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Bayesian calibration of dynamic compression experiments on the Sandia Z Machine

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NNSA National Nuclear Security Administration

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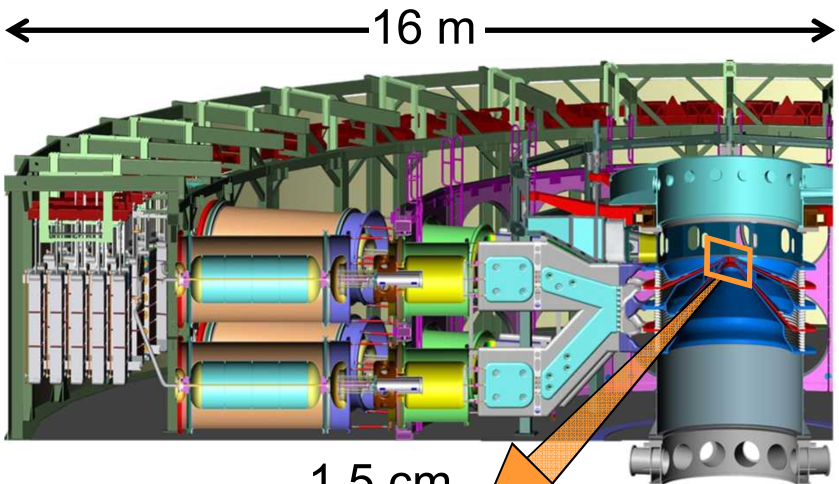
Acknowledgments

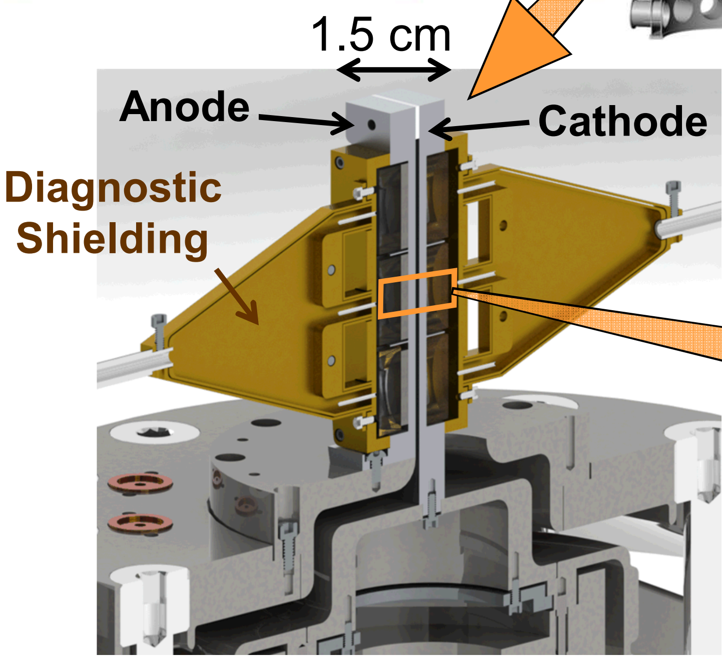
- Laura Swiler
  - Dakota (Bayesian code) implementation
- Lauren Hund
  - Statistical model development

Outline

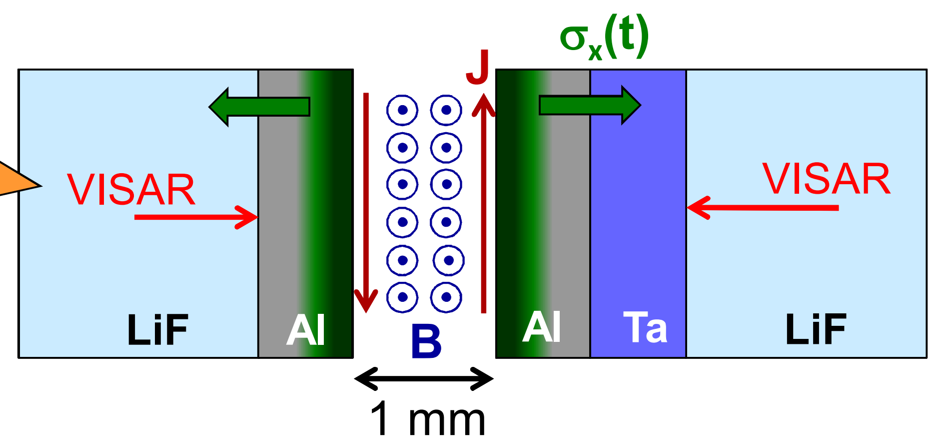
- Experimental configuration and data
  - Ramp compression of tantalum to 2.5 MBar
- Bayesian calibration methodology
  - Can we extract EOS information with quantified uncertainties?
- Results
  - 298K isotherm compared to data in the literature

