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Automated Generation of Tabular Equations of State with Uncertainty Information

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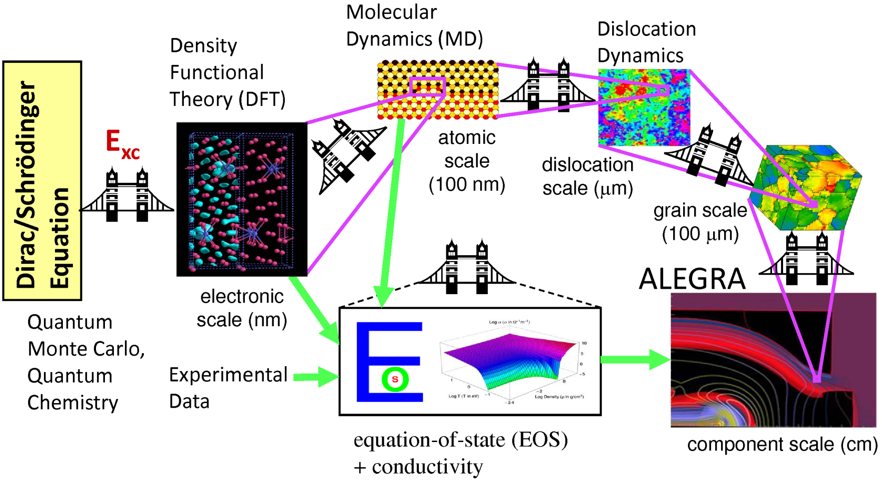
EOS Development Paradigm



- Recognize EOS multi-scale character – initially neglect strength effects.
- Provide quantitative error estimates to continuum analysts based upon fundamental measurements and calculations of the EOS.
- Preserve model providence throughout the process.
- Usable system for generation and use of the EOS.

Tabular EOS UQ System

Software Package	Output
EOS model library and data	Proposal model (XML input deck)
Bayesian inference using Markov Chain Monte Carlo	Extensive sampling of Posterior Distribution Function (PDF)
EOS Table building	Topologically equivalent tables for each sample
PCA analysis	Mean EOS table + most significant table perturbations
Hydrocode + Dakota	Cumulative Distribution Function for quantities of interest

- First half of system utilizes analytic EOS models.
- Last half of system utilizes tabulated EOS models.
- Uncertainty information transferred from parametric to thermodynamic space.

What Does "EOS Model" Mean?

XML input deck is the (meta-)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

EOS table and interpolation scheme is the real "EOS model"

- Codes actually query it for thermodynamic closure states
- Example: pick on Kerley's 3700 and Sandia's codes
  - ALEGRA simulation with 3700 and backup linear interpolation
  - ALEGRA simulation with 3700 and sound speed modifications
  - CTH simulation with 3700 and bad state clipping
  - Saying "Aluminum 3700" describes none of these accurately
  - They are not even the same as Kerley's model used to build 3700

Can the XML input really be the "EOS model"?

- Tabulation must be representative of original models
- Consistency between EOS build tools and hydrocode interpolation
- System must be automated – no by-hand modifications
- Provide no incentives for fiddling by the hydrocode/analysts

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Aluminum Example Case

Test multi-phase aluminum model:

- Semi-empirical solid-liquid-gas model
  - Cold curve uses polynomial expansion form
  - FCC solid phase uses the Debye model
  - Fluid phase uses Bushman-Lomonosov-Fortov model
- 37 parameters in total
- Range of interest to 150 kK and 20 g/cm^3

Multiple sets of data used for calibration:

- 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

Recording the Art of EOS Building

Expert modeler decisions (often visually based):

- Appropriate models to use
- Stability and physicality requirements
- Relative weighting of data sets
- How well models should agree with data

Bayes' rule allows inferring parameters' posterior distribution function (PDF) using data and prior knowledge:

posterior, likelihood, prior, normalization

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

The expert's art must be encoded in the XML input for automation of PDF sampling and table building.

