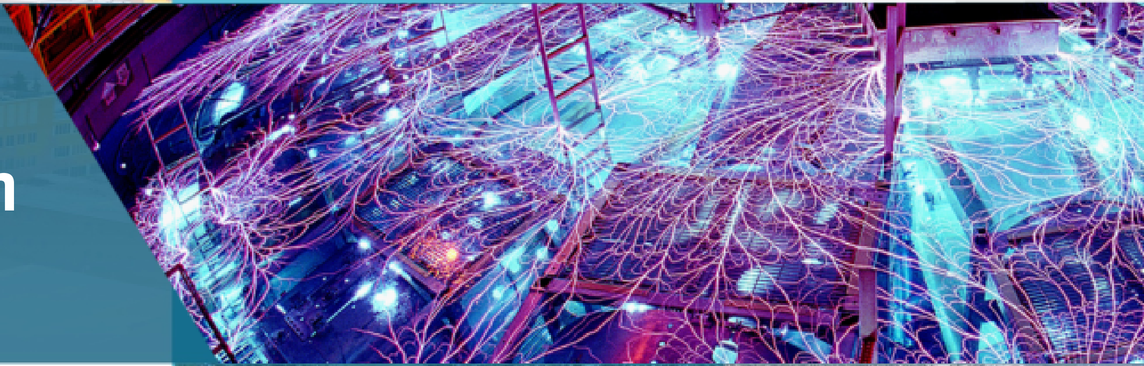
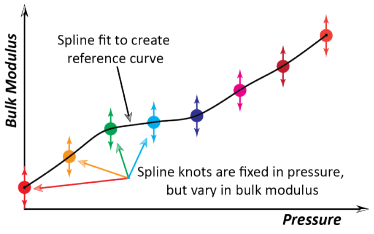
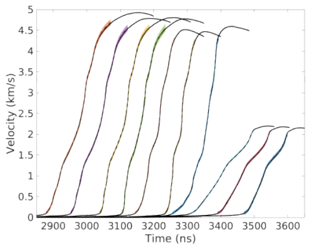
SAND2022-9209C

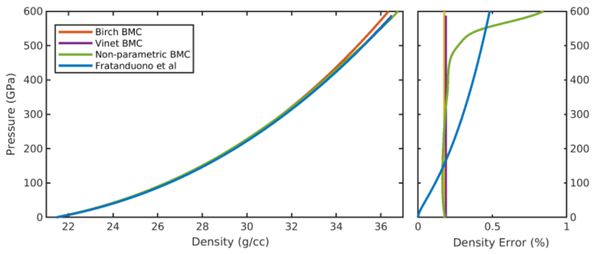
Sandia National Laboratories

Bayesian methods to extract cold curves from shockless compression experiments on the Z machine









Justin Brown, Jean-Paul Davis, Gabriel Huerta, James Tucker, Kurtis Shuler

SHOCK'21: 22nd Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, Anaheim, California July 11 – 15, 2022

Session L05: Strength 1

Platinum 3, 2:30-3:00

U.S. DEPARTMENT OF ENERGY NNSA

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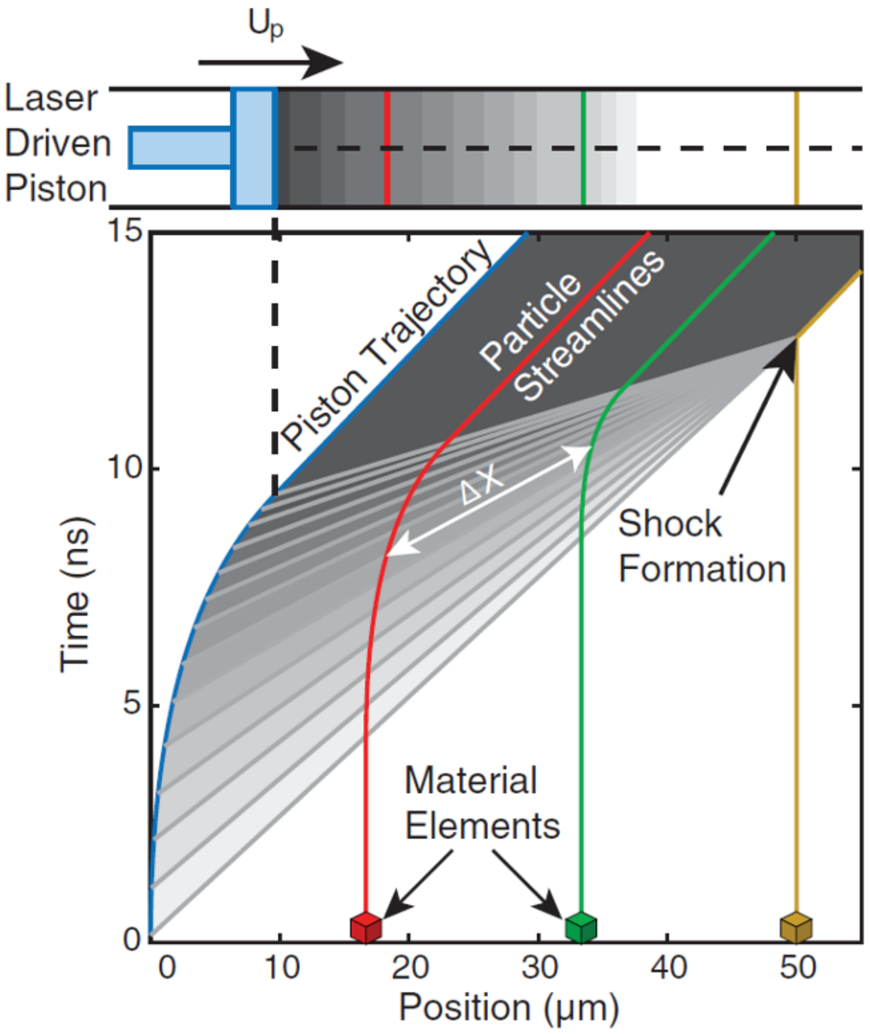
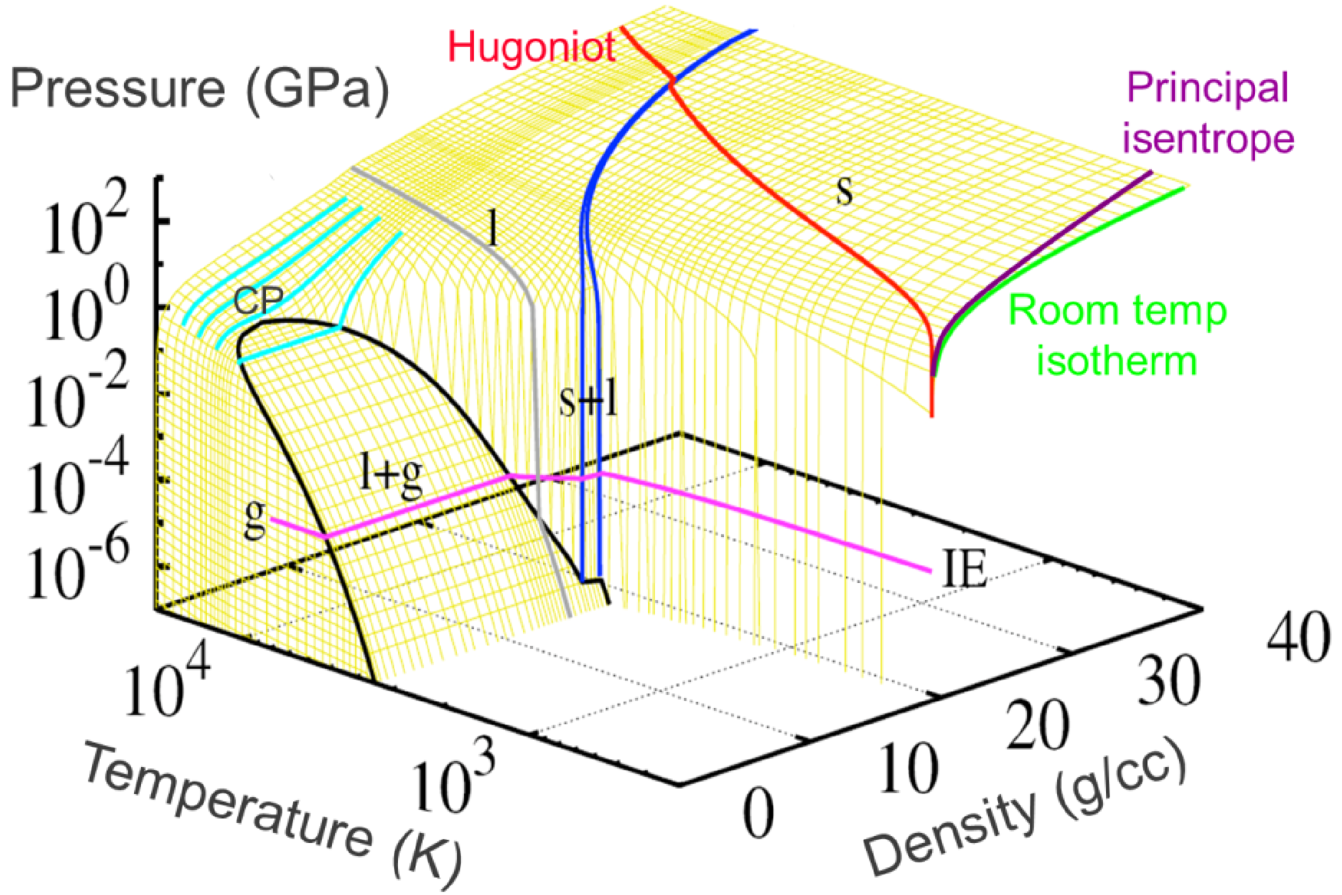
Shockless compression probes a high-pressure low-temperature region of phase space

