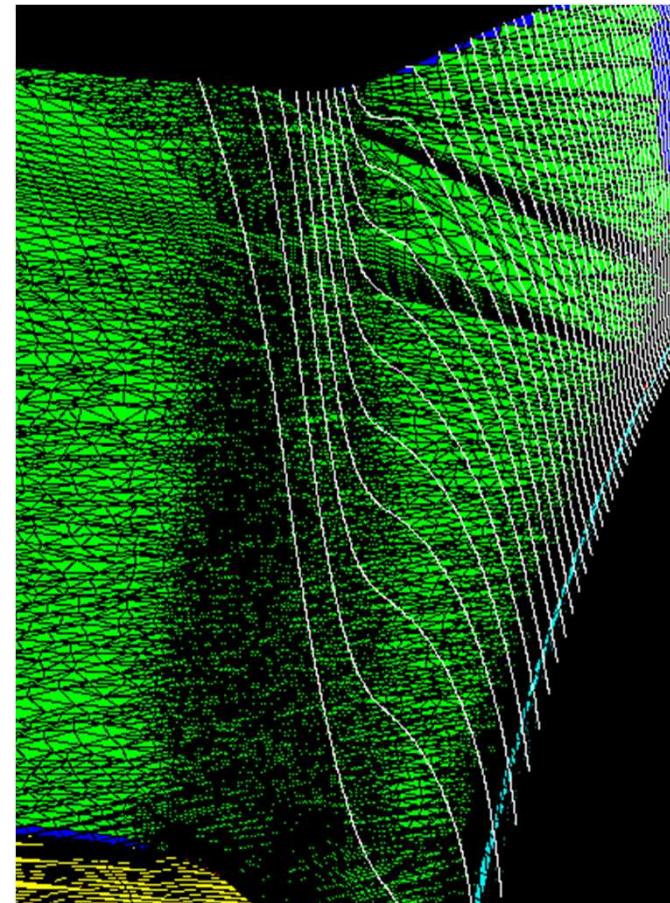


$$\mathbb{T} = \bar{\mathbb{T}} + \sum_k \xi_k \mathbb{T}_k$$

# Multiphase Tabular Generation and Representation: AI UQ enabled table

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

- Current wide range UQ AI 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  
9

# Develop surrogate random variable distributions

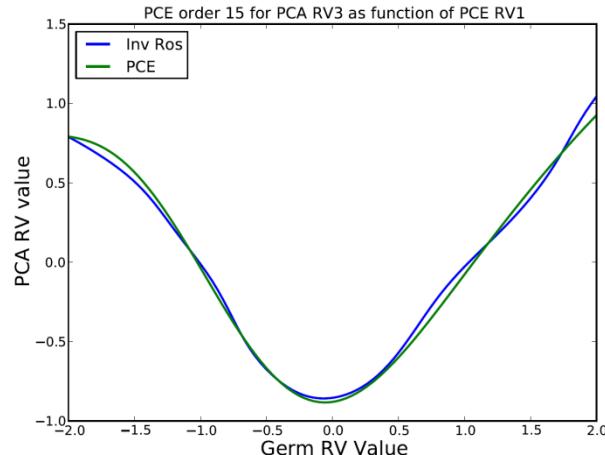
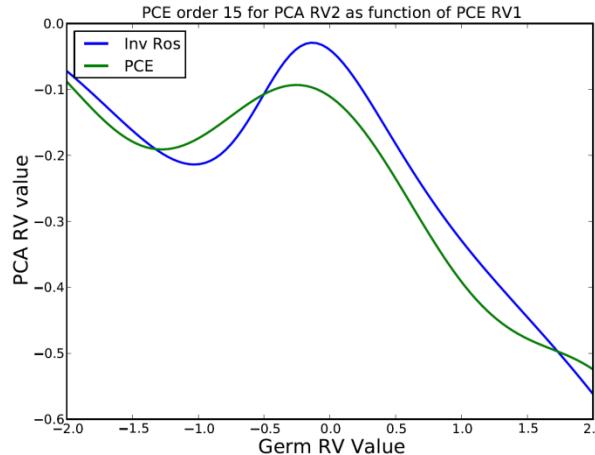
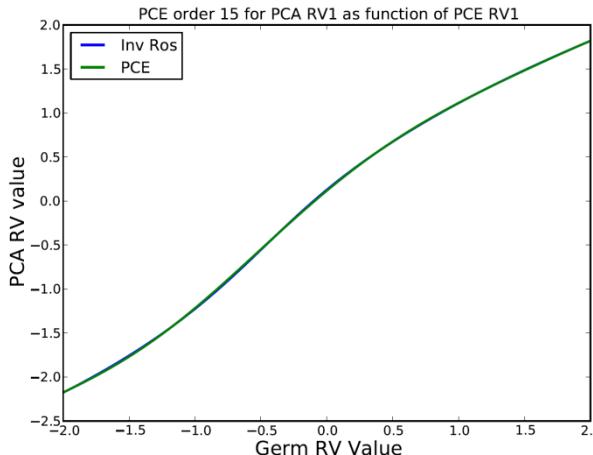
$$T = \bar{T} + \xi_1 T_1 + \xi_2 T_2 + \xi_3 T_3 + \dots$$

