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# An Uncertainty Quantification System for Tabular Equations of State

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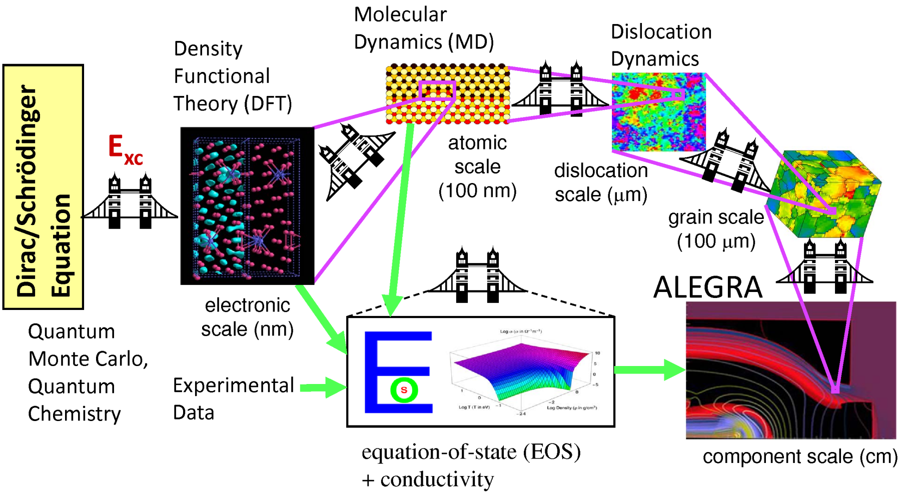
# Motivation




Goal: Provide quantitative error estimates to the continuum analysts based upon fundamental measurements and calculations 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.

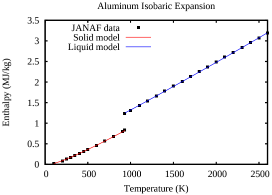
# EOS Data and Model

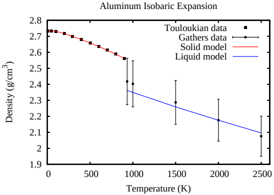
## Test multi-phase aluminum model:

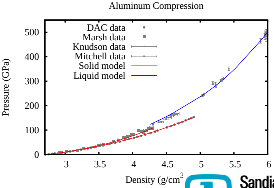
- Semi-empirical solid-liquid-gas model
  - Cold curve uses polynomial expansion form
  - FCC solid phase uses the Debye model
  - Fluid phase uses Bushman-Lomonosov-Fortov model
- 30 parameters in total
- Range of interest to 40 kK and 10 g/cm$^3$

## 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



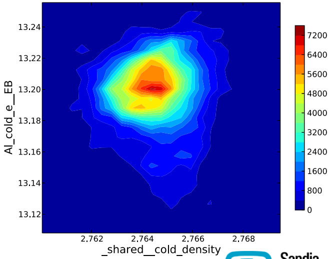



# Bayesian Inference of Parameters

$$\underbrace{p(\lambda|D)}_{\text{posterior}} = \frac{\overbrace{p(D|\lambda)}^{\text{likelihood}}\,\overbrace{p(\lambda)}^{\text{prior}}}{\underbrace{p(D)}_{\text{normalization}}}$$

Bayes' rule gives posterior distribution function (PDF):

- Represents belief in parameter values $\lambda$ given data $D$.
- Adaptive Markov Chain Monte Carlo used to sample the PDF.
- Starting point obtained via optimization.
- Difficult due to ill-constrained and magnitude differences of parameters.
- Must enforce stability and physicality constraints on model via priors
- Successfully applied on the 30 parameter example aluminum model.
- Marginal distribution of two cold curve parameters indicate their lack of correlation