The Sandia Z machine

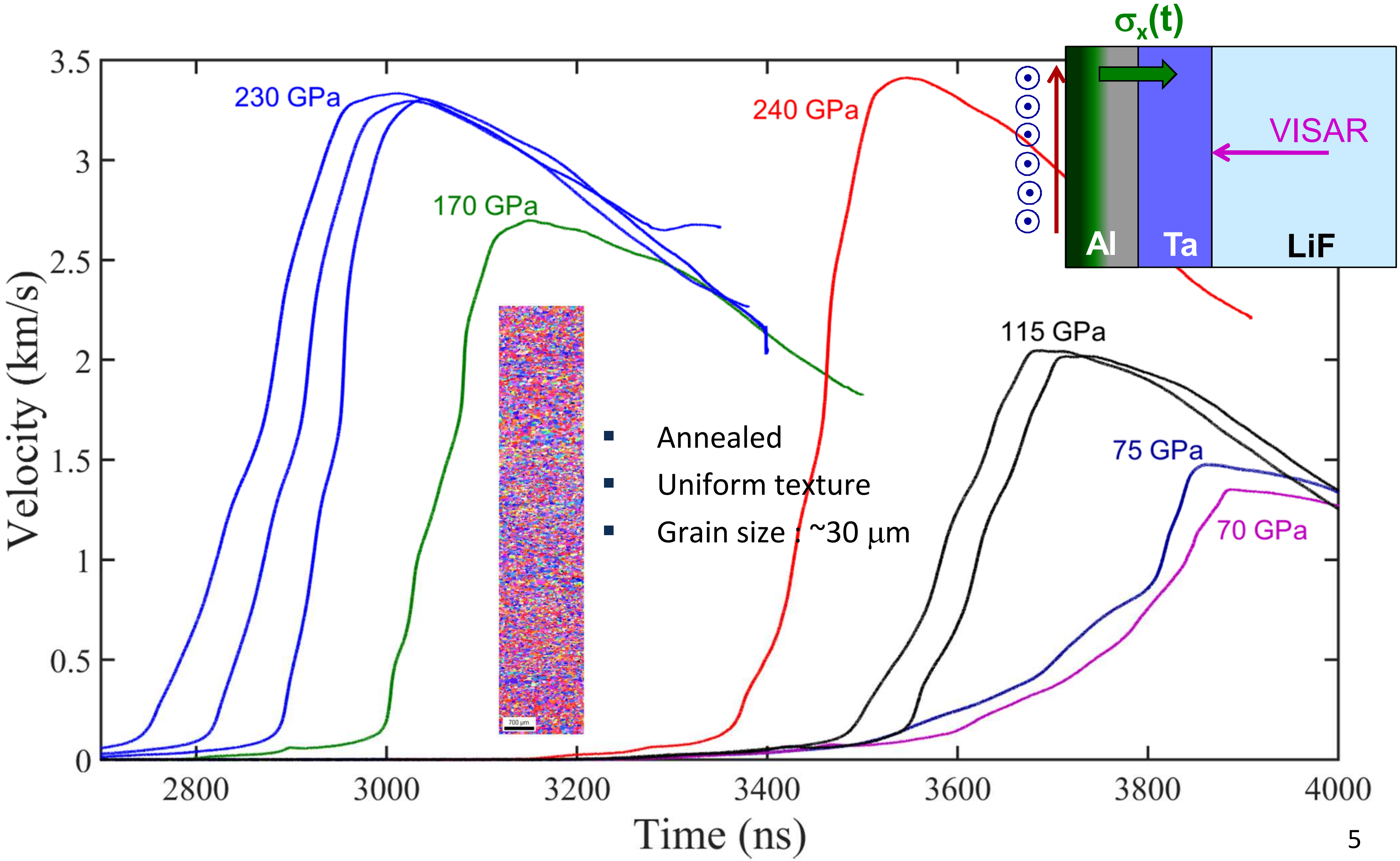




- Current pulse of up to 26 MA delivered to parallel flat-plate electrodes shorted at one end
- Controllable pulse shape, rise time 100 – 1200 ns
- Ramped magnetic (J x B) force induces ramped stress wave in electrode material
- Stress wave propagates into ambient material, ahead of diffusion front

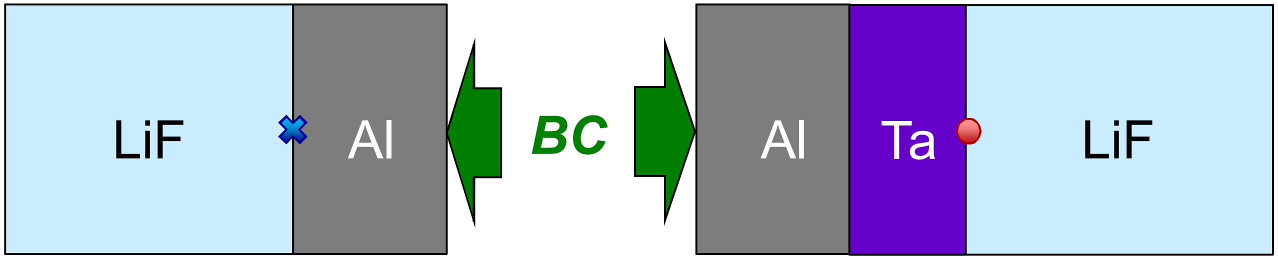


Tantalum Ramp compression measurements have been made between peak stresses of 70-240 GPa



- Annealed
- Uniform texture
- Grain size : ~30 μm

Inverse problem definition



Simulation inputs (vector: γ)

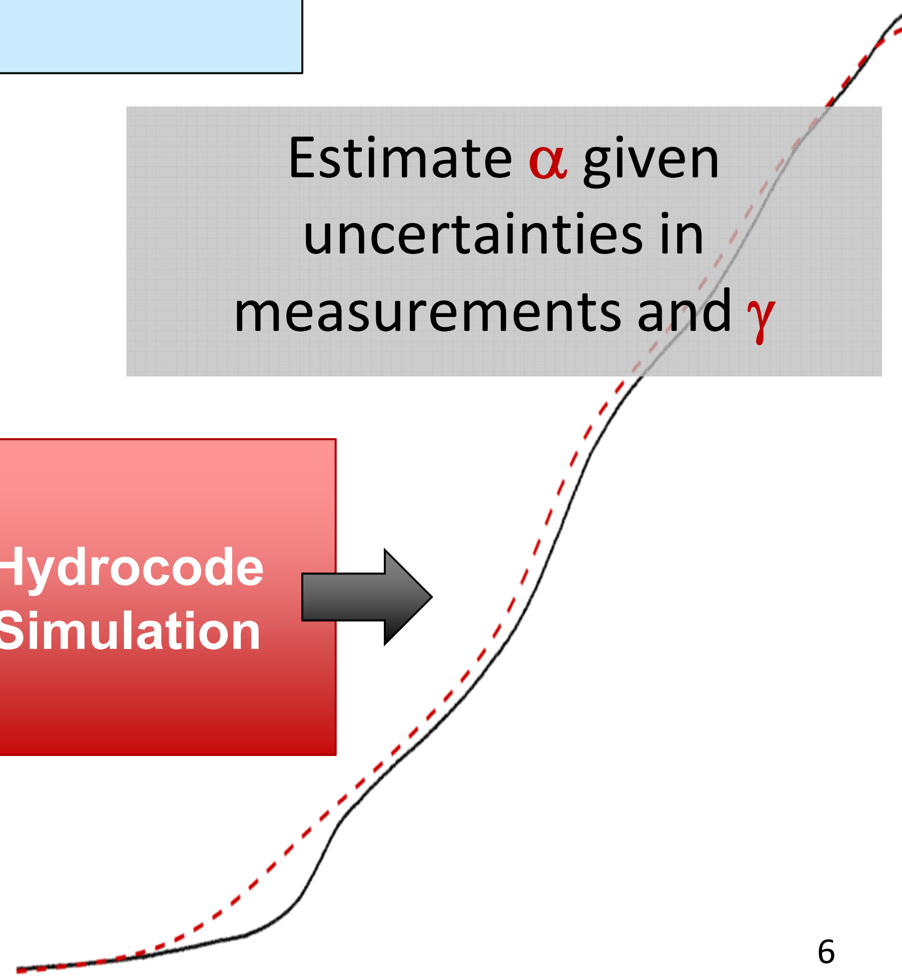
- Boundary conditions
- Metrology
- Material models (standards)
  - EOS, conductivity, strength

Model parameters (vector: α) (unknown sample)

- EOS, strength, kinetics

Hydrocode Simulation

Estimate α given uncertainties in measurements and γ



Statistical Model

- Computer model : $V^S(\cdot)$ is a deterministic mapping from $\{\boldsymbol{\gamma}, \boldsymbol{\alpha}\} \rightarrow V_i^S$
- Experiment model : $V_j^E(t, \boldsymbol{\gamma}_j, \boldsymbol{\alpha}) = V_j^S(t, \boldsymbol{\gamma}_j, \boldsymbol{\alpha}) + \delta(t, \boldsymbol{\gamma}_j, \boldsymbol{\alpha})$

  j = 1,…,J indexes the experiment
- Model for discrepancy : $\delta(t, \boldsymbol{\gamma}_j, \boldsymbol{\alpha}) = \mathrm{MVN}(0, \boldsymbol{\Sigma}_j)$

  Σ_j is the experimental variance
- Nuisance parameter prior : $\boldsymbol{\gamma}_j \sim f_{\boldsymbol{\gamma}}(\cdot)$, $f_{\boldsymbol{\gamma}}$ is known
- Physical parameter prior : $\boldsymbol{\alpha} \sim f_{\alpha} \propto 1$, non – informative