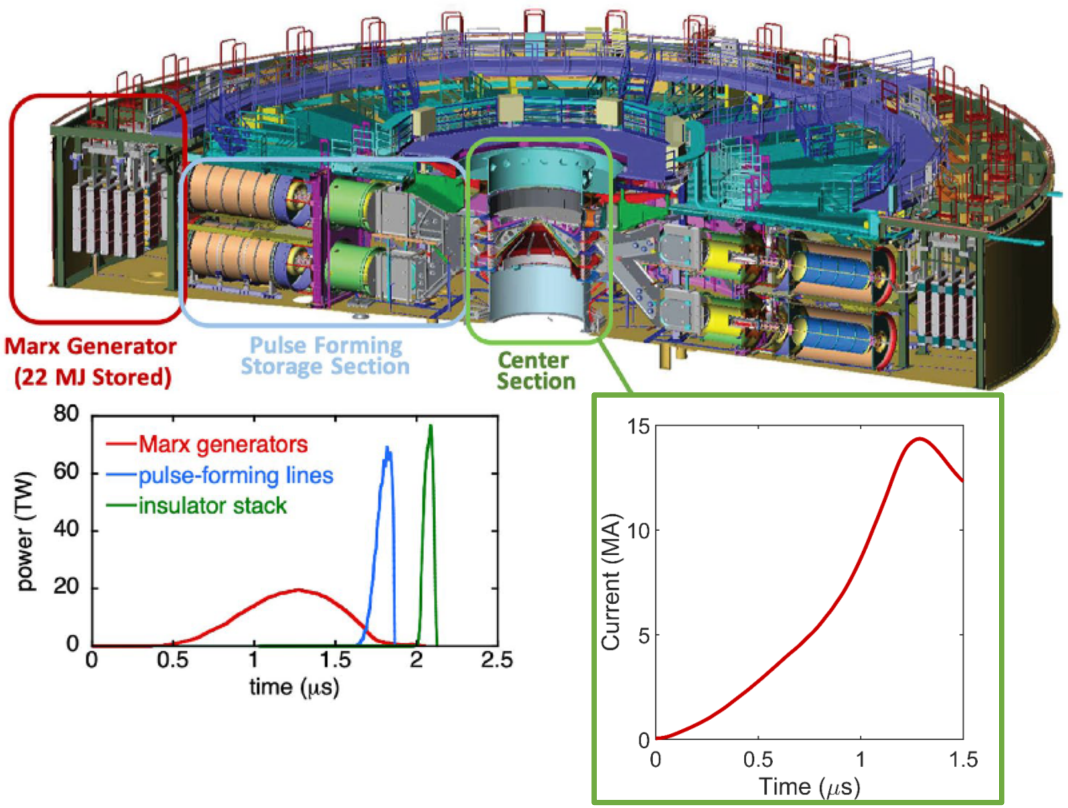


*Fratanduono et al., Science, **372**, 1063-1068 (2021)*

Generic phase diagram showing different dynamic paths

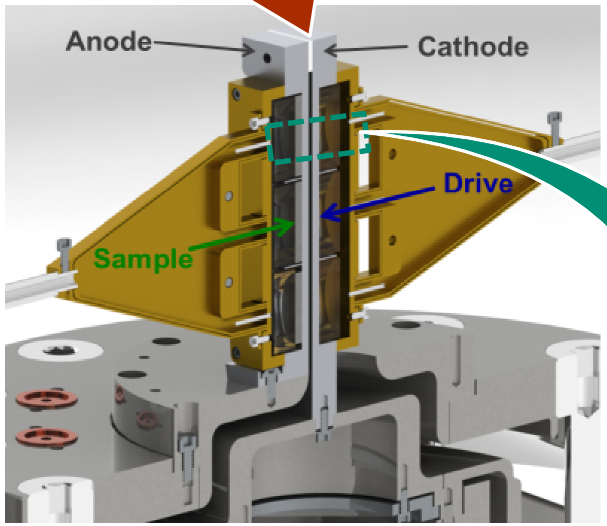


Sandia's Z-Machine can be used to shocklessly compress materials to multi-megabar pressures

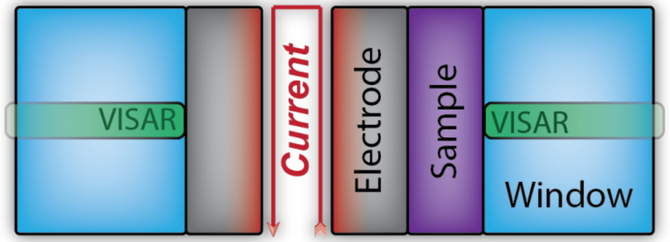


Sinars et al., Phys. Plasmas, ***27***, *070501 (2020)*

Z generates a shaped current that drives a ramped pressure pulse



Each drive and sample measurement located along the height is designed to be 1D



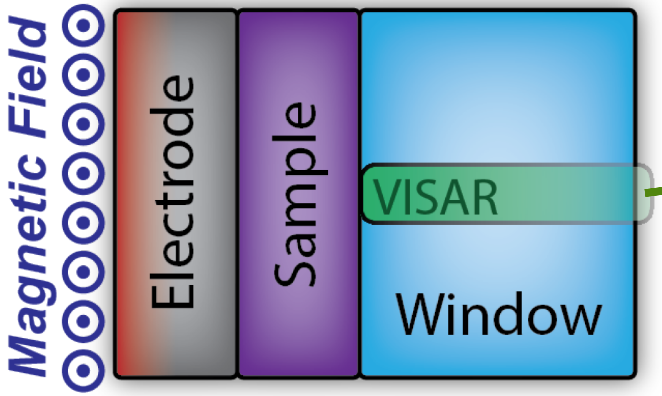
Bayesian calibration offers an avenue to untangle the physics contributing to the measured velocity

Experimental configuration leads to an inverse problem: optimize the sample response to match the measured velocity

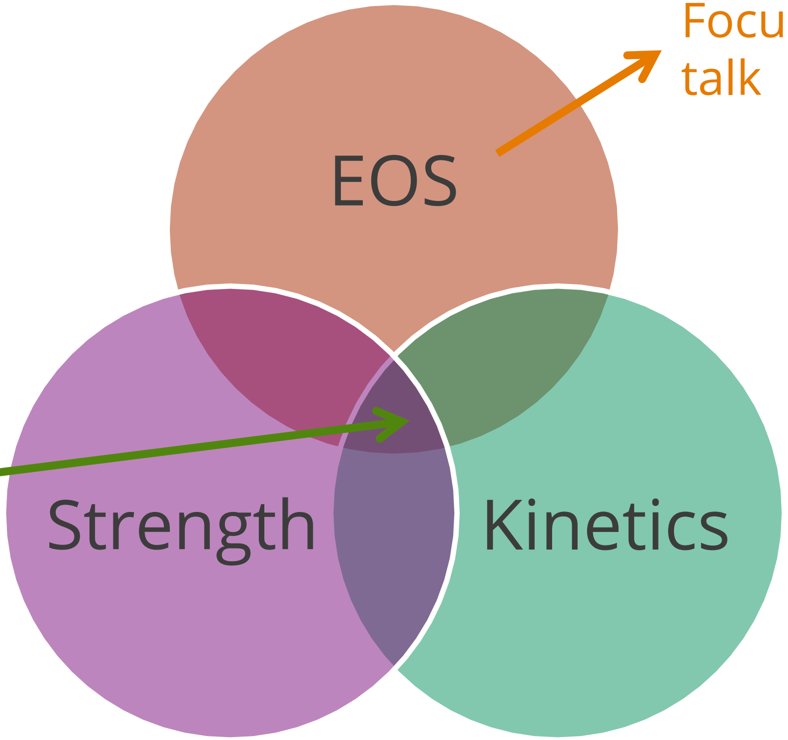
Bayesian calibration offers advantages in solving this problem:

- Include all sources of uncertainty (B-field, thicknesses, timing, standard models, etc.)
- Include all sources of data
- UQ is built-in

The measured velocity captures limited information about the complete response of the material



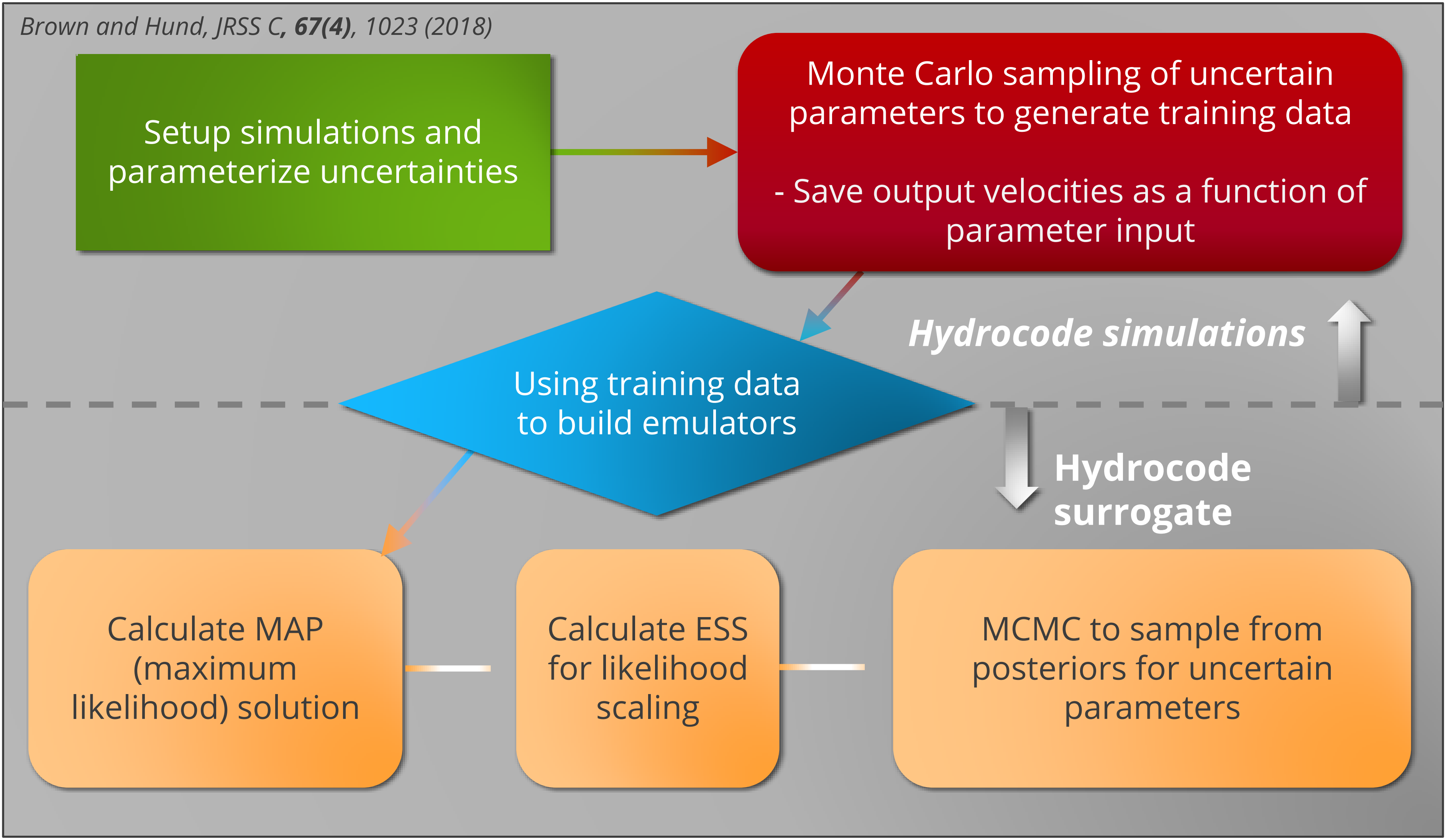
What we measure



Focus of this talk

W. Schill, “Simultaneous Bayesian calibration of strength, kinetics, and phase boundaries,” July 13th, O03.0001, 9:15-9:30

Previous work has established the methodology to solve the Z inverse problem using Bayesian calibration



Relatively standard approach except:

1. Hydrocode simulations are too slow, so an emulator is built
2. Deal with auto-correlation of the measured velocity

What this gives: probability distribution for parameters of a given model of interest

Outline

Introduction

- Ramp compression and the Z machine
- The Z inverse problem and established Bayes techniques