- 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  $\xi_i$  which are zero mean and unit co-variance (Not necessarily independent)
- One can assume 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 independent but still preserve ordered dependencies.

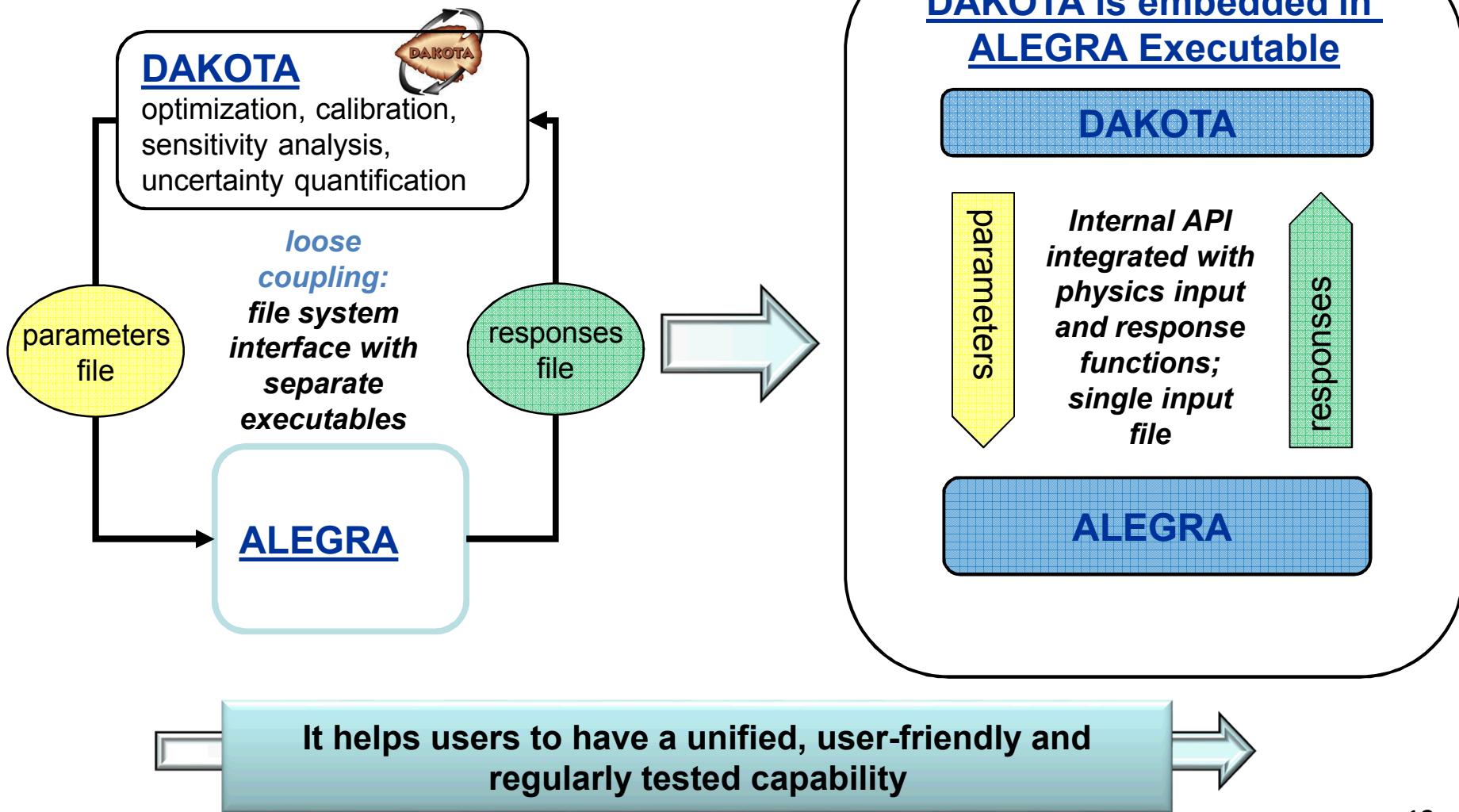
$$\xi_i(\boldsymbol{\eta}) = \sum_{j=0}^{\binom{K+r}{r}-1} a_j \psi_j(\boldsymbol{\eta})$$