Residuals are defined using the Mahalanobis distance

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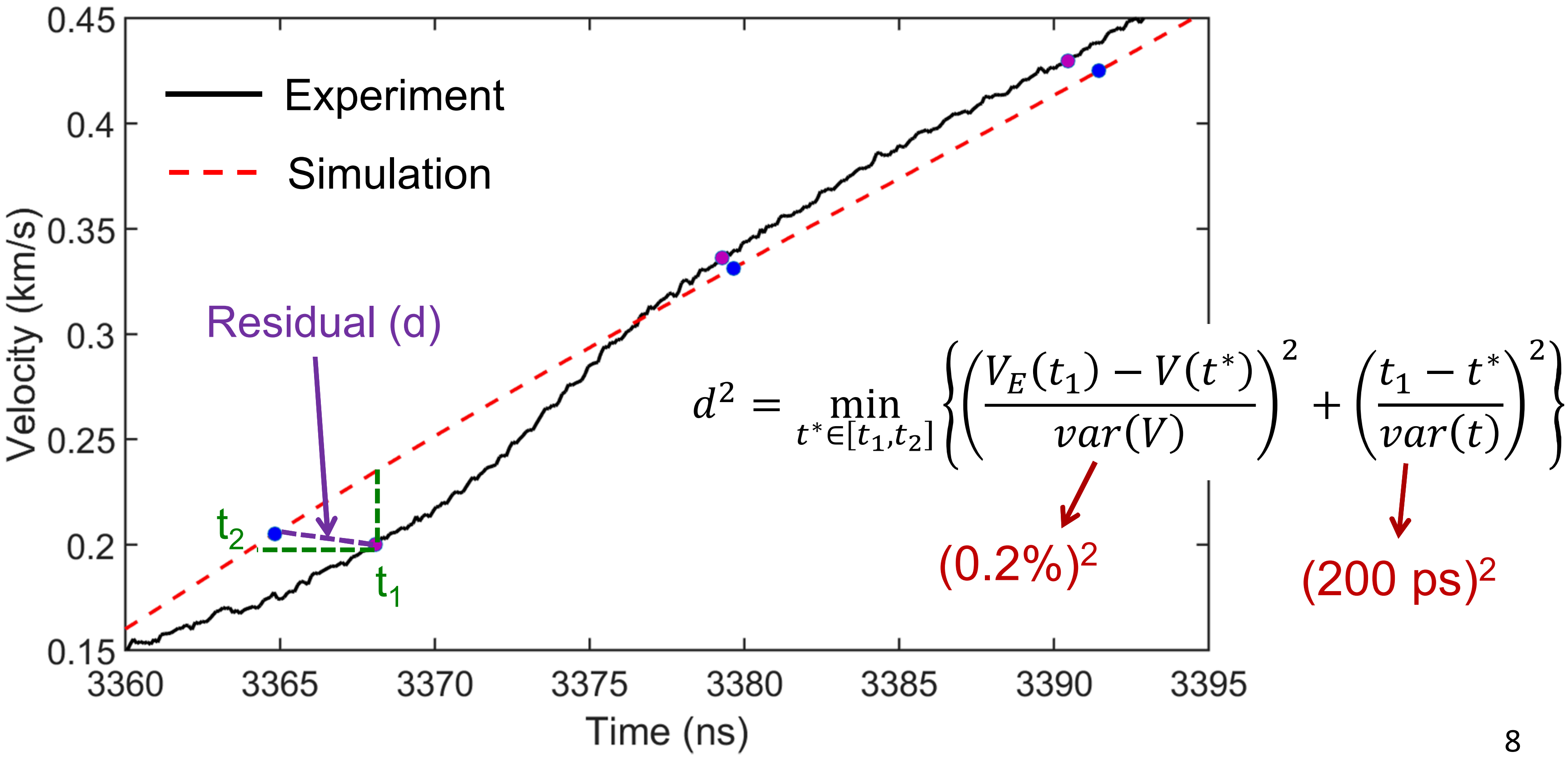
- Incorporates experimental uncertainties in both time and velocity
- Provides robustness to problems with shocks



$$d^2 = \min_{t^* \in [t_1, t_2]} \left\{ \left(\frac{V_E(t_1) - V(t^*)}{var(V)} \right)^2 + \left(\frac{t_1 - t^*}{var(t)} \right)^2 \right\}$$

Application of Bayes' Rule

Likelihood

Posterior

Prior (Guess for probability distribution of α)

$$P(\boldsymbol{\alpha}|V_E) = \frac{P(V_E|\boldsymbol{\alpha})P(\boldsymbol{\alpha})}{\mathrm{P}(V_E)}$$

Evidence (that data was generated by the model)

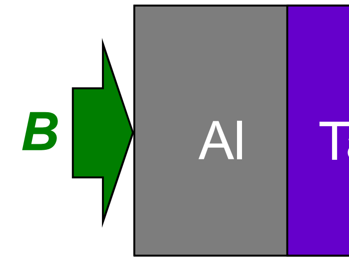
Likelihood function : product of normal probability density functions

$$P(V^E|\boldsymbol{\alpha}) = \prod_{k=1}^{n} \frac{1}{\sqrt{(2\pi)^n|\boldsymbol{\Sigma}_d|}} exp\{-\boldsymbol{r}^T\boldsymbol{\Sigma}_d^{-1}\boldsymbol{r}\}$$

Covariance matrix of Gaussian data uncertainties

Vector of n residuals between simulation and experiment

Model and parameter setup



Nuisance parameter priors (Gaussian)

	Mean	Standard Deviation
Initial Density	16.55 g/cc	0.4 %
Electrode thickness	0	1.5 μm
Sample thickness	0	1.5 μm
B-Field scaling	1	0.4 %

x 13 experiments = 40 nuisance variables!

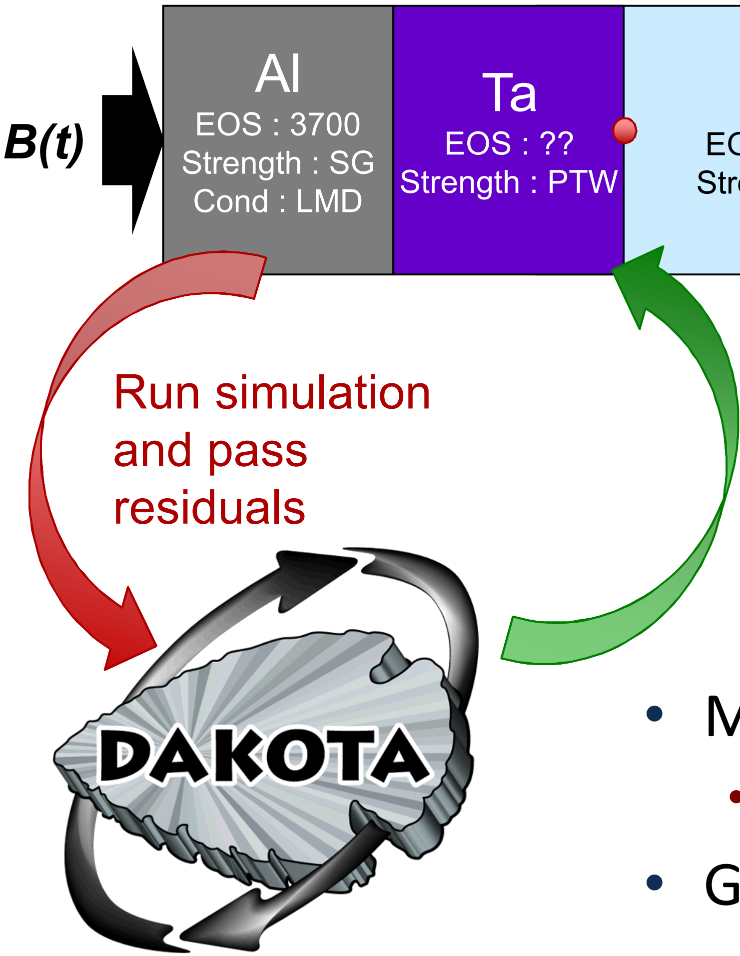
EOS model : Vinet

$$P_{ref}(\rho) = 3B_0 \left(\frac{1-\eta}{\eta^2}\right) e^{\frac{3}{2}(B_0'-1)(1-\eta)}, \qquad \eta = \left(\frac{\rho_0}{\rho_0}\right)^{\frac{1}{3}}$$

Uniform model priors	
Bulk modulus (B_0)	155 – 215 GPa
Pressure derivative (B_0’)	2.9 – 4.9

