Sandia National Laboratories

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EFFICIENT APPROACH FOR GENERATING TRANSPORT COEFFICIENT DATASETS FOR UNCERTAINTY QUANTIFICATION OF MAGNETOHYDRODYNAMIC SIMULATIONS

Presenting: Luke Stanek

In collaboration with: William Lewis, Joshua P. Townsend, Kyle Cochrane, Christopher Jennings, and Stephanie Hansen

High-Energy-Density Science Seminar Series

Livermore, California, August 1st, 2024

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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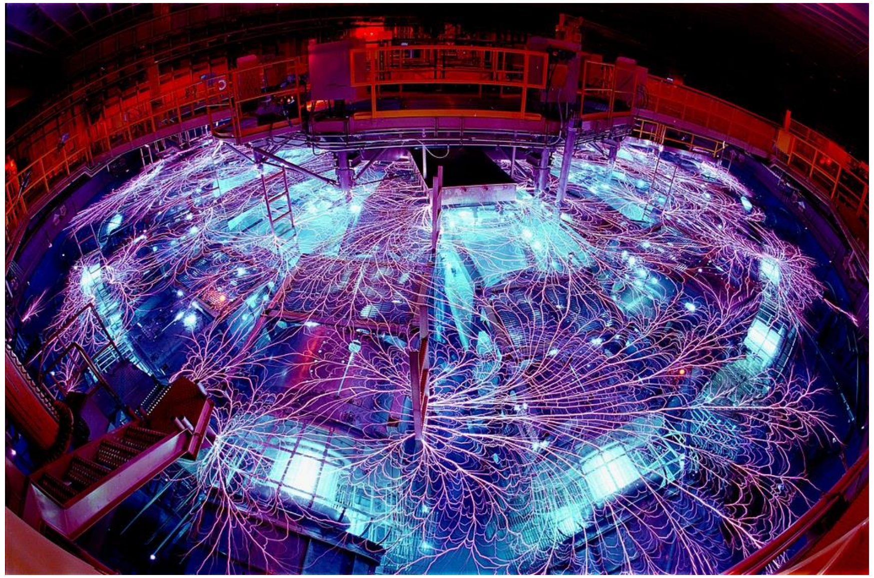
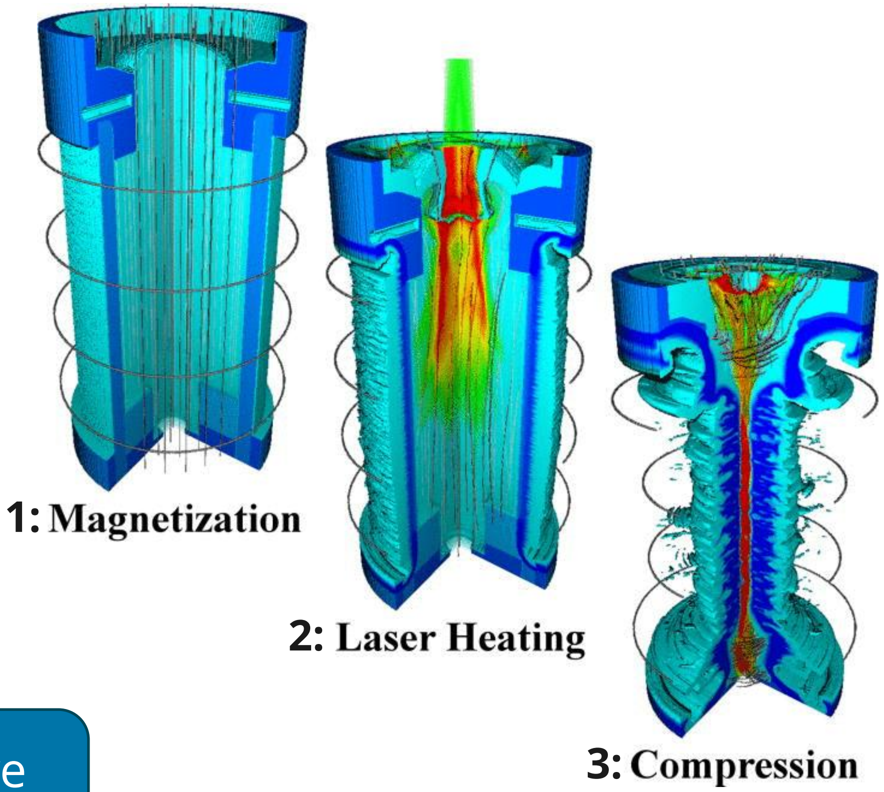
The pulsed power sciences center explores a multitude of applications through experiments and theory

Experiments on the Z machine provide data for:

- nuclear fusion research,
- material properties at high-energy-density conditions,
- and fundamental science applications.