EOS calibration of a simple material: tantalum

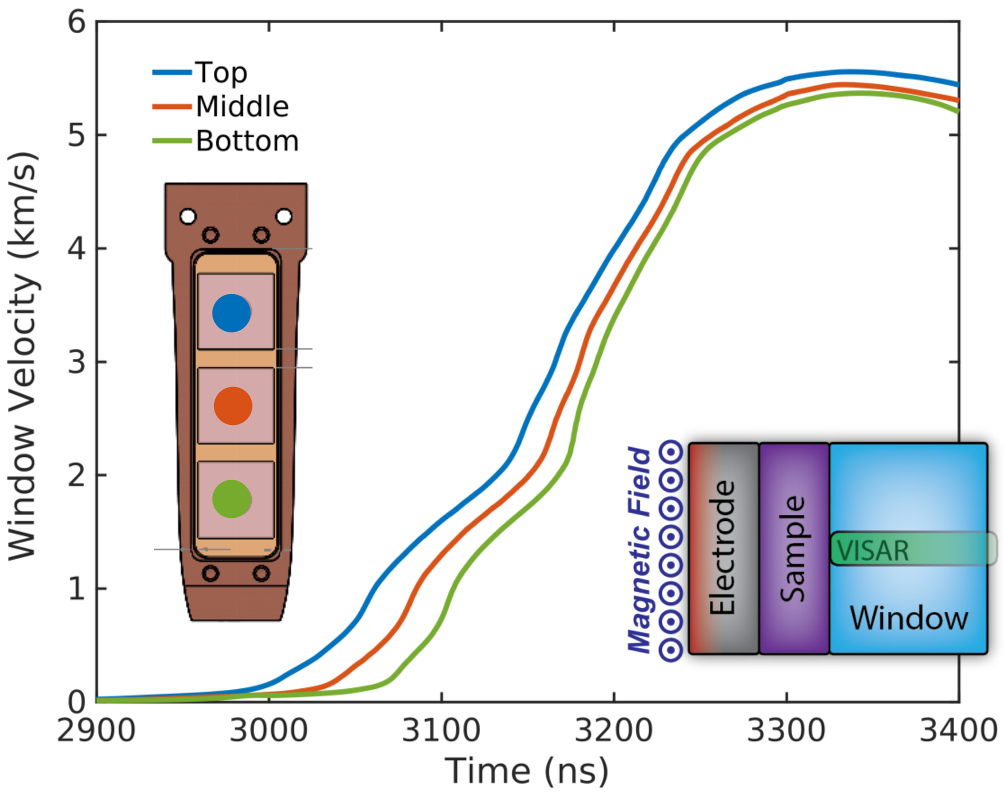
- Parametric EOS models ☹
- Proposed non-parametric form ☺

More practical examples on:

- Platinum – a lot of data and deep dive into uncertainty quantification
- Tin – Complex material with multiple phase transformations

Practical example: Ta cold curve, Vinet model

3 shockless velocity measurements from 1 experiment on Ta to 5 MBar



$$\eta = \left(\frac{\rho_0}{\rho}\right)^{\frac{1}{3}}$$

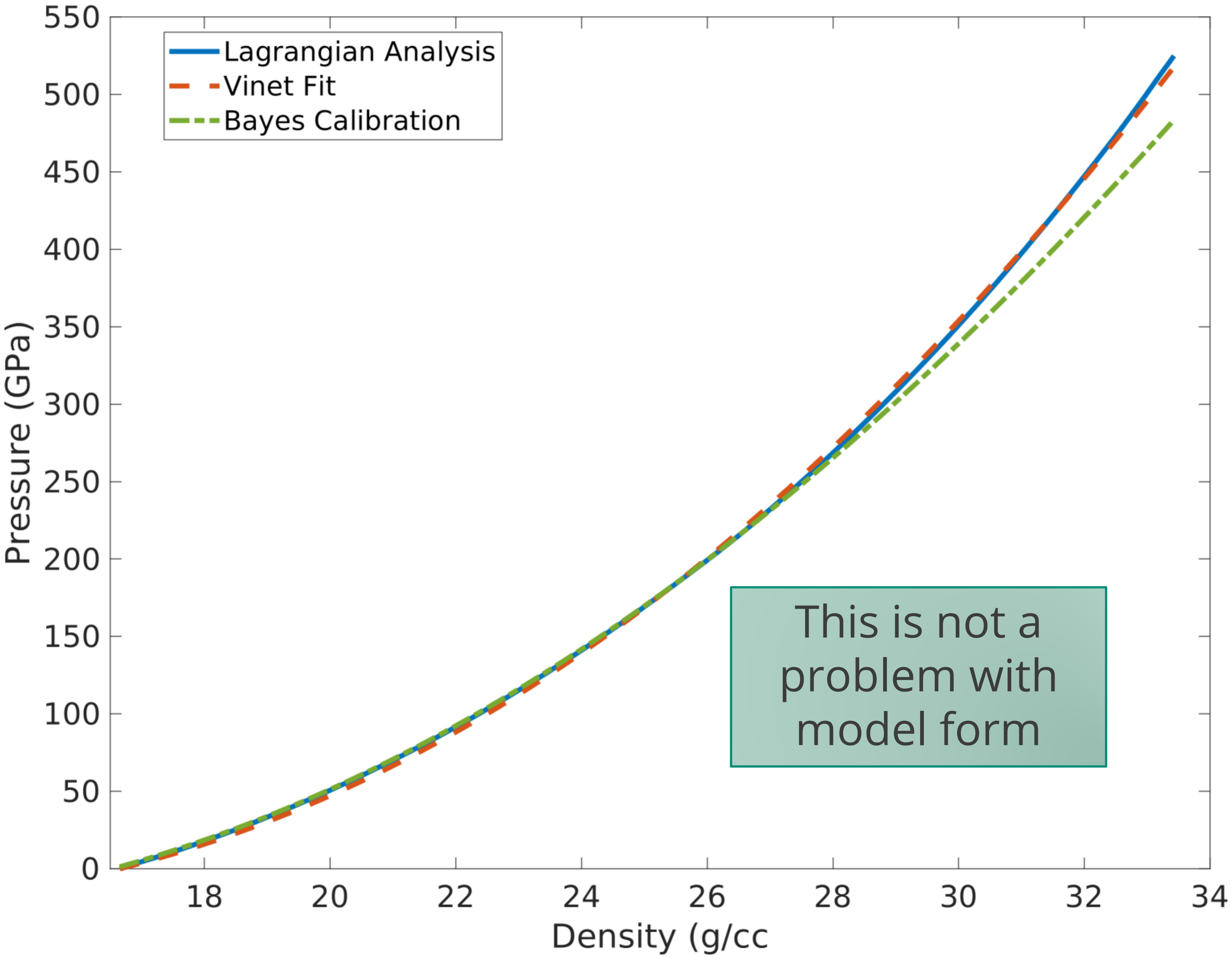
$$P(\rho) = 3B_0\left(\frac{1-\eta}{\eta^2}\right) exp\left\{\frac{3}{2}(B_0' - 1)(1-\eta)\right\}$$

Uncertain parameter specification (priors)

Experimental uncertainties	
Electrode thickness	1.5 microns
Sample thickness	1.5 microns
Magnetic field	0.4%
Relative timing	0.2 ns

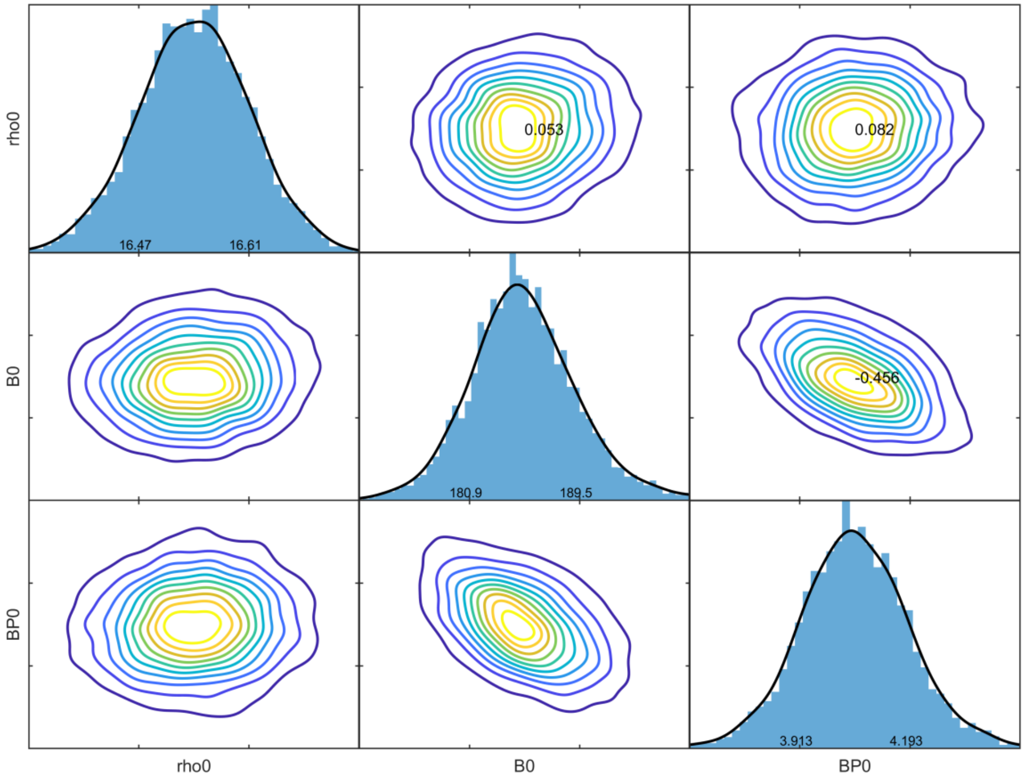
Physical Parameters		
Initial Density	16.65 ± 0.5% g/cc	→ Immersion measurement
Bulk Modulus (B_0)	195.7 ± 10 GPa	→ Ultrasonics
B_0'	[1.9, 5.9]	→ Easily encompasses measurements