2 parameter estimation

Posterior is solved using a combination of codes



Determine next set of parameters to simulate: Markov Chain Monte Carlo (MCMC) update

LASLO MHD code

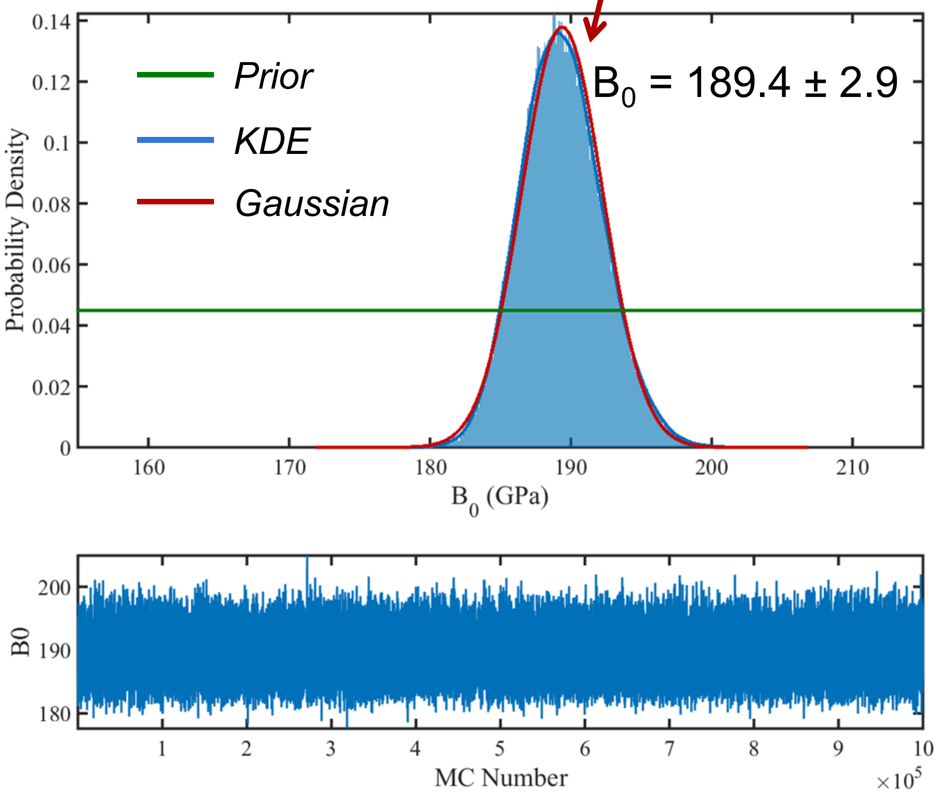
- 1D Lagrangian simulations
- 1 μm mesh

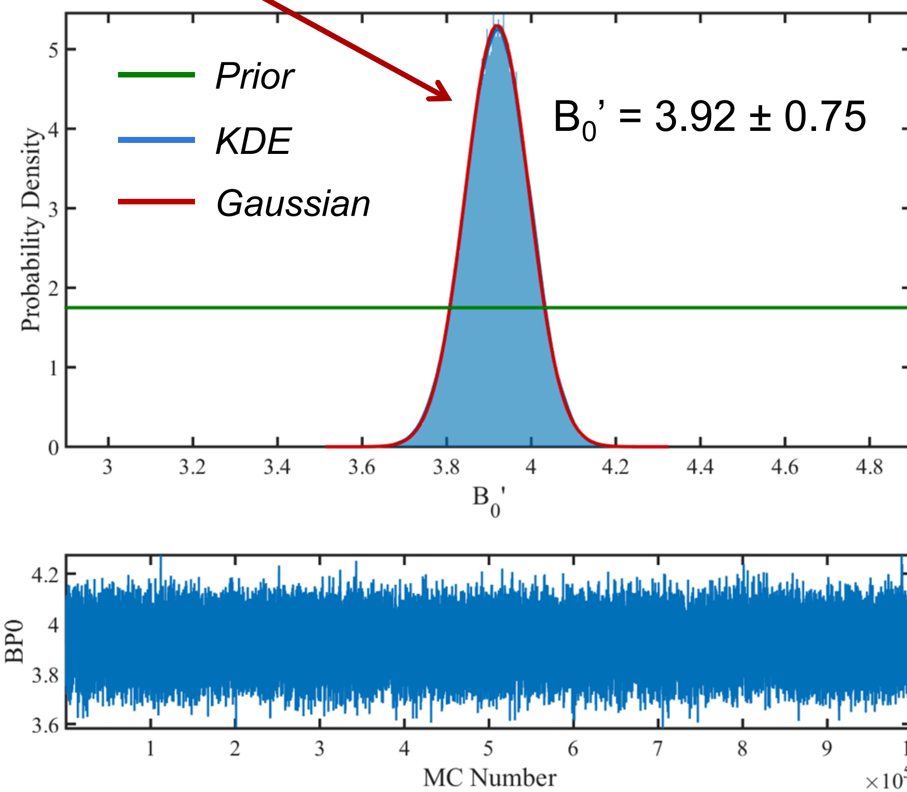
Dakota optimization code

- Metropolis-Hastings MCMC sampler
  - Standard technique for solving for posterior
- Gaussian process (GP) emulators
  - Monte Carlo (LH) sampling of parameter space

Calibration parameter Markov chains

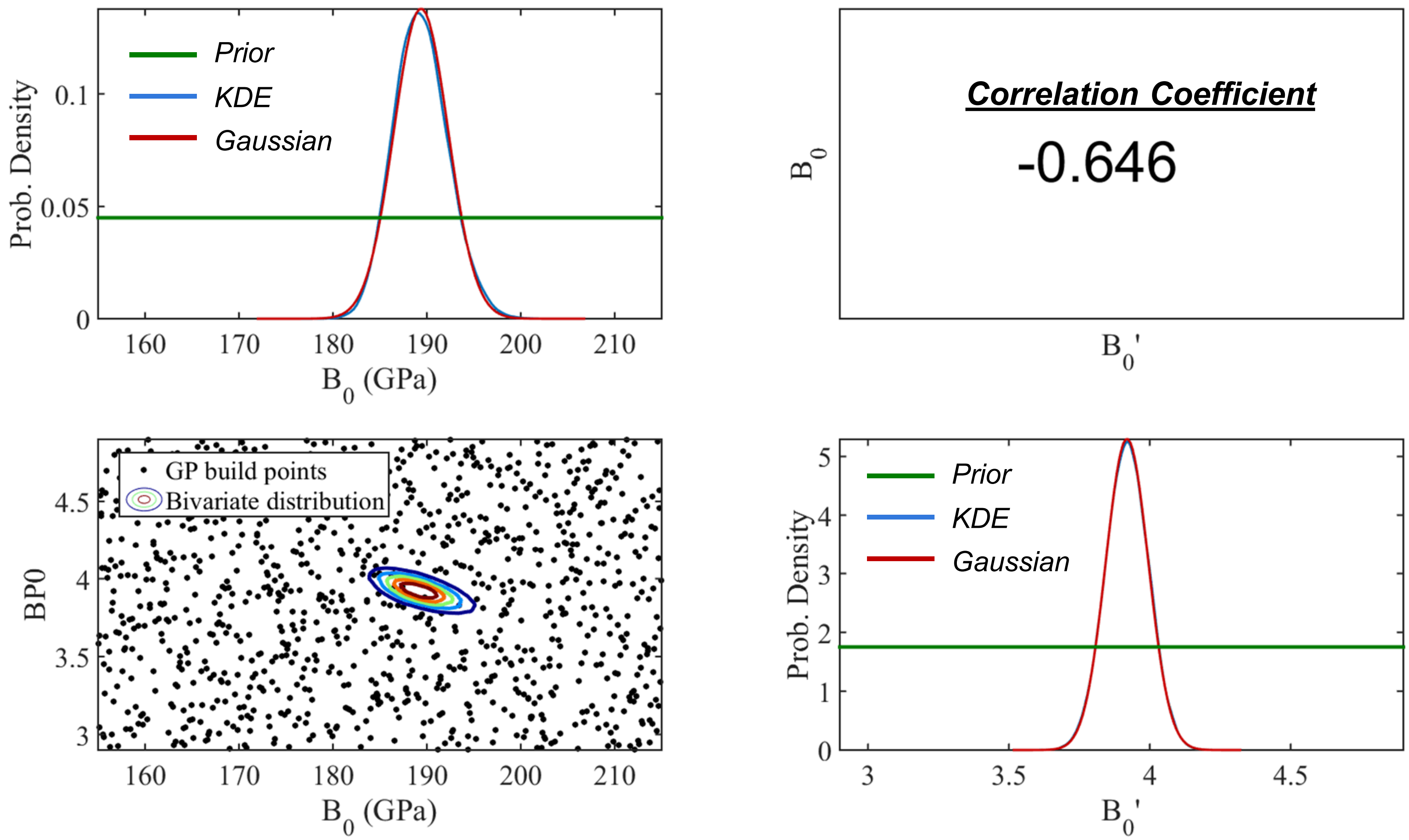
$$P_{ref}(\rho) = 3B_0 \left(\frac{1-\eta}{\eta^2}\right) e^{\frac{3}{2}(B_0'-1)(1-\eta)}, \qquad \eta = \left(\frac{\rho_0}{\rho_0}\right)^{\frac{1}{3}}$$