# Rosenblatt transformation needs more samples

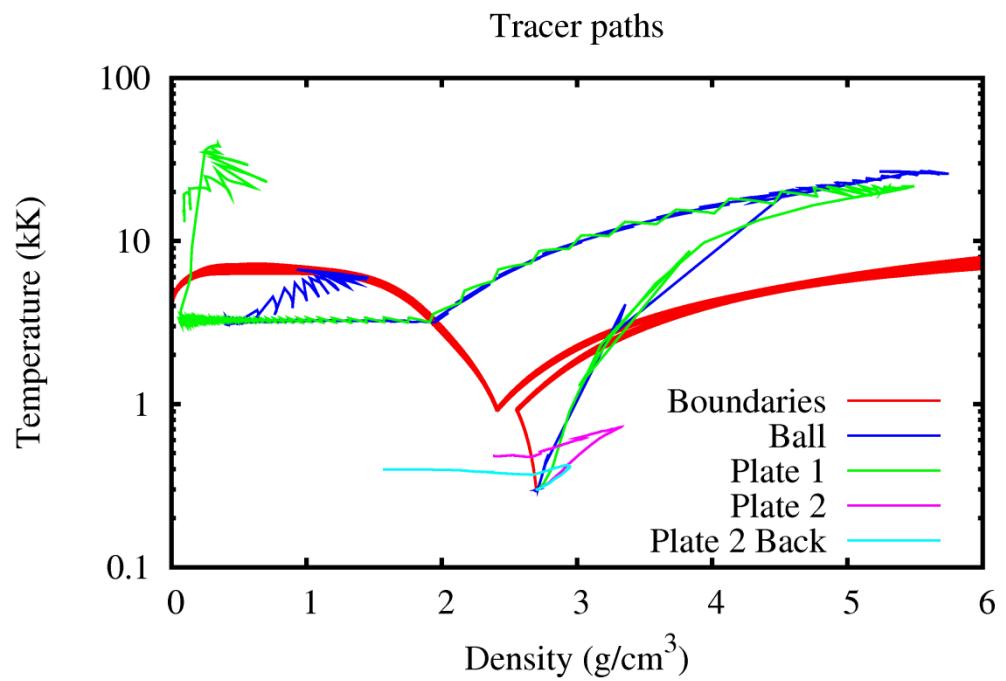
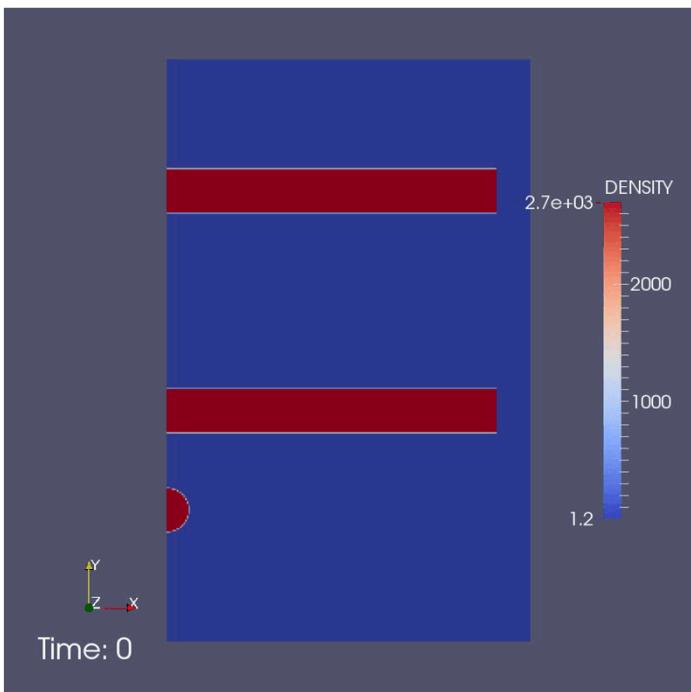
- The Rosenblatt transformation seems to do quite well in the main components. I.e. relating the first mode to the first PCE dimension.
- However, the coupling terms between the different modes are much more nonlinear, and seem a bit noisy. Even 15<sup>th</sup> order PCE does not seem to be sufficient.
- 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