Ta Vinet model calibration is deceiving



This is not a problem with model form

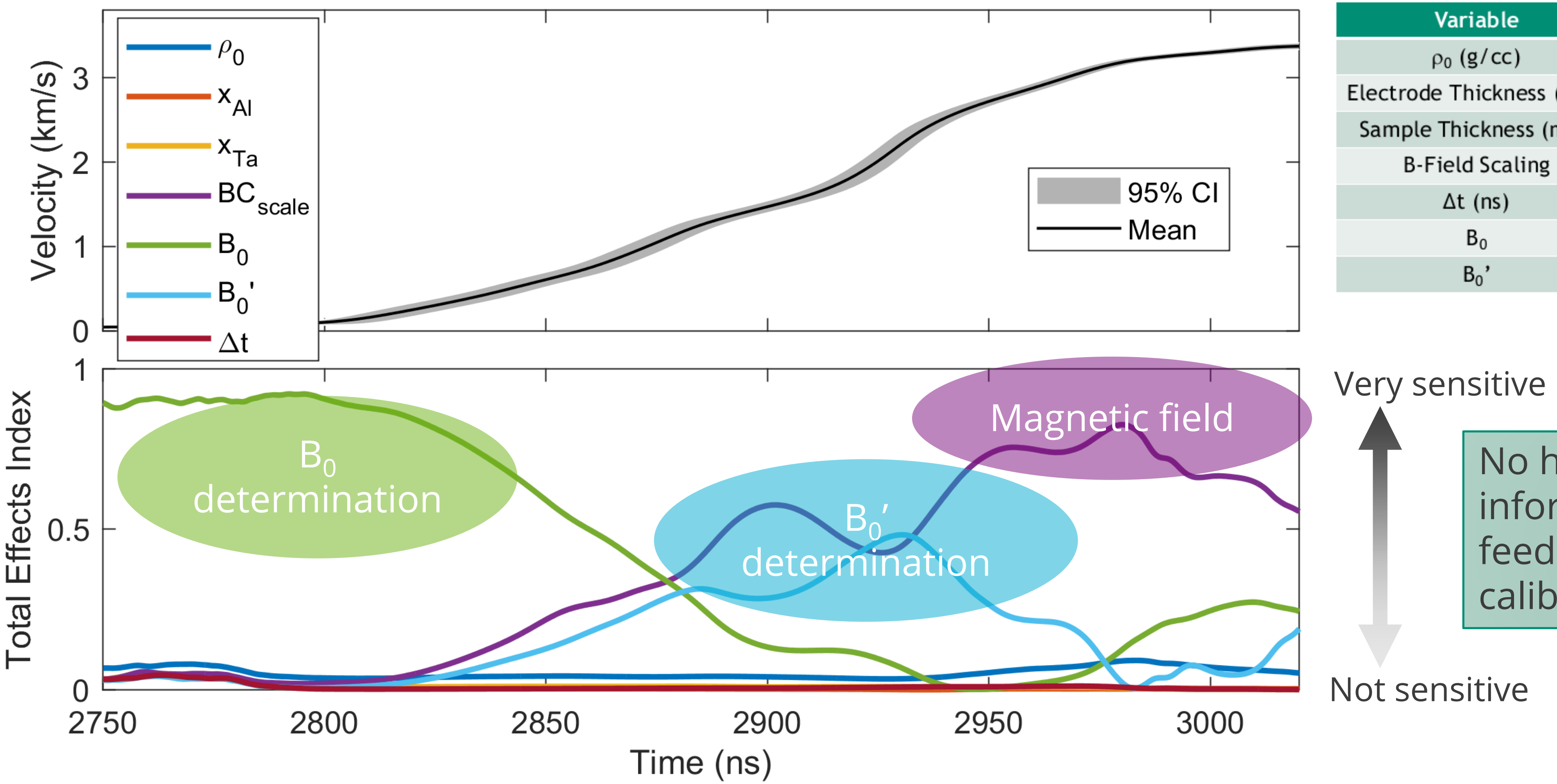
Posterior distributions for the Vinet parameters



Sensitivity analysis demonstrates the inference is not influenced by high pressure portion of the velocity

Global variance-based sensitivity analysis (Sobol)

- Gives an indication for which parameters are identifiable within the calibration



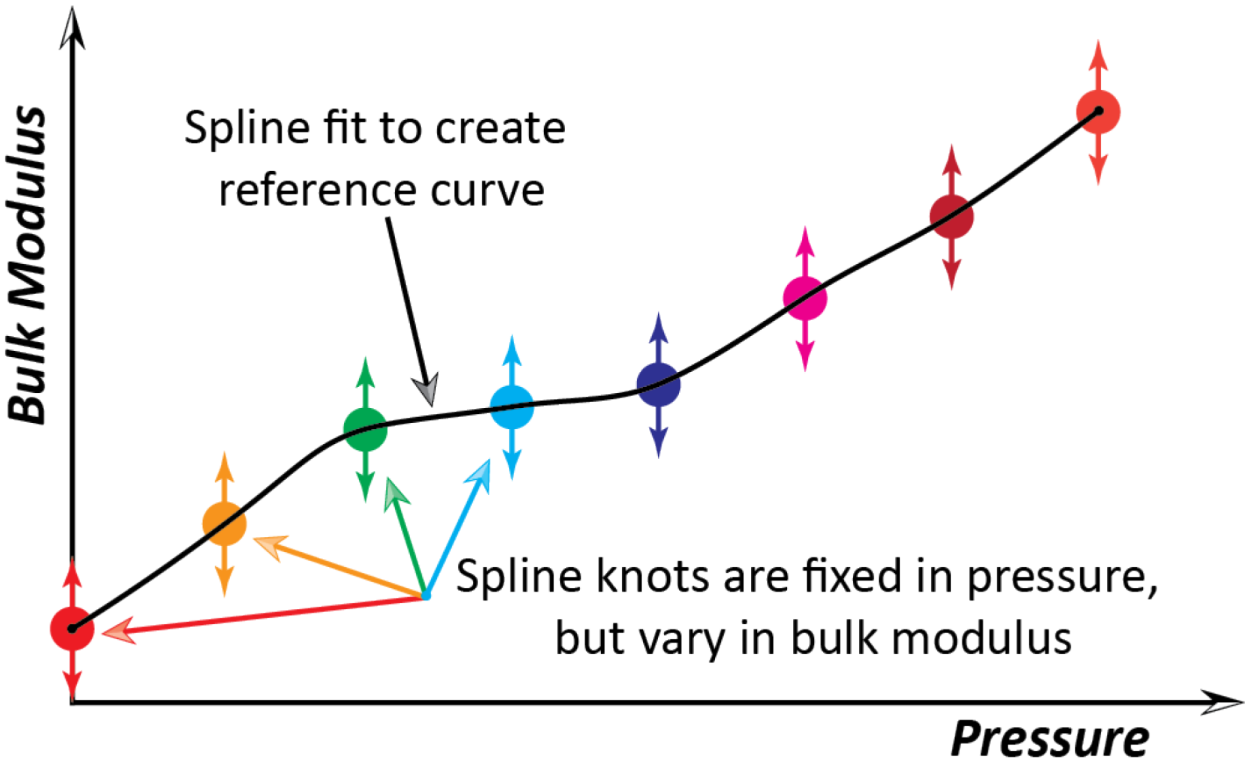
Prior Distributions

Variable	Mean	Std Deviation
ρ_0 (g/cc)	16.55	0.0662
Electrode Thickness (mm)	2.0054	0.0015
Sample Thickness (mm)	1.5002	0.0015
B-Field Scaling	1.0	0.004
Δt (ns)	0	0.2
B_0	195.6	4.7
B_0'	3.5	0.1

No high-pressure information is feeding into the calibration!

A non-parametric form for the cold curve was developed to localize compressibility sensitivities

If available, we like to use a calibrated strength model, so this inherently removes the strength effects, and we are truly calibrating the cold curve

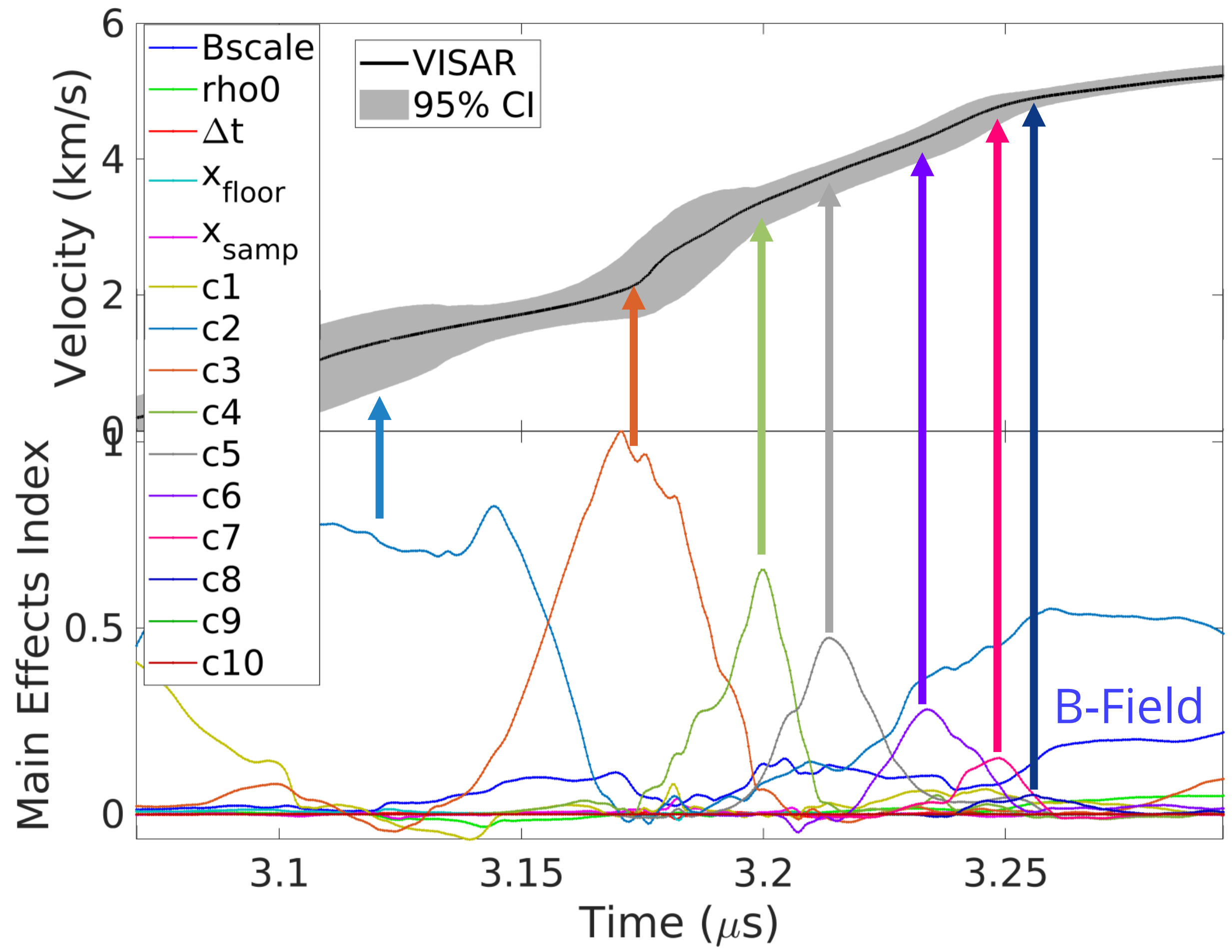


Cold curve serves as the reference curve and is defined by a series of 'knots'

- The space is arbitrary, but we've found B-P works well
  1. Intuitive space representing what we hope to learn from these experiments
  2. Taking derivatives to solve for wavespeed has been problematic. Fewer numerical issues with choosing a variable directly related to wavespeed and integrating for the rest of the thermodynamic variables.
- The 'knots' serve as the parameters which are allowed to move up and down.
  - Pchip interpolation used to solve for the reference curve.
- Mie-Gruneisen approximation used to solve for thermal response.
  - Assumed $\gamma\rho = \gamma_0\rho_0$ and constant specific heat.