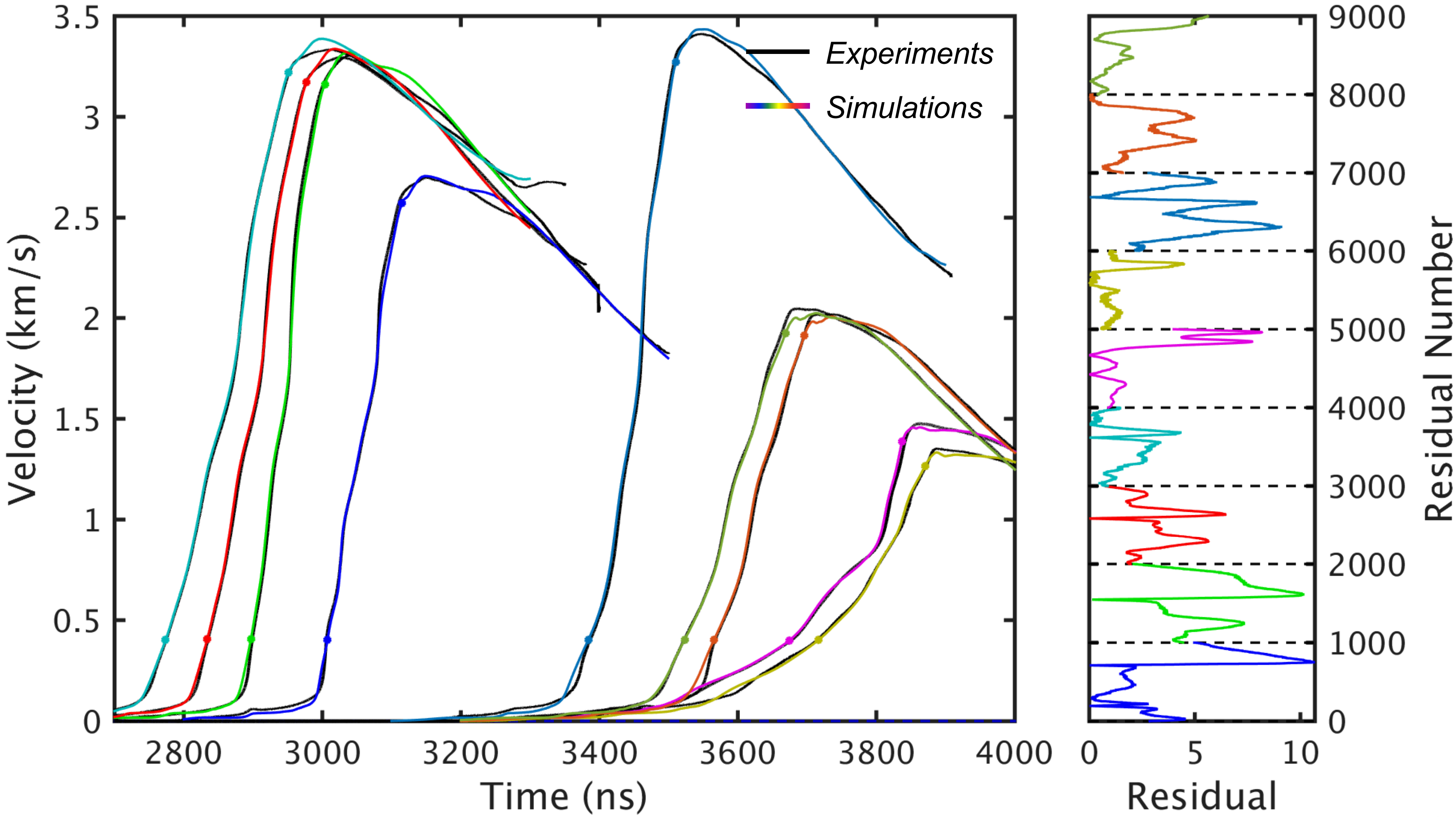


Marginal distributions illustrate parameter correlations

- The inference accounts for correlation between all 40 nuisance parameters as well!