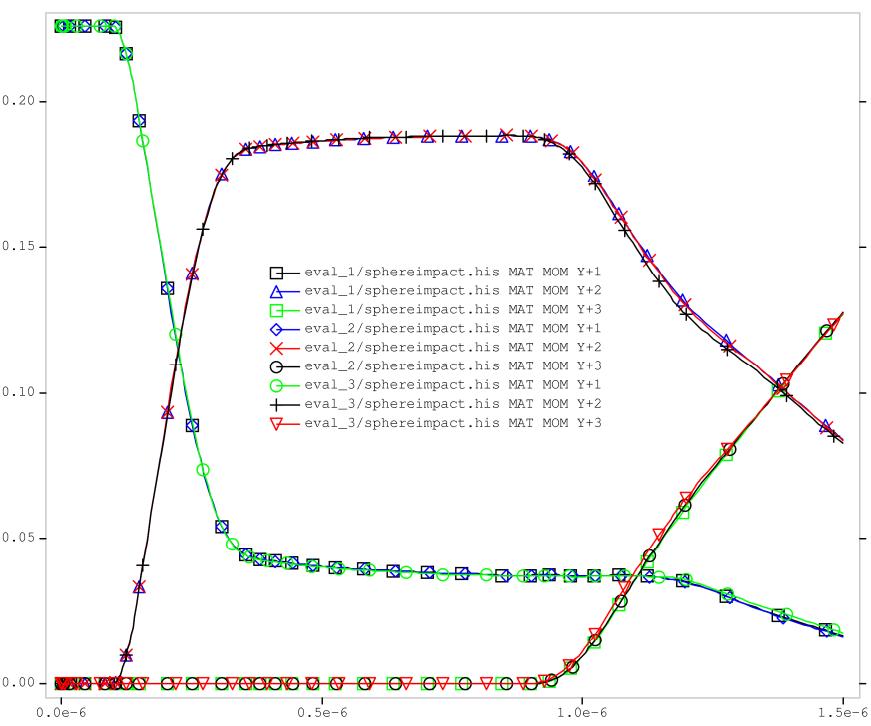
# 2mm diameter Al ball impacting spaced Al plates at 20 km/s in air background. Termination at 1.5 $\mu$ s.



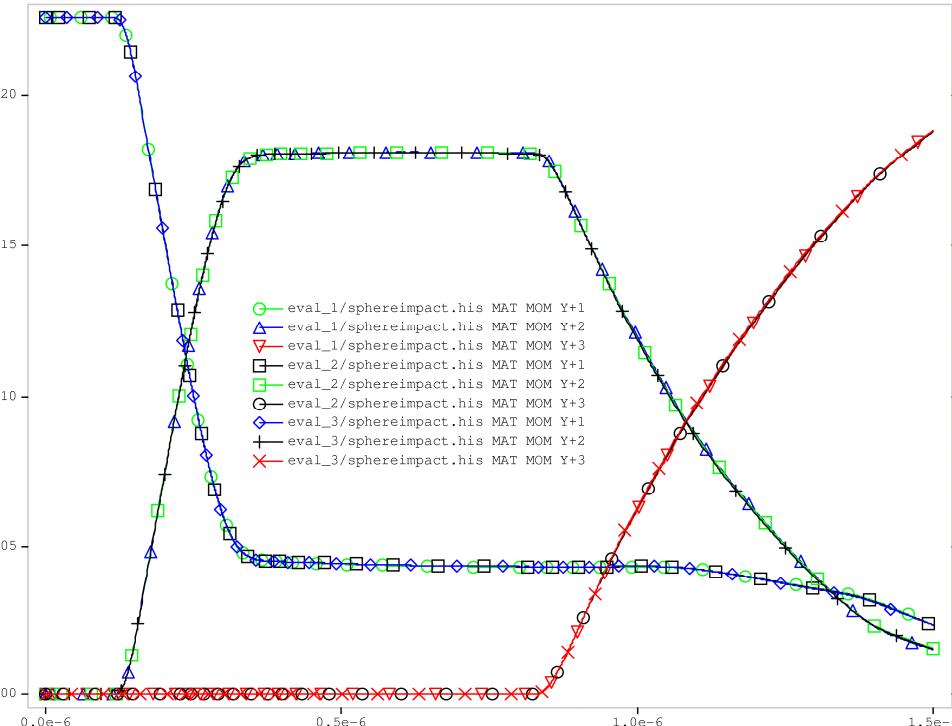
Phase boundary lines of PCA source EOS files are shown along with phase space trajectory of tracers (mean table,  $\text{csmin}=0$ ,  $\text{mfac}=4$ ).