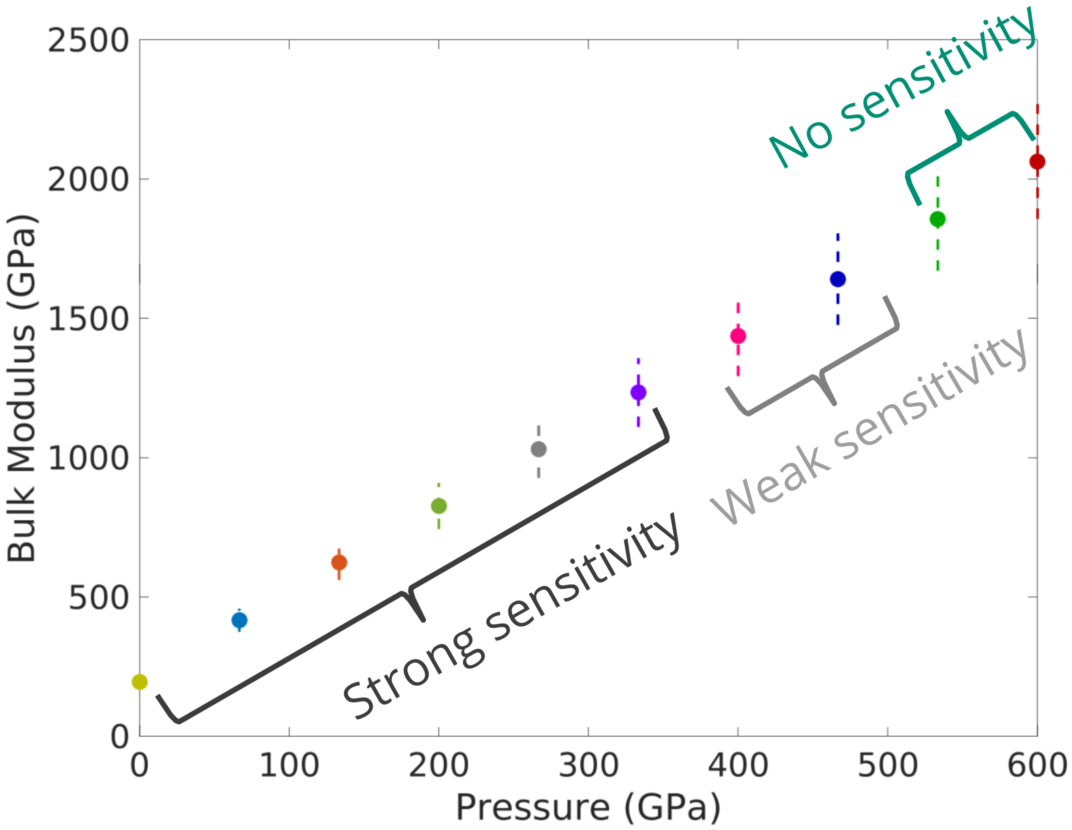
Ta sensitivity analysis for non-parametric cold curve shows localization to specific velocities

Sensitivity analysis suggests we should be able to accurately identify parameters to ~300 GPa with high accuracy and 500 GPa with reduced accuracy.



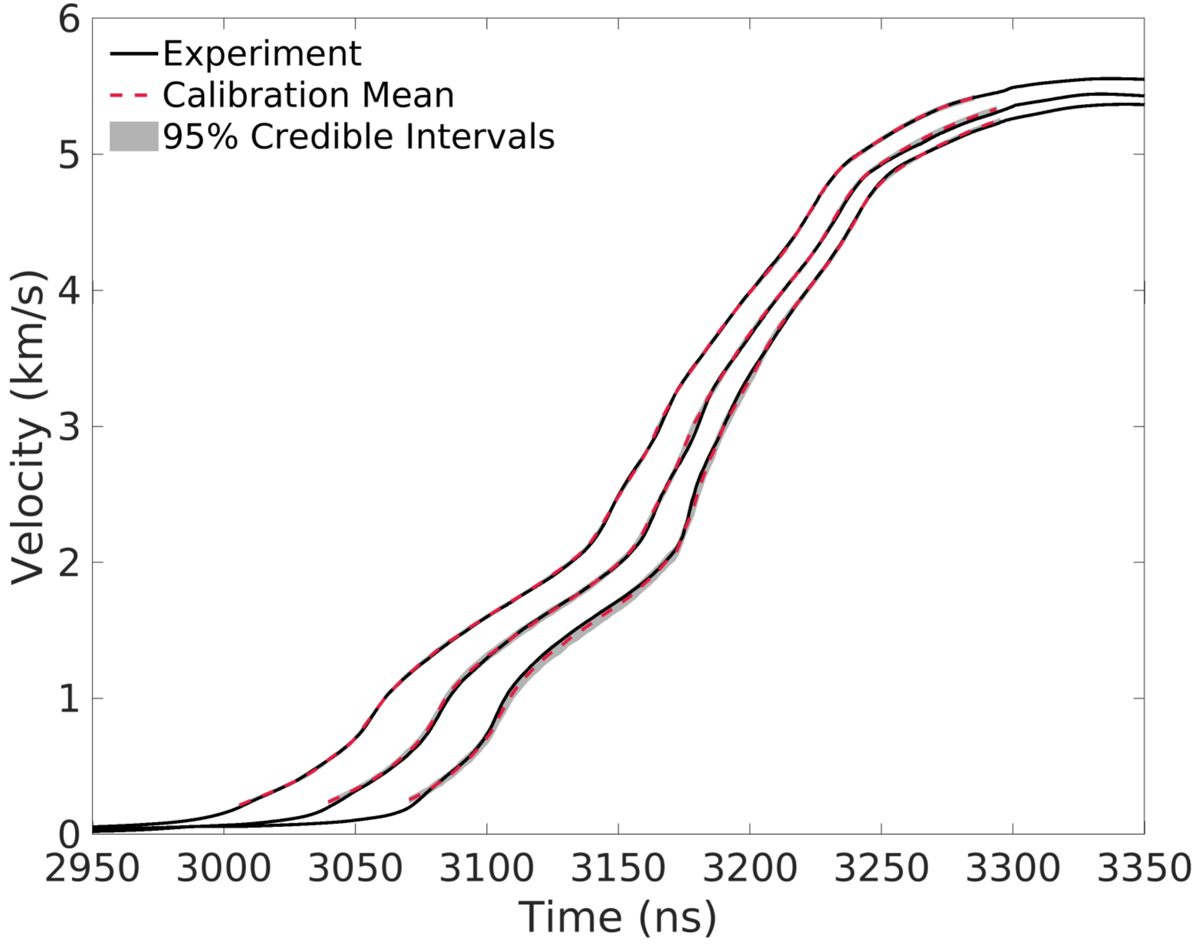
Input Normal Distributions

Variable	Mean	Std Deviation
B-Field Scaling	1.0	0.004
C1-C10	1.0	0.05

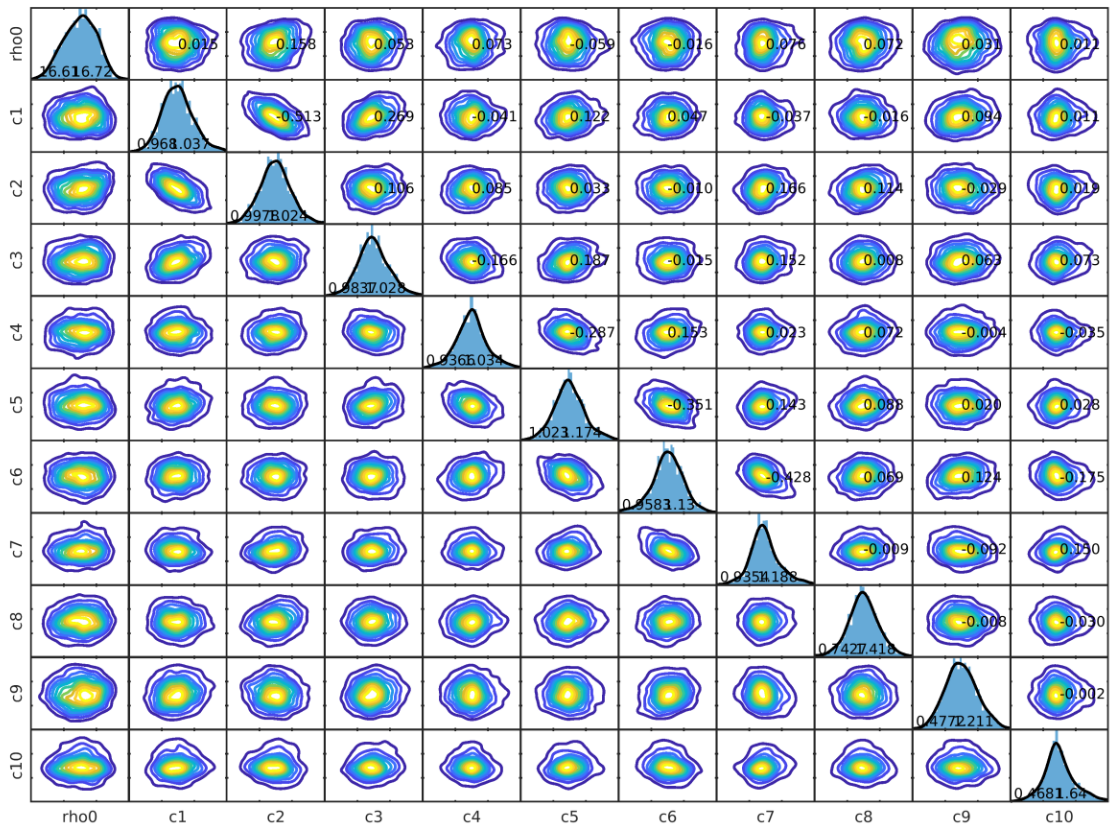


Calibration results for the arbitrary cold curve

No discrepancies between experiment and simulation



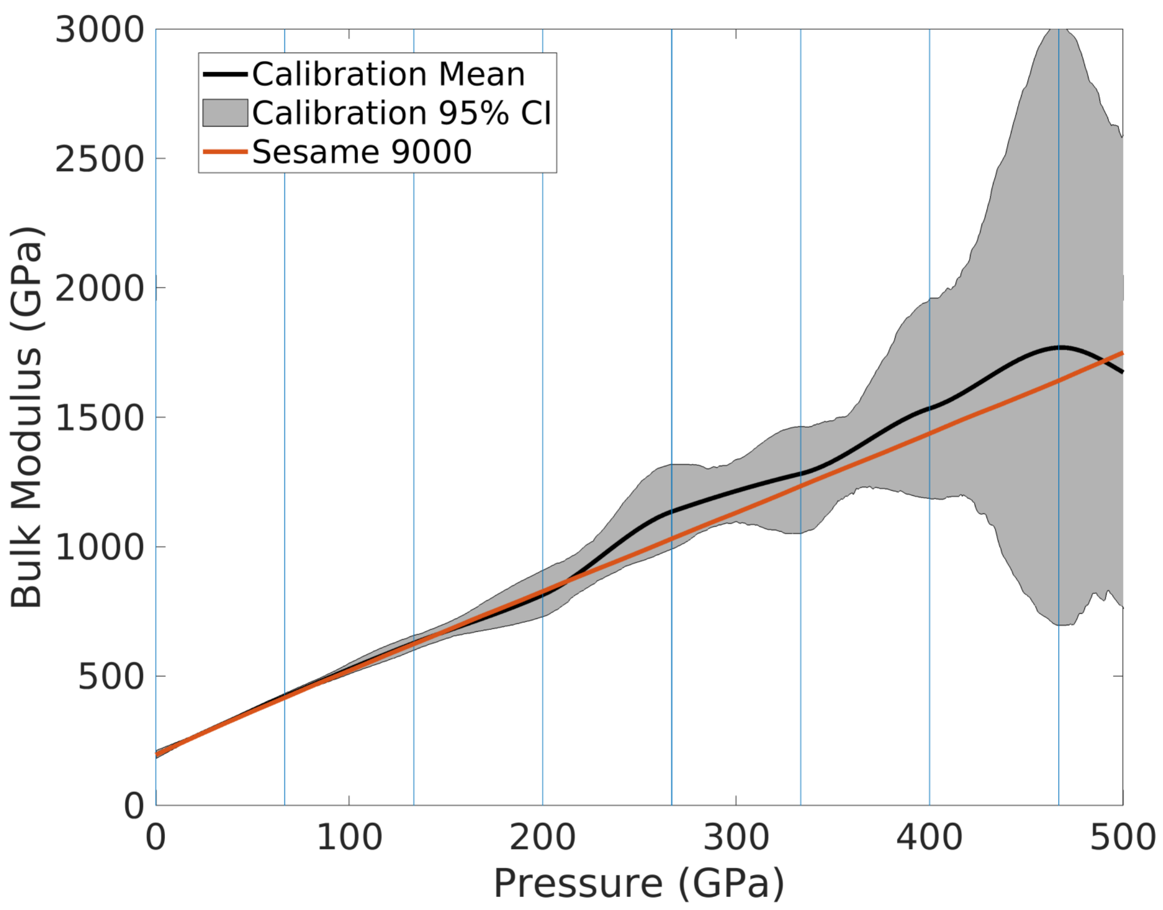
Physical parameter space is large but tractable