- All invalid parameter sets must be rejected in the inference
- Likelihood contains weighting of data
- Prior contains conditions on physicality (rejection criteria)
- Expert still must guide the system to a good starting point, the Maximum A Posteriori (MAP) value

Physicality Conditions

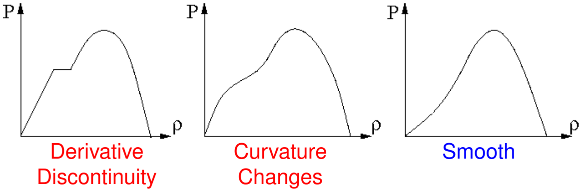
Thermal and mechanical stability:

- Heat capacity and bulk modulus must be positive
- Applied to pure phase regions (i.e. not transitions)
- Particularly important for regions without calibration data

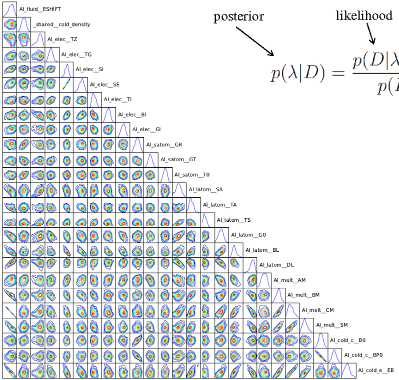
Smoothness of phase boundary lines:

- Boundaries must not have discontinuities
  - They indicate problems with model parameters or solvers
  - Prevents later problems with curve approximation and tabulation
- Boundaries should not have multiple curvature changes
  - One sign change allowed along boundaries
  - Physical for vapor dome, other lines may still be questionable
  - With few exceptions more changes are unphysical
- Applies to vaporization, melt, polymorphic transitions
- Derivatives sampled along phase boundaries

Vapor dome example:



Al EOS Model Inference



posterior, likelihood, prior, normalization

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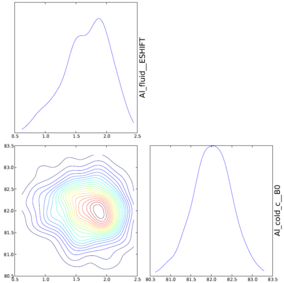

Al EOS 25 parameter inference

A marginal distribution

- Use adaptive Markov Chain Monte Carlo scheme to reduce number of steps
- Start chain from optimized MAP parameters
- PDF evaluations may be parallelized to enable long chains ($\sim$4.5M steps for this EOS, one serial evaluation is approximately 2 sec.)
- Each posterior evaluation is roughly equivalent to generating an entire EOS table and having an expert check it for correct behavior.

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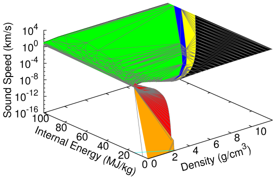
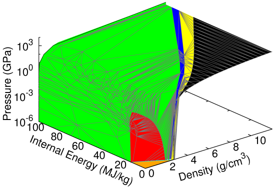
UTri EOS format for Tabulation

- Unstructured triangular mesh in density-internal energy space.
- All desired thermodynamic quantities tabulated at mesh nodes.
- Uses linear interpolation on triangles.
- May add mesh nodes to reduce error with respect to model below a certain tolerance.
- Accurate EOS tables correctly represent the very small thermodynamic sound speed in certain mixed phase regions, with precise phase jumps.
- Prescribed accuracy means tabulation error may be quantified and/or eliminated from uncertainty considerations.



Phases

solid
fluid
melt
vaporization
sublimation
off table



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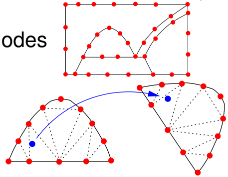
Tabulation Complexities

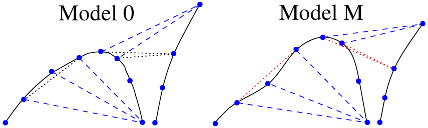
Must build N topologically equivalent UTri tables with similar accuracy:

- Triangular mesh in density-internal energy space
- All thermodynamic quantities tabulated at mesh nodes
- First, adaptively mesh boundaries
- Second, adaptively mesh phase regions

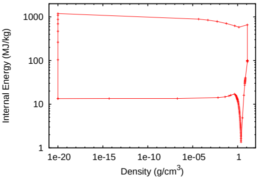


Phase region complexities:

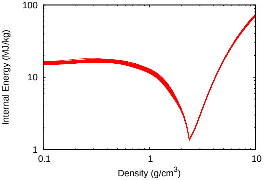
- Constrained Delaunay triangulation used as transfer function
- Extreme non-convexity in individual phase regions
- Computation chain must be parallelized for many tables



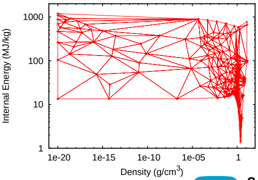
Aluminum fluid region:



Mesh 0 boundary (1.0 tolerance)



70 other boundaries



Mesh 0 grid

Tabular UQ Representation

Principal Component Analysis (PCA) used for tabular dimension reduction of N tables:

- Export truncated set of mode table that capture most details (i.e. eigenspectrum energy)
- Multi-precision floating point necessary due to dynamic range of tables
- Using log of density and energy ensures positivity
- Parallel processing of singular value decomposition matrix creation important
- Random variables ξ_i are uncorrelated, zero mean, unit standard deviation, but not necessarily independent
- Kernel density estimator and Rosenblatt transformation using Hermite Polynomial Chaos Expansion (PCE) representation may provide a similar system with independent random variables η.
- PCA solver currently scales as MN^2, limiting the practical number of samples.

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

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

$$z = \bar{z} + \tilde{U}\Sigma\xi$$

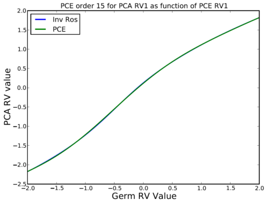
$$= \bar{z} + (Z - \bar{z}\mathbf{1}^T)H^{1/2}\tilde{V}\xi$$

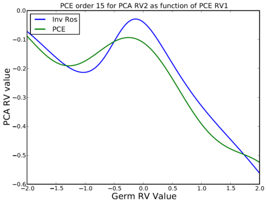
$$\mathbb{T} = \bar{\mathbb{T}} + \sum_k \xi_k \mathbb{T}_k$$

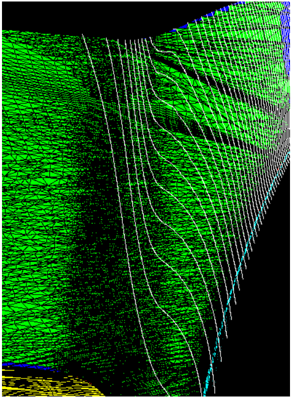
$$\xi_i(\boldsymbol{\eta}) = \sum_{j=0}^{\binom{K+r}{r}-1} a_j \psi_j(\boldsymbol{\eta})$$

AI UQ Enabled Table

- Tabulated 442 samples from chain.
- Accuracy set to 0.01 relative tolerance.
- 7 modes in PCA above 10^{-3} energy cutoff.
- Rosenblatt transformation works well with main components, i.e. relating first PCA random variable (RV) to first PCE RV.
- Coupling terms between different order RVs much more nonlinear.
- Need more samples, higher order PCEs, and possibly another mapping approach.







Pressure isobars of mean table in density-internal energy space

Summary

System for multi-phase tabular EOS with embedded UQ provides:

- Reproducibility and documentation of tabular model generation process.
- More precise EOS surface representation including phase boundaries.
- Embedded UQ information in the EOS table.
- Usable EOS representation for UQ enabled continuum analysis.
- Clarification between EOS model and data uncertainties relative to other analysis uncertainties.

Next steps:

- Build a PCA/Rosenblatt EOS representation based upon $\sim$10,000 samples
- Implement other closure models (i.e. conductivity) into the same consistent framework.
- Long term, work toward providing UQ enabled strength modeling.