# 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 is center quadrature point)
- Shown here are material momentum plots at factors of 1 and 4 times resolution.
- Sample output time histories are a good way to gain perspective on what might be important.



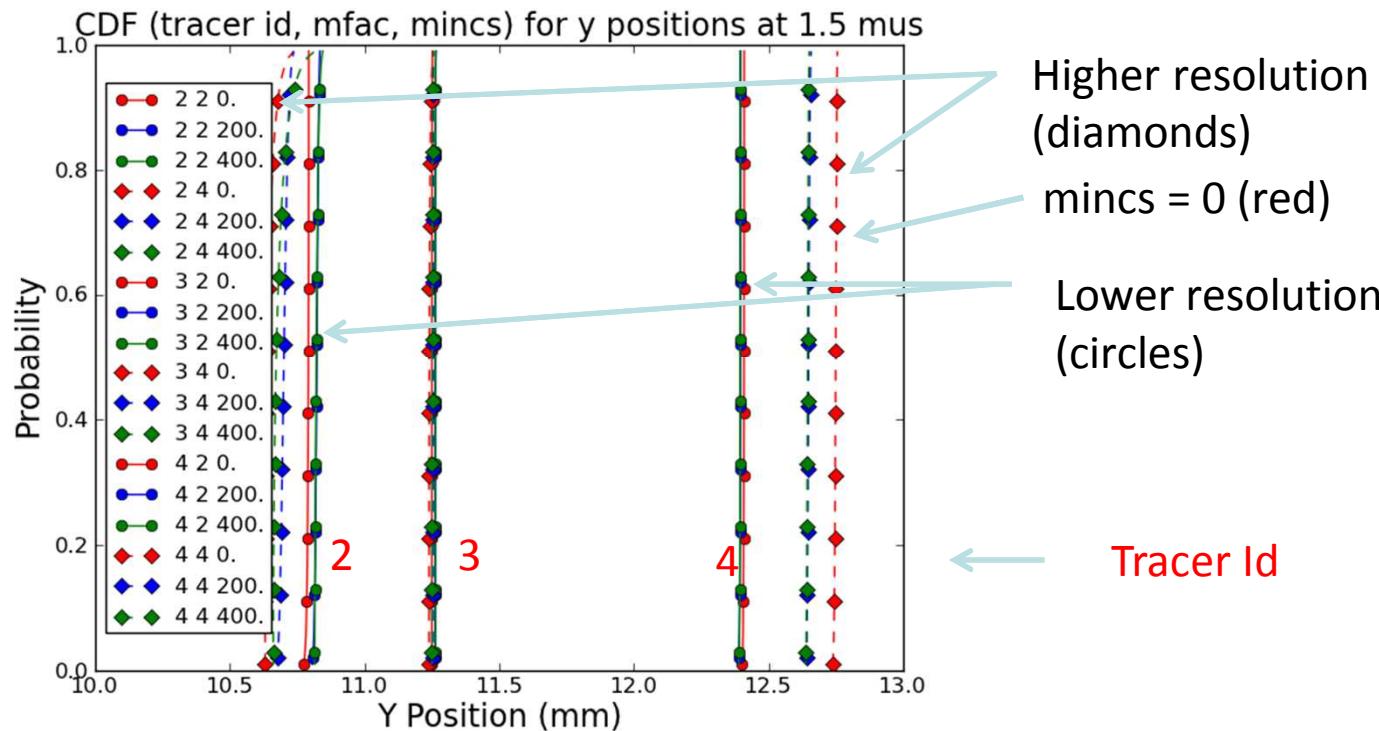
Low resolution



4 times resolution

# Uncertainty analysis using UQ enabled AI 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 uncertainties (e.g. mesh resolution (mfac), numerical or modeling constants (mincs)).
- 2) Conclusions will depend 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.