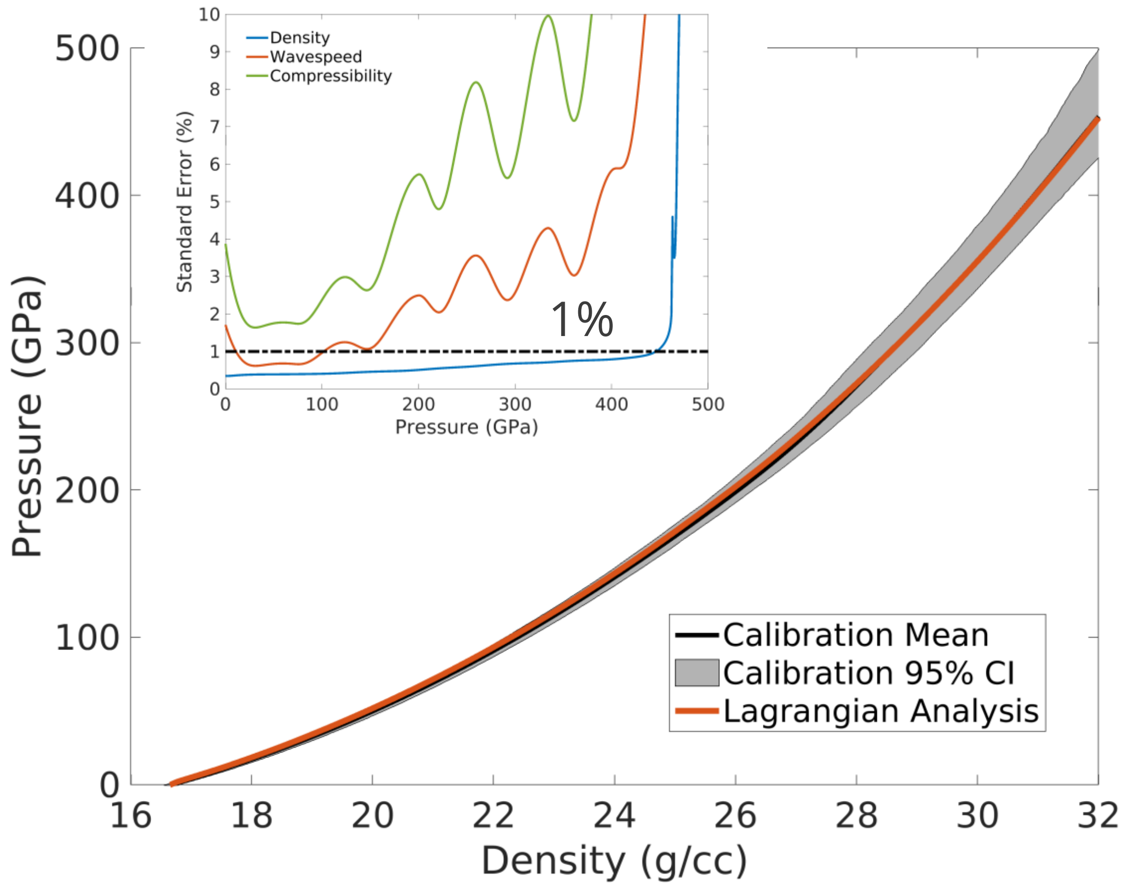


Calibration results for the arbitrary cold curve

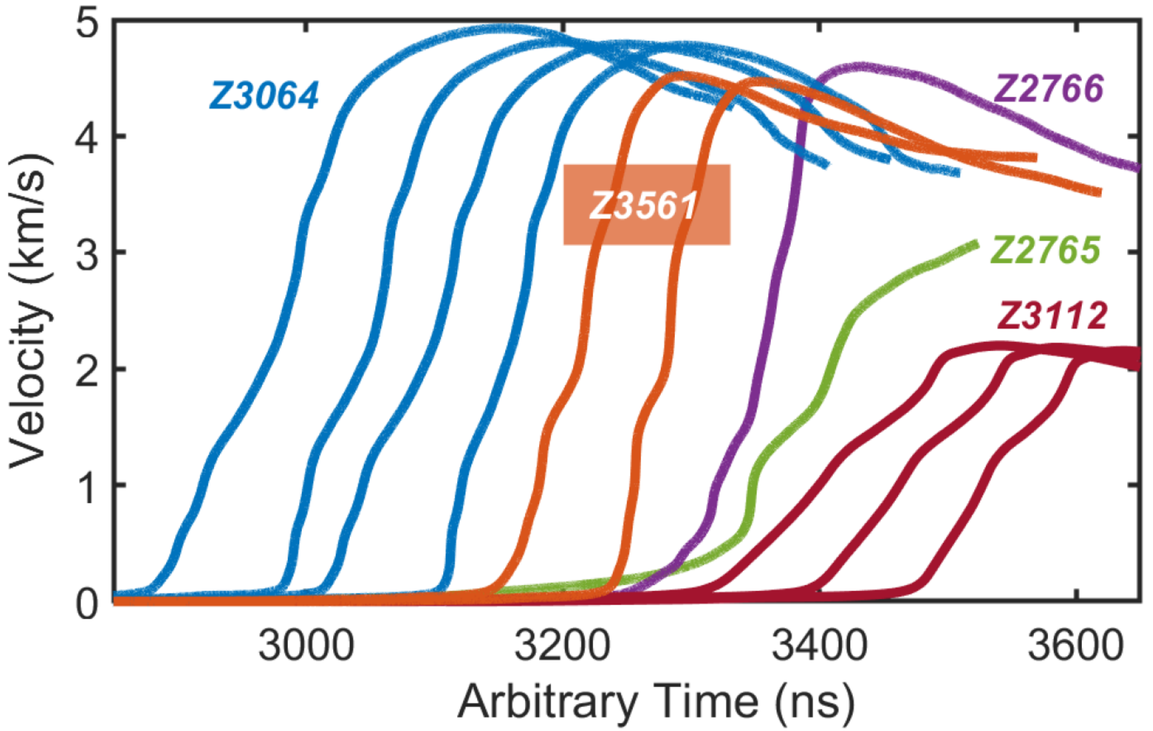
Errors blow up past 400 GPa, consistent with the sensitivity analysis

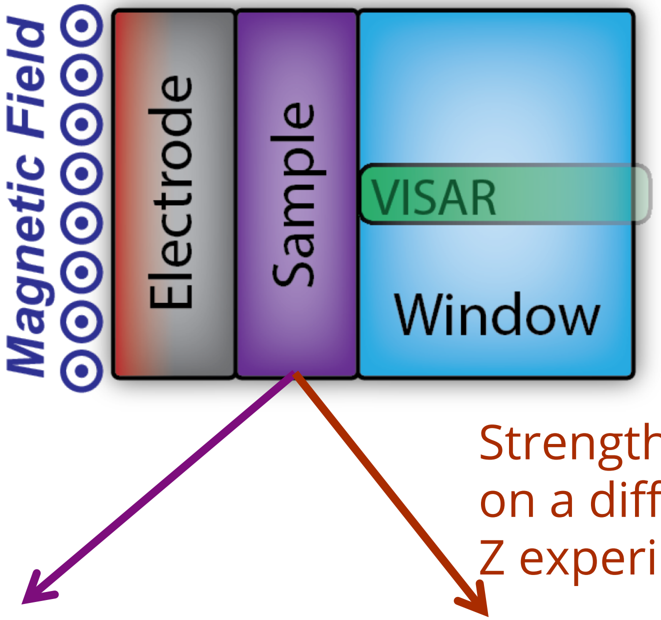
Now the analytic and Bayes approaches agree!





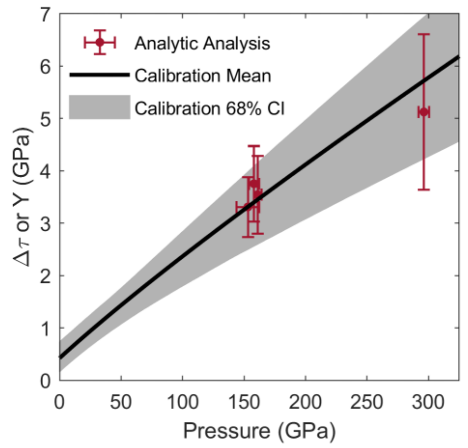
11 Platinum measurements have been obtained over 5 experiments to pressures of 600 GPa