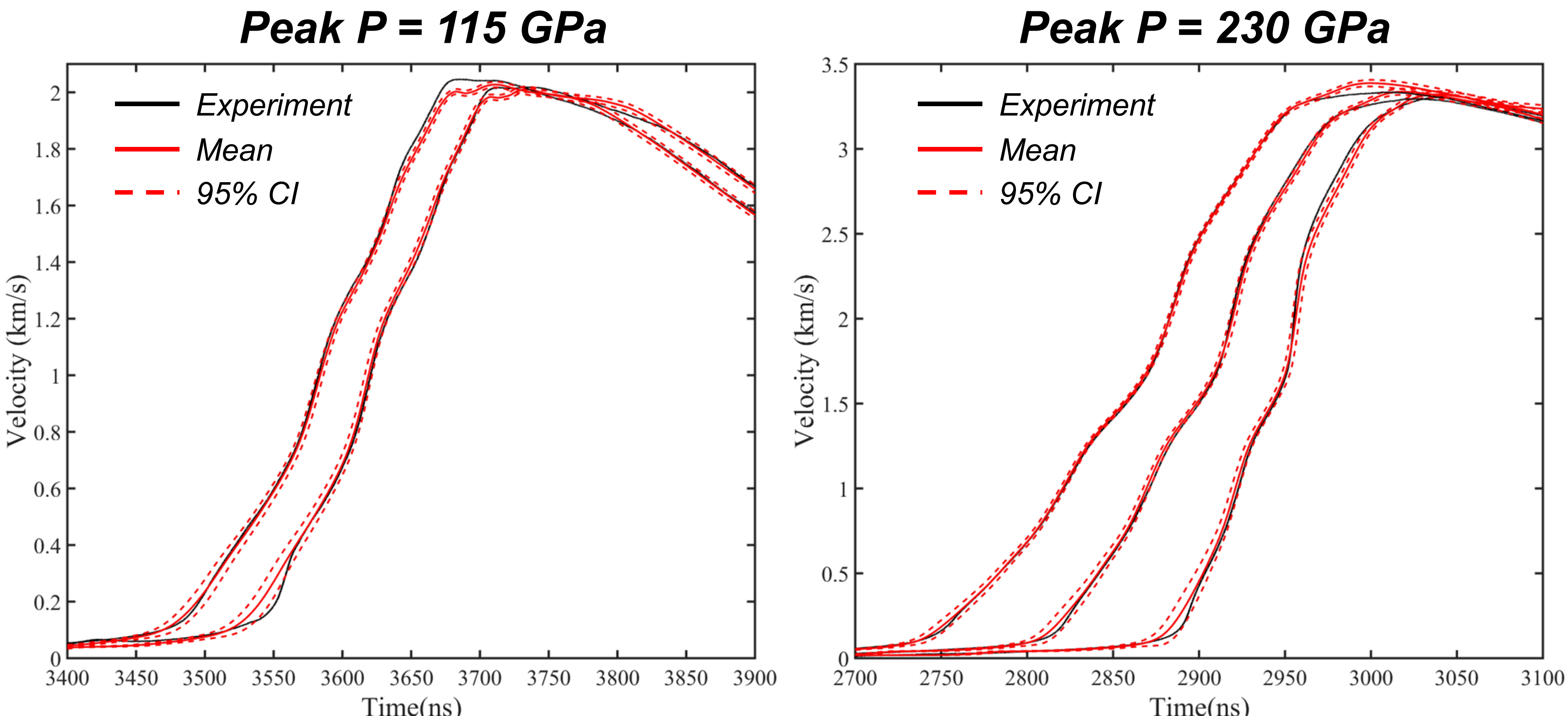


Simulated velocities profiles using mean calibration parameters



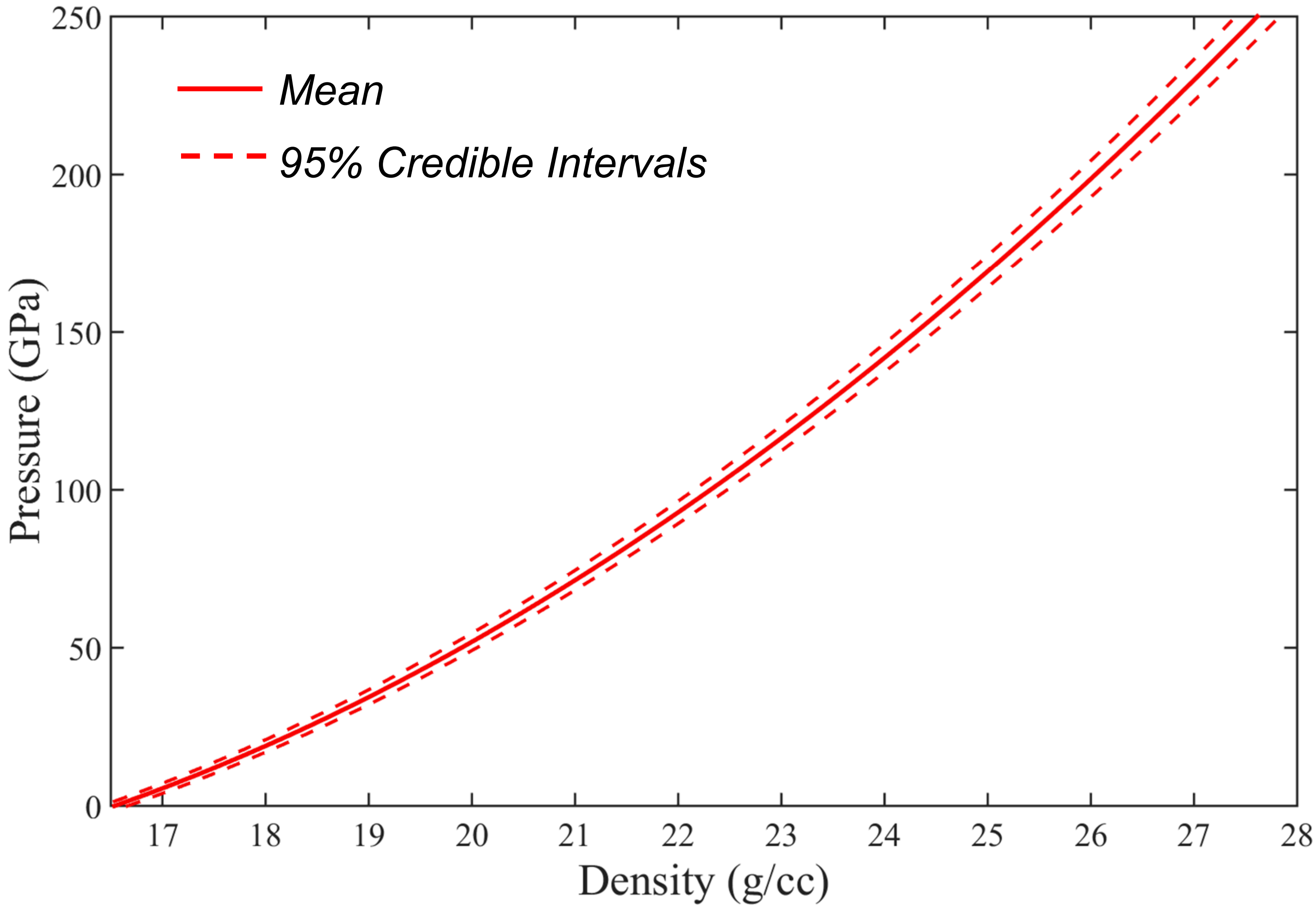
Credible interval calculations illustrate coverage of the calibration

