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# Accounting for Data Uncertainty in Making and Using an EOS

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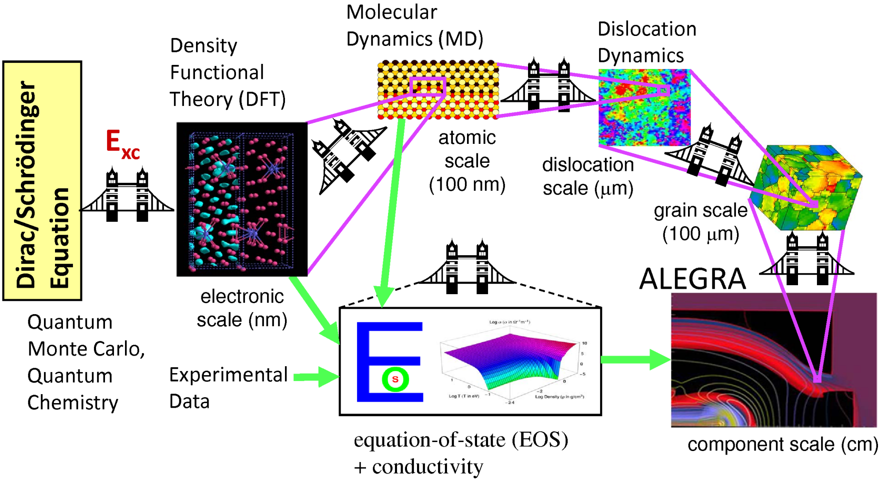
# EOS Development Paradigm




- 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.
- Focus herein will be on the first steps involving data

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# 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

# 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:

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

## 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

# Bayesian Inference

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

Bayesian "objective" is the posterior distribution function (PDF):

- Attempt to find the most likely parameters and their distribution, allowing UQ practices to be employed
- Often sampled with Monte Carlo methods but can also be optimized directly with gradient methods
- Typical to work with logarithm of PDF and ignore normalization

# Constructing Bayesian Likelihood

Calculate likelihood:

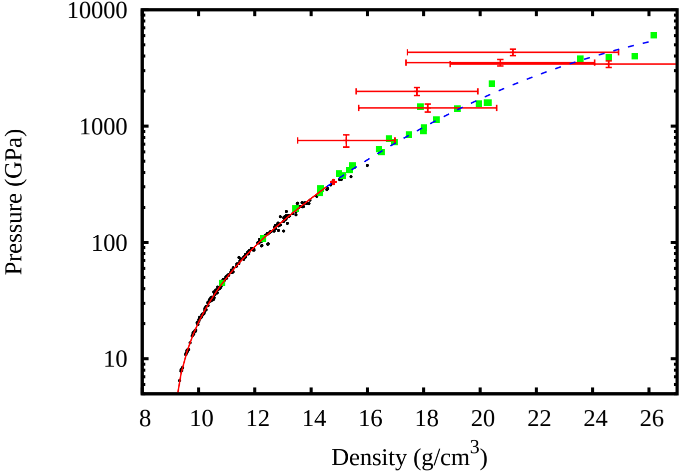
$$\log(p(D|\lambda)) = -\frac{1}{2}\left[\frac{D-\bar{D}}{\sigma_D}\right]^2 - \frac{1}{2}\log\sigma_D^2$$

- Simple Gaussian noise models currently supported
- Noise model hyperparameter $\sigma_D$ often can be fixed
- $\sigma_D$ may be specified either as specific values or a relative weight
- Gaussian statistics with fixed hyperparamters gives least-squares
- Every data source is cast into this framework, from cold curves to shock data to phase boundaries
- Using surrogate models for data can make sense when many and/or scattered point are available

# Surrogate Data Example

Principal Hugoniot data for copper:

- Surrogate model is linear or quadratic $u_s$-$u_p$ form
- Points sampled from surrogate for inclusion in likelihood
- $\sigma_D$ is chosen based upon spread of data from surrogate



# Constructing Bayesian Prior

Calculate prior:

$$\log(p(\lambda)) = -\frac{1}{2}\left[\frac{\lambda-\bar{\lambda}}{\sigma_\lambda \bar{\lambda}}\right]^2 + \texttt{conditions}(\lambda)$$

- Simple Gaussian priors and bound constraints currently supported for parameters
- Various uses include constraining parameters to certain ranges or eliminating unphysical models

Conditions:

- Act as rejection criteria (very small probability)
- Encode physicality requirements on the model
- Requirements ranked in prior contribution to aid in sampling
- Can still make sampling and optimization difficult
- Moving from discrete to smooth engagement of conditions would likely improve these difficulties

# Physicality Conditions

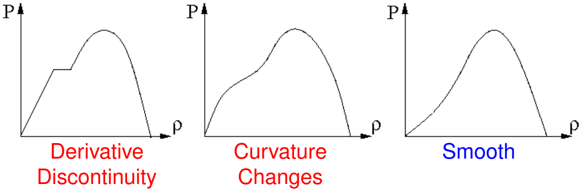
## Thermal and mechanical stability:

- 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:



# 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

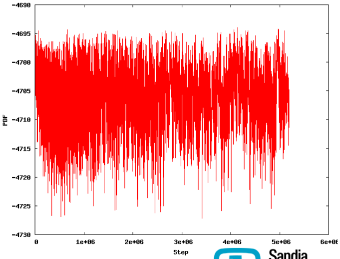
# Optimizing the Posterior

## Optimization and Sampling:

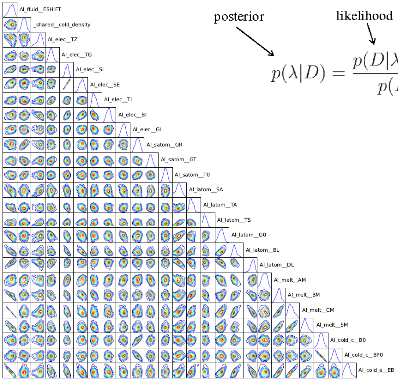
- PDF is optimized as in normal EOS development
- Hand tuning of parameters or automated methods used
- Methods: gradient based, genetic algorithms, simulated annealing
- All suffer curse of dimensionality in finding global optimum

## Maximum A Posteriori (MAP) parameters:

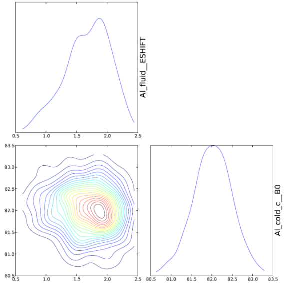
- Normal EOS development gives the expert opinion “best” model.
- Sampling the PDF via Markov Chain Monte Carlo (MCMC) verifies this opinion is represented (the “art” has been recorded) in the statement of the likelihood and prior probabilities.
- MCMC burn-in with significant change in the PDF indicates a “better” model.
- The verified best model is the starting point for the remaining UQ process.



# Al EOS Model Inference




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




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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# Summary

Dealing with data uncertainty in creating EOS models:

- The data needs to be treated on the same footing as the rest of the modeling process
- Expert opinion on model agreement with data must be recorded
- Automated processes must reproduce the expert opinion
- Physical constraints on models are an implicit form of data in this system
- Sampling of the PDF provides the foundation for propagating the data uncertainty to inform uncertainty in engineering outputs.

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