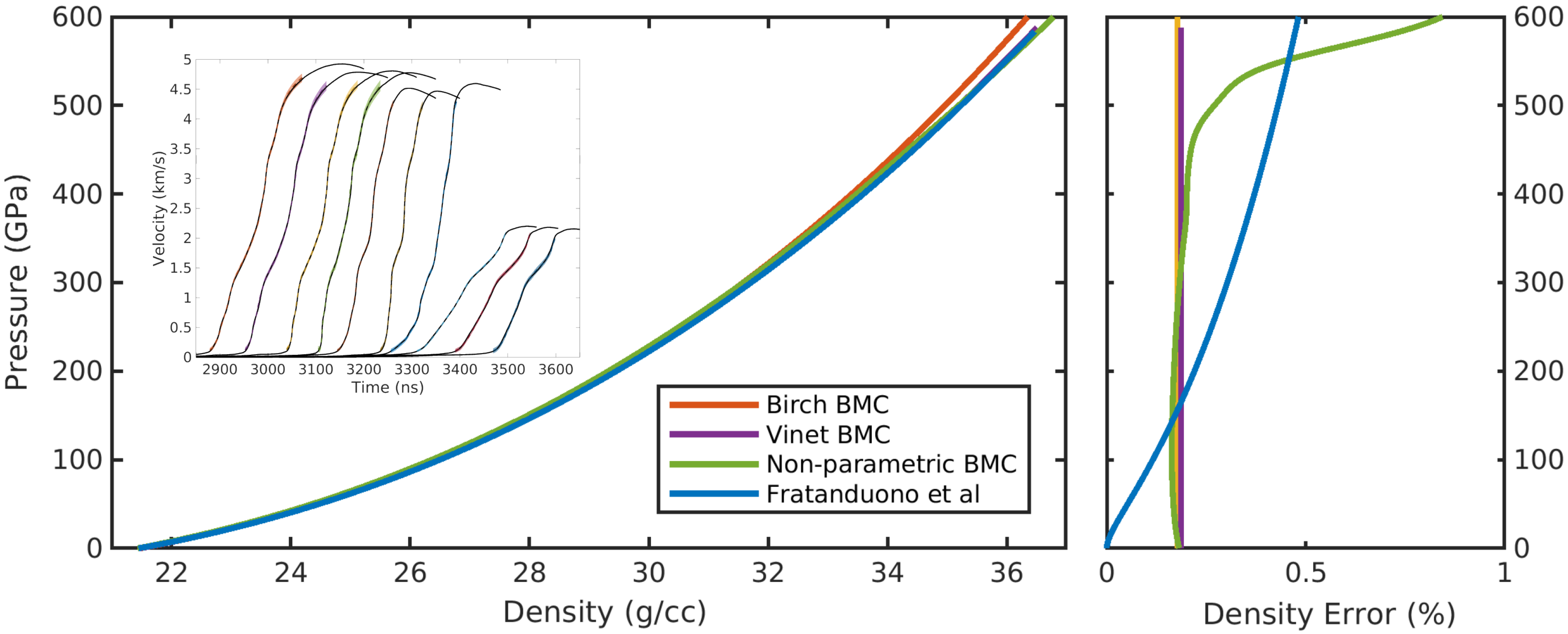
Strength fixed based on a different type of Z experiment

Unknown is EOS

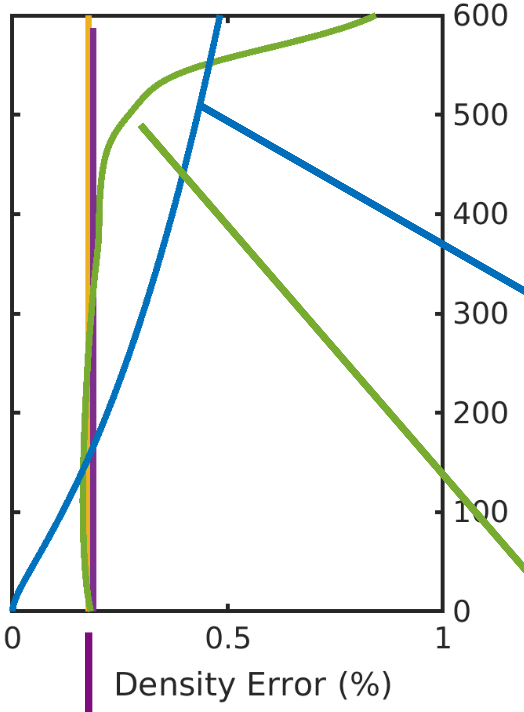


J-P Davis, "Refined measurement of the compressibility of solid platinum under ramped compression to 500 GPa at the Z machine," July 11th, E04.0001, 2:00-2:15

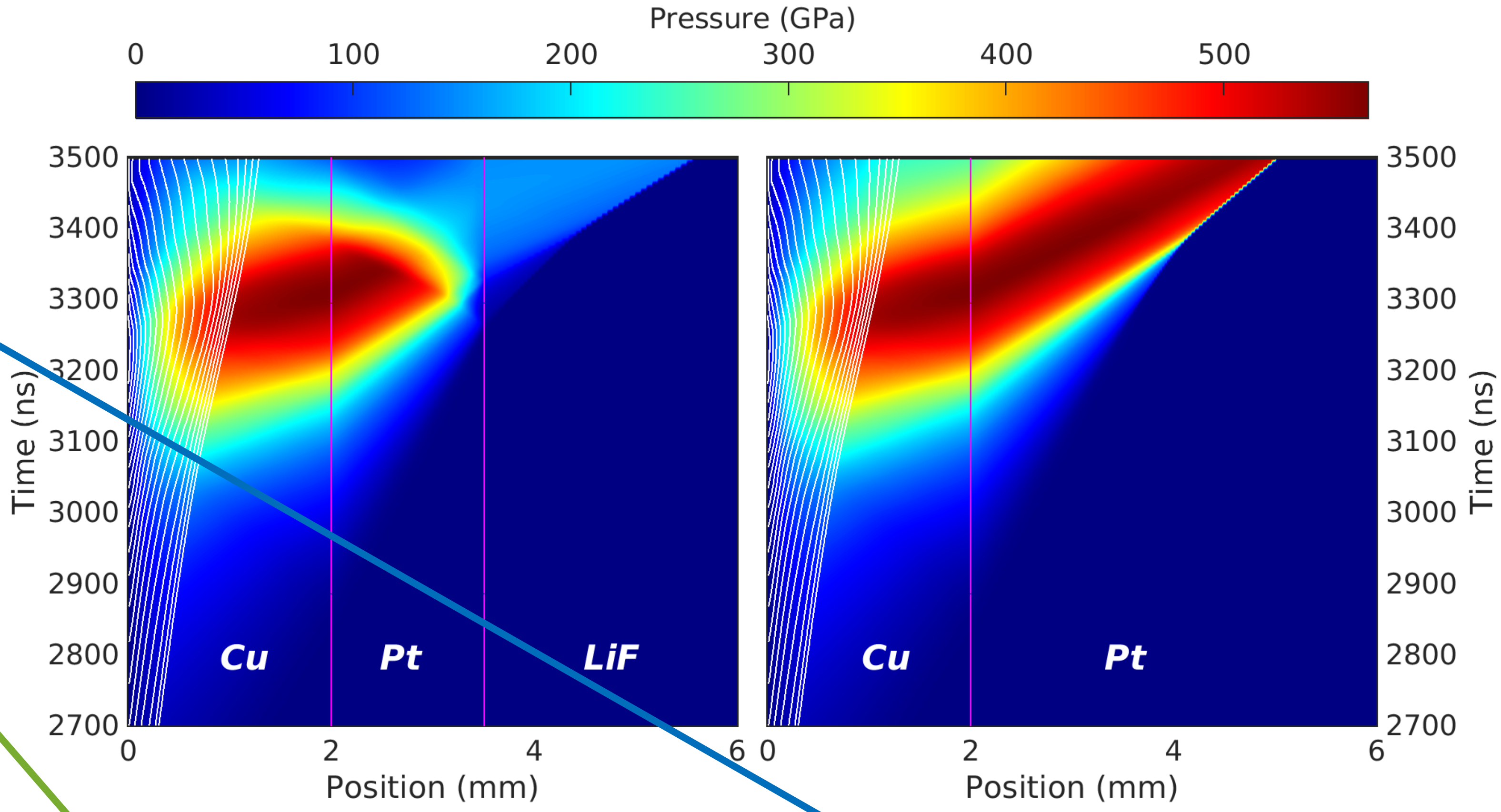
Bayes calibration over the Pt data is in good agreement with traditional analysis methods, but the nature of the high pressure errors are very different



Uncertainties are dramatically different between the methods



$$P(\rho) = 3B_0\left(\frac{1-\eta}{\eta^2}\right) exp\left\{\frac{3}{2}(B_0' - 1)(1-\eta)\right\}$$



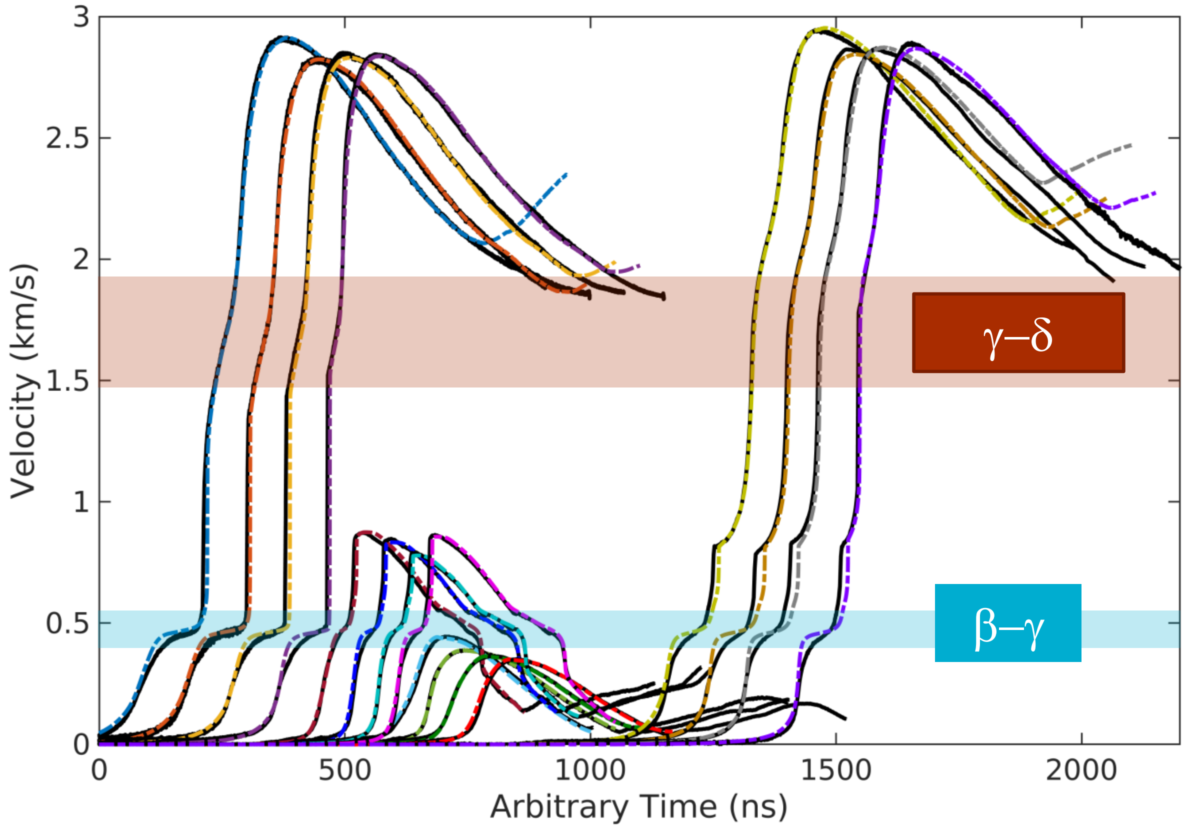
Wave interactions in the real experiment