- Propagation of the Markov chain to the simulated velocities



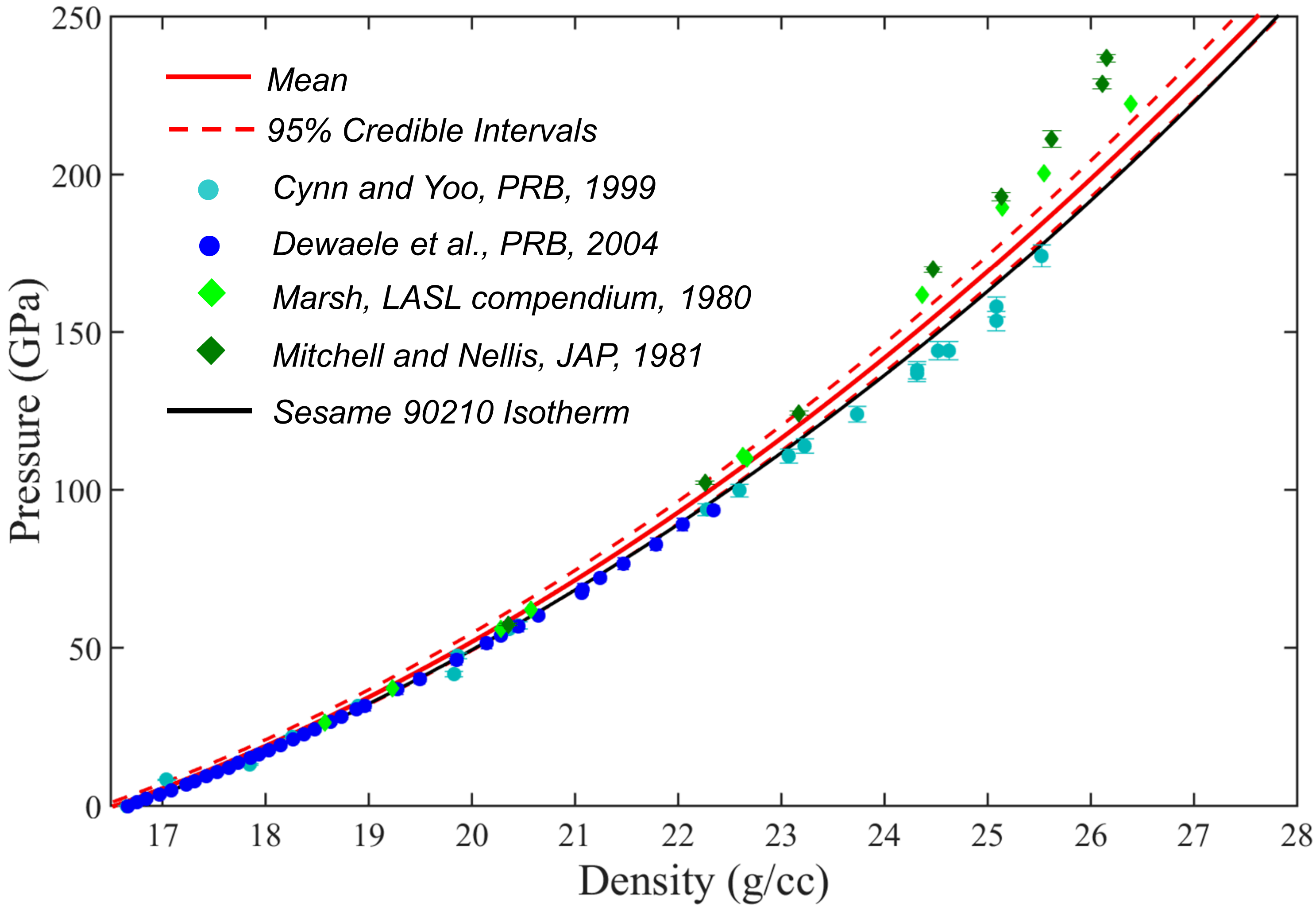
Calibrated reference isotherm

- Markov chain was propagated directly through the model



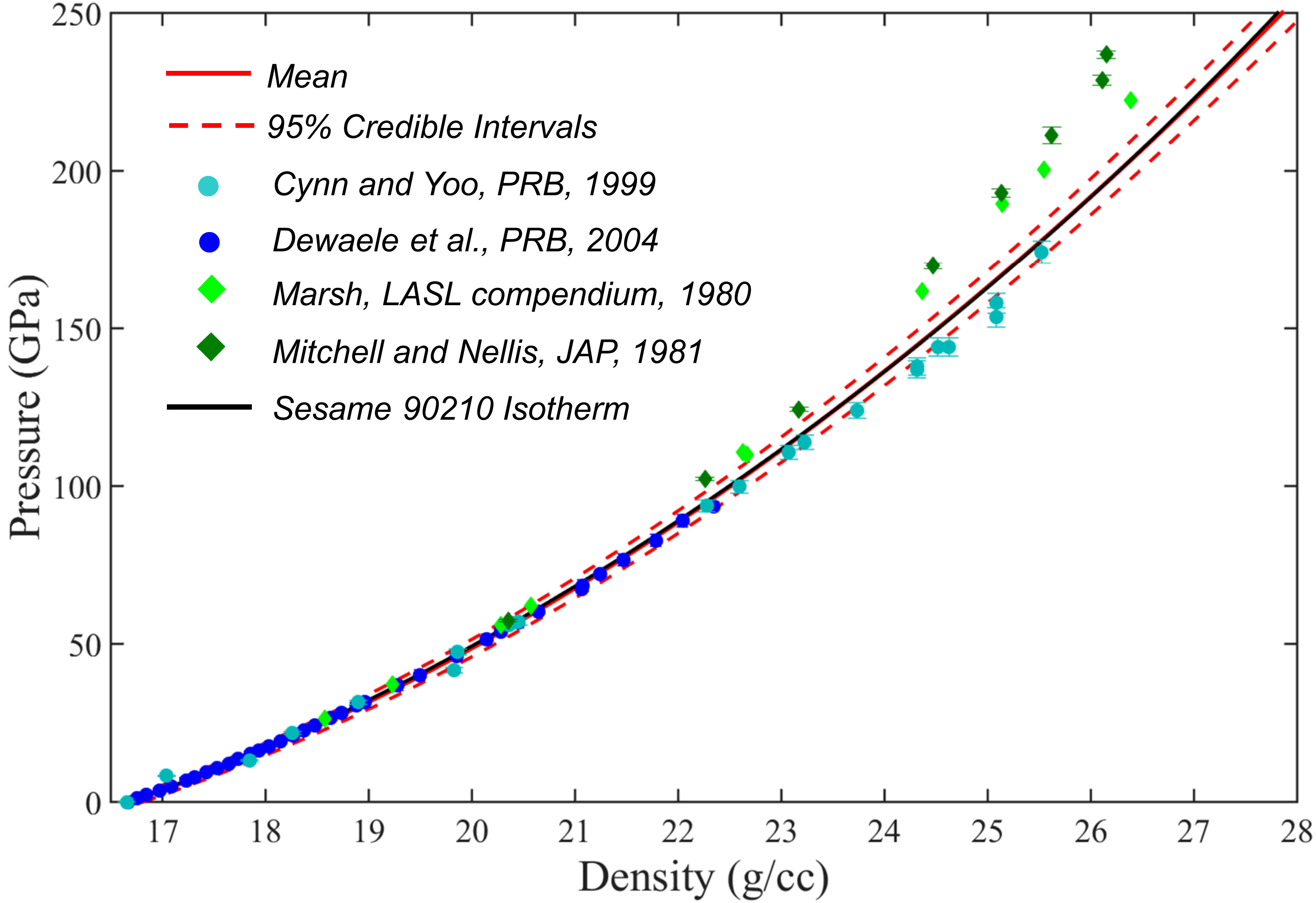
Calibrated reference isotherm

- In good agreement with DAC and Hugoniot measurements



Calibrated reference isotherm

- Shifting the reference density 0.7% to match the DAC/tabular values results in excellent consistency



Summary

- Presented a Bayesian methodology for parameter estimation of velocimetry based dynamic materials experiments
  - Still working on validation and verification of the method
  - Still working on accurate modeling of the model discrepancy for predictive calculations

- Demonstrated the technique on ramp compressed tantalum to 250 GPa (6 experiments and 9 measurements)
  - For an assumed strength model, we produced a reduced isotherm with quantified uncertainties
  - In excellent agreement with previous EOS work

Posterior is sampled using Markov Chain Monte Carlo (MCMC)

- We want to sample from the posterior distribution:

$$P(\boldsymbol{\alpha}|V_E) \propto P(V_E|\boldsymbol{\alpha})P(\boldsymbol{\alpha})$$

- Solution : construct a Markov chain which has an equilibrium distribution equal to the posterior

Markov chain: $\pi(\alpha_{i+1}|\alpha_1, \alpha_2, \ldots \alpha_i) = \pi(\alpha_{i+1}|\ \alpha_i)$