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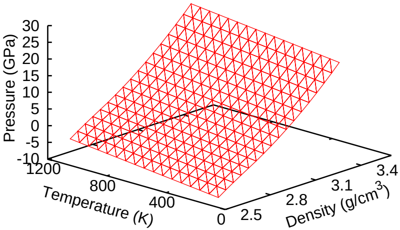
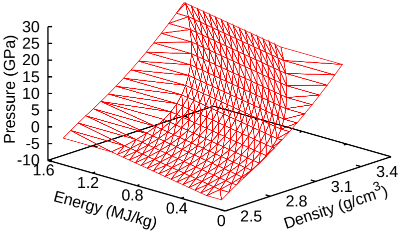
# Tabular Representation

New unstructured triangular (UTri) format essential:

- Uses linear interpolation on triangles
- Non-rectangular grid easily follows phase boundaries capturing derivative discontinuities
- Adaptation allows for storage efficiency while ensuring a desired tabulation accuracy
- Tabulates in both the $(\rho, T)$ and $(\rho, E)$ phase spaces
- All desired variables tabulated simultaneously

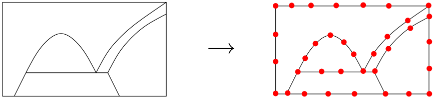
Example pressure surfaces in $(\rho, T)$ and $(\rho, E)$ spaces:



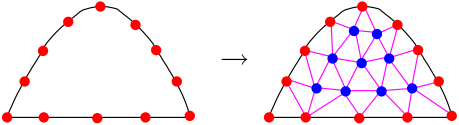



# Smooth Mesh Generation

N sample tables with consistent topologies:



Adaptively mesh boundaries: linear map of node locations between sample tables



Adaptively mesh phase regions: interior nodes mapped using a Laplace-Beltrami smoother with phase boundary points as boundary conditions

$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial \xi^{\alpha}}\left(\sqrt{g}g^{\alpha\beta}\frac{\partial x^{i}}{\partial \xi^{\alpha}}\right) = 0$$

Smoothing of mesh points eliminates noise from PCA.

# Tabular UQ Analysis

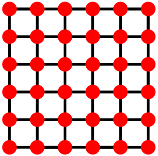
Use Principal Component Analysis (PCA) to look for a tabular representation with reduced dimensionality:

- Start with representative sample of tables (e.g. MCMC chain states)
- Perform PCA:

$$\bar{z} = ZH^{1/2}\mathbf{1}/\mathbf{1}^T H\mathbf{1}$$

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

Nx

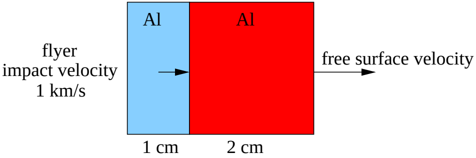


$$z = \bar{z} + U\Sigma\xi = \bar{z} + G^{-1/2}\tilde{U}\Sigma\xi = \bar{z} + (Z - \bar{z}\mathbf{1}^T)H^{1/2}\tilde{V}\xi$$

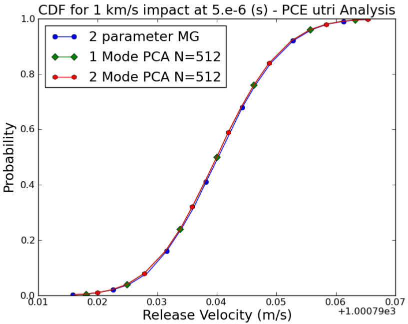
- Choose a truncated set of modes to export in tabular form
- In the hydrocode, an EOS table is generated at start up for each sample run with the user selecting the number of modes to be used: $T = \bar{T} + \sum_k \xi_k T_k$
- Random variables $\xi_k$ are uncorrelated, zero mean, unit variance, but not necessarily independent

# Example Results

## Simple flyer plate impact problem:




- Measure free surface velocity at back of target
- Results shown for a two parameter Mie-Grüneisen model



# Summary

- Tabular EOS UQ system developed
- Supports multi-phase EOS models with many uncertain parameters
- Enabled by underlying unstructured triangular table format
- Robustness issues need to be worked out before realizing full production system
  - Stable and physical behavior of models for arbitrary parameter choices
  - Determining good starting points for the MCMC chain
  - More efficient table generation
  - Proper conditioning of variables for the PCA step
  - Examine the assumption of Gaussian distributions