Wave interactions in the analytic analysis

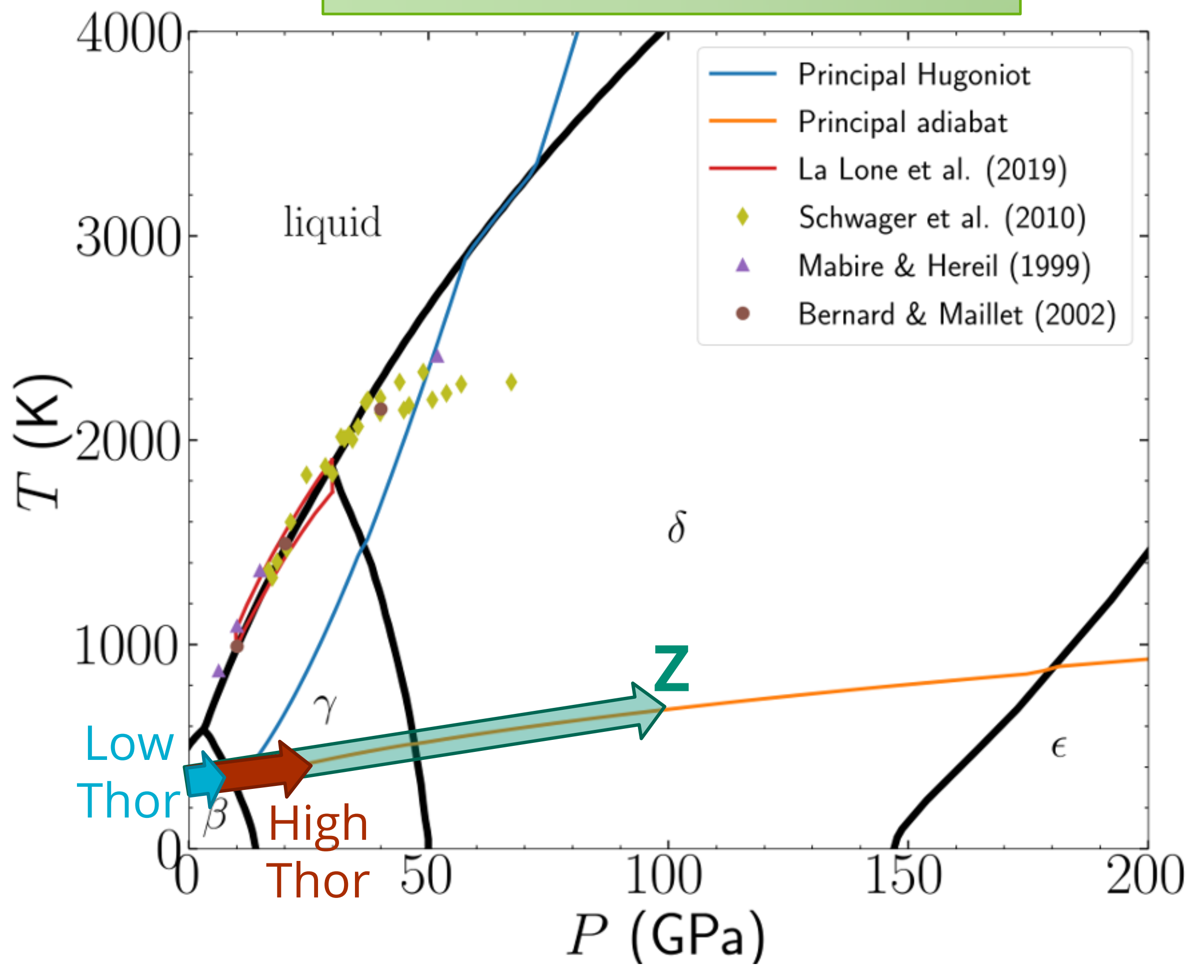
This calibration method can be extended to complex scenarios such as phase transformations

Data with a clear phase transformation

Combining data across multiple experiments

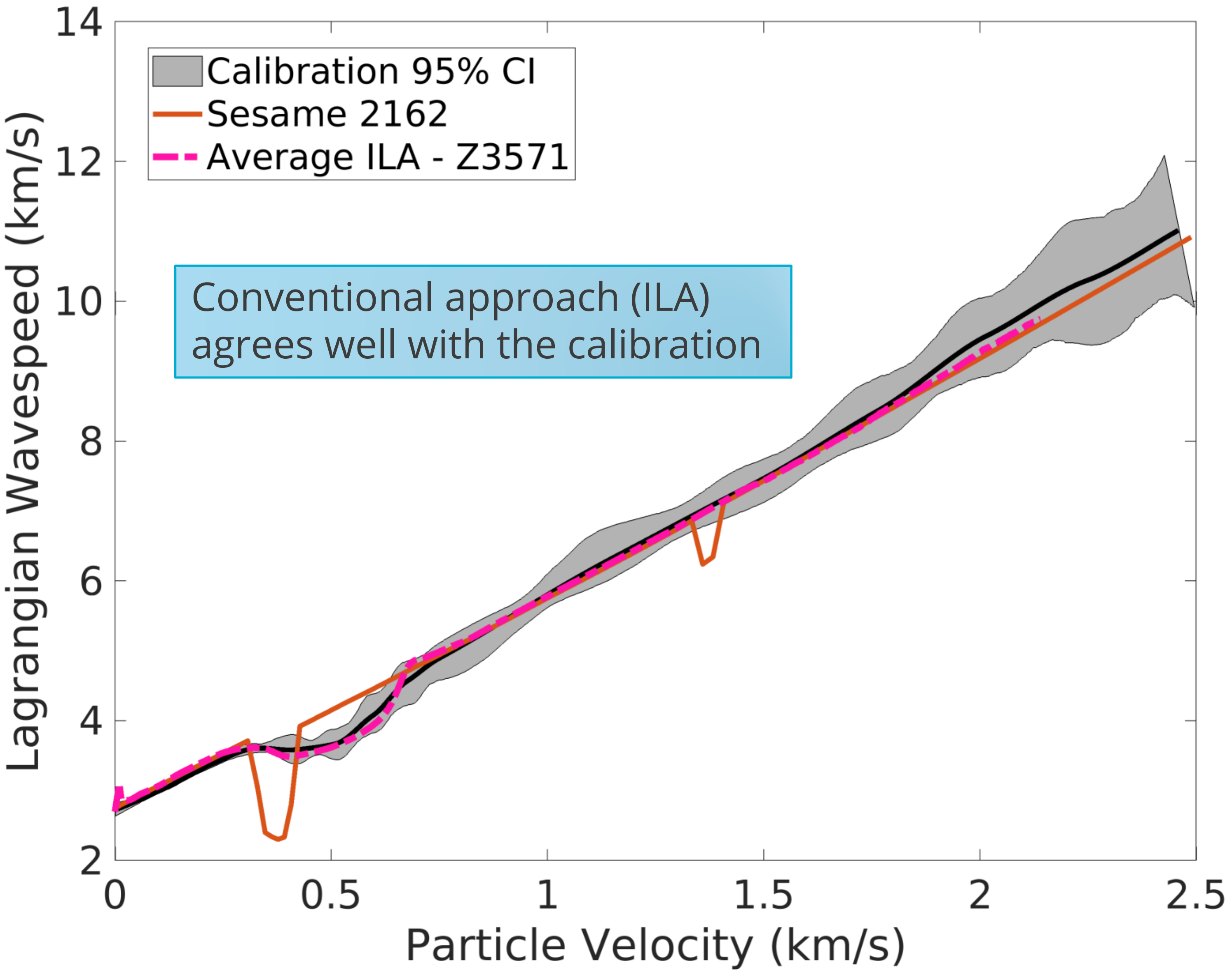


Sesame 2162 Tin EOS



*Rehn et al., PRB **103**, 184102 (2021)*

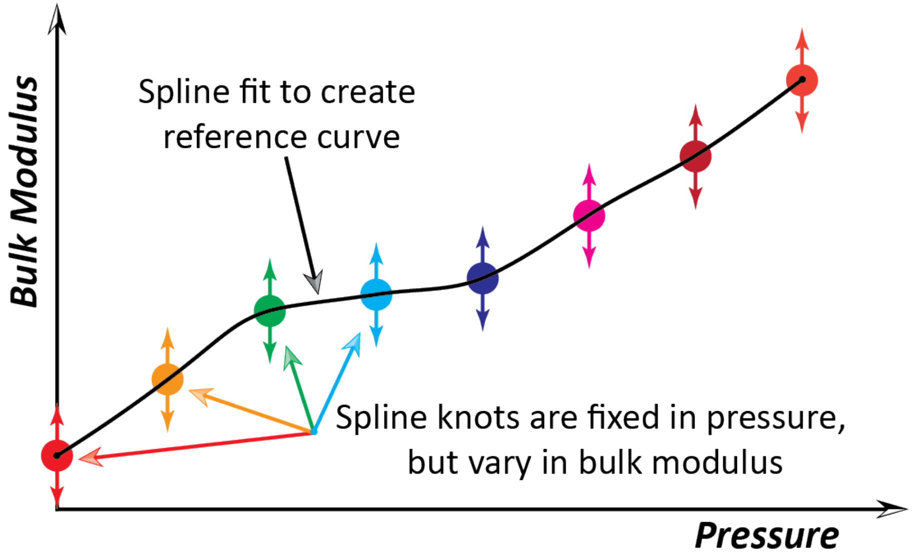
The non-parametric approach is flexible enough to handle non-monotonicity in the response

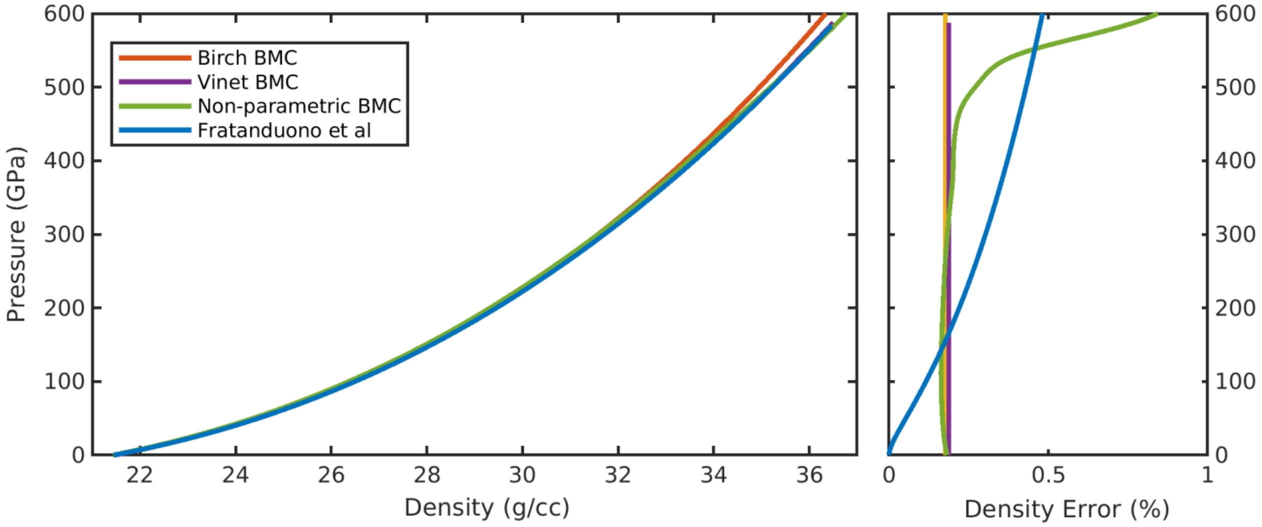


Conclusions

Presented a non-parametric Bayesian calibration method to extract the cold curve from ramp compression experiments on the Z machine

- All the advantages of going Bayesian: incorporate all data and prior knowledge, complete description of all of the errors, inherent UQ
- Full sensitivity over the entire measured response
- Better error quantification when compared to traditional analysis methods





THANK YOU