Random walk; next state only depends on previous one

- Metropolis algorithm defines states in the chain:

$$R = \frac{P(V_E|\alpha_{i+1})}{P(V_E|\alpha_i)}$$

→

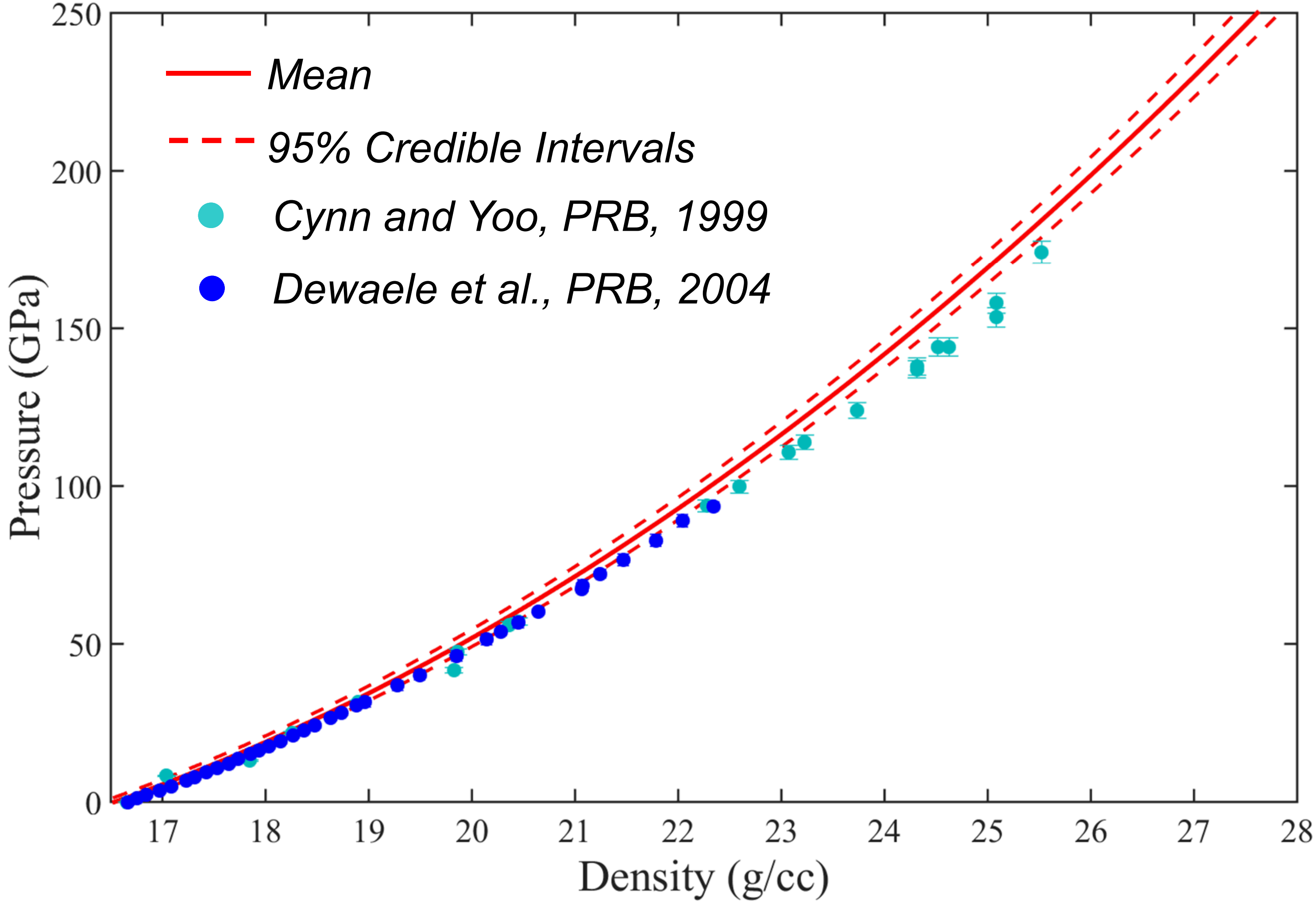
Accept α_{i+1} if R > 1

Reject with probability R if R < 1

Metropolis et al., "Equations of State Calculations by Fast Computing Machines", JCP, 21(6),1953.

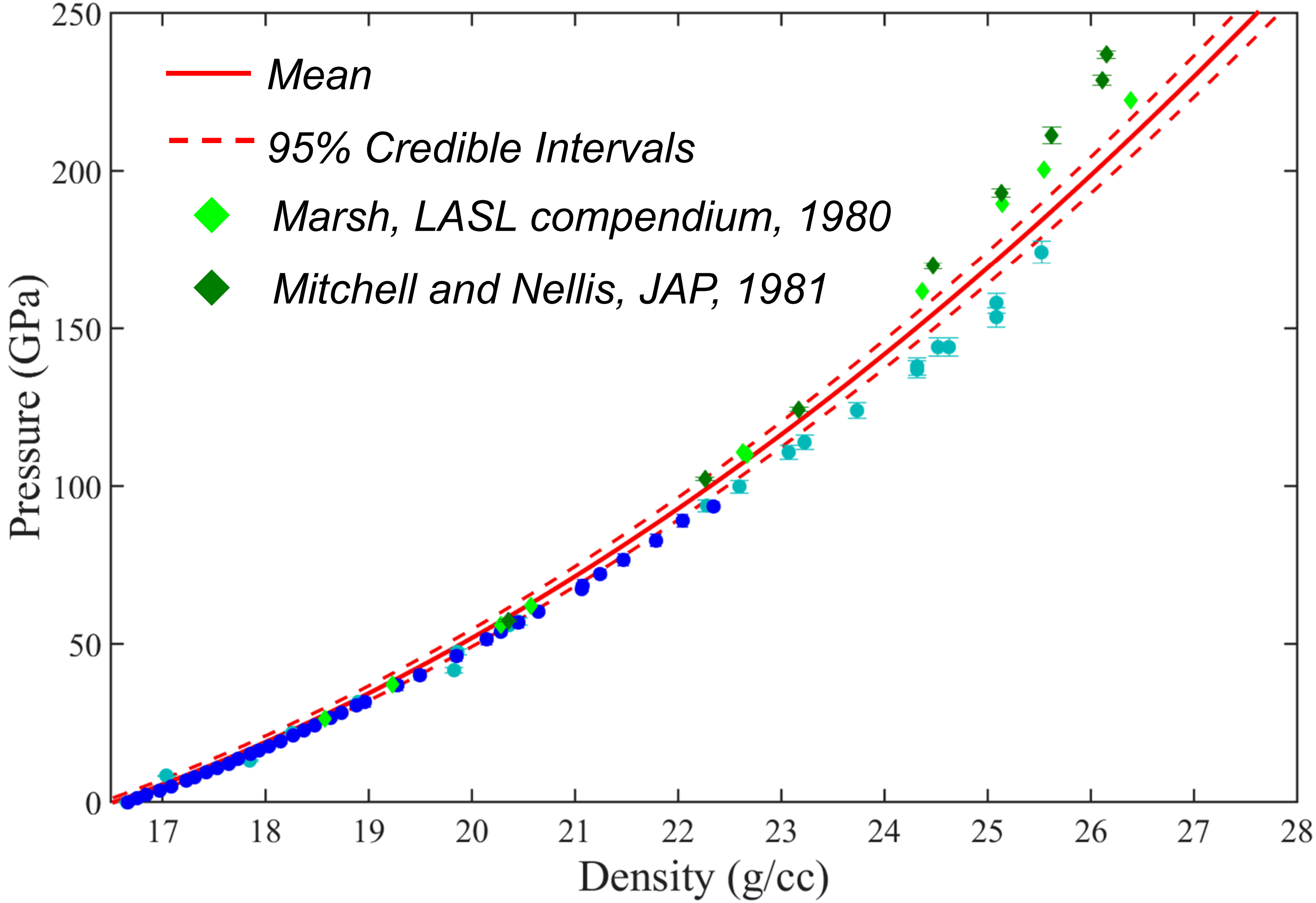
Calibrated reference isotherm

- In good agreement with DAC data



Calibrated reference isotherm

- In good agreement with Hugoniot data



Calibrated reference isotherm

- In good agreement with Lagrangian analysis