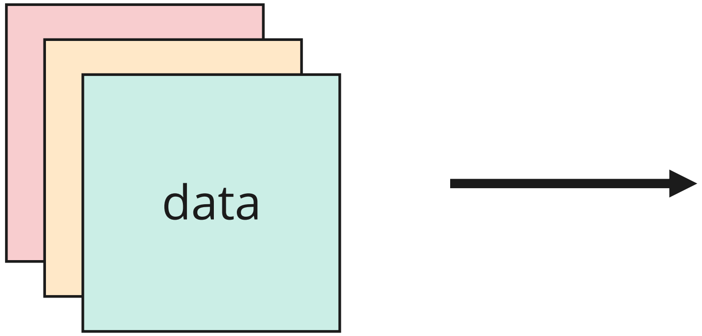


The Z machine compresses fusion fuel contained in a beryllium can (liner).

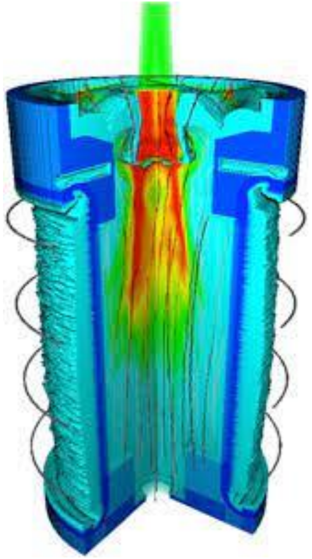


With nearly every experiment, simulations are carried out to compare theory and experiment.

My work involves quantifying the uncertainty from material models and simulations



Input data for simulations (e.g., equations of state and transport coefficients, opacity)



Magnetohydrodynamic (MHD) simulations of experiments

MagLIF simulation by Chris Jennings

Outline

1. *Producing* transport coefficients accurately and rapidly;
2. *using* transport coefficients in hydrodynamic simulations.

Outline

1. *Producing* transport coefficients accurately and rapidly;
2. *using* transport coefficients in hydrodynamic simulations.

Background: transport coefficients quantify how a fluids respond due to gradients in the fluid variables

$$\mathbf{j} = -C\nabla X$$

generic expression for *linear* transport coefficients

How do we compute transport coefficients?

Some common choices of X yield familiar expressions:

$$\mathbf{j}_D = -D\nabla\rho$$

Fick's law; D is the self-diffusion coefficient.

$$\mathbf{j}_\kappa = -\kappa\nabla T$$

Fourier's heat law; κ is the thermal conductivity.

$$\mathbf{j}_\sigma = -\sigma\nabla\phi$$

Ohm's law; σ is the electrical conductivity.

Charged-Particle Transport Coefficient Comparison Workshop: comparing approaches for generating data

High Energy Density Physics 37 (2020) 100905

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Review of the first charged-particle transport coefficient comparison workshop

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workshop held in 2016

RESEARCH ARTICLE | MAY 02 2024

Review of the second charged-particle transport coefficient code comparison workshop

Special Collection: Charged-Particle Transport in High Energy Density Plasmas

Lucas J. Stanek; Alina Kononov; Stephanie B. Hansen; Brian M. Haines; S. X. Hu; Patrick F. Knapp; Michael S. Murillo; Liam G. Stanton; Heather D. Whitley; Scott D. Baalrud; Lucas J. Babati; Andrew D. Baczewski; Mandy Bethkenhagen; Augustin Blanchet; Raymond C. Clay, III; Kyle R. Cochrane; Lee A. Collins; Amanda Dumi; Gerald Faussurier; Martin French; Zachary A. Johnson; Valentin V. Karasiev; Shashikant Kumar; Meghan K. Lentz; Cody A. Melton; Katarina A. Nichols; George M. Petrov; Vanina Recoules; Ronald Redmer; Gerd Röpke; Maximilian Schörner; Nathaniel R. Shaffer; Vidushi Sharma; Luciano G. Silvestri; François Soubiran; Phanish Suryanarayana; Mikael Tacu; Joshua P. Townsend; Alexander J. White

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Phys. Plasmas 31, 052104 (2024)
https://doi.org/10.1063/5.0198155

workshop held in 2023

wide range of conditions for 2 elements

Summary of workshop cases.

Element	Density (g/cm^3)	Temperature (eV)
C	0.1, 1, 10, 100	0.2, 2, 20, 200, 2000
H	0.1, 1, 10, 100	0.2, 2, 20, 200, 2000
CH	0.1, 1, 10, 100	0.2, 2, 20, 200, 2000

targeted conditions for 6 elements

Priority Level	Case ID	Element(s)	$n_{species}$ (cm^{-3})	ρ_{total} ($g\ cm^{-3}$)	T (eV)
1	H1	H	5.98×10^{23}	1	2
1	C1	C	5.01×10^{23}	10	2
1	CH1	CH	4.63×10^{22}	1	2
1	Al1	Al	6.03×10^{22}	2.7	1
1	Cu1	Cu	8.49×10^{22}	8.96	1
1	HCu1	HCu	1.68×10^{22}	1.8	1
2	Be1	Be	1.23×10^{23}	1.84	4.4
2	CH2	CH	4.16×10^{22}	0.9	7.8
2	Au1	Au	5.91×10^{22}	19.32	10
2	H3	H	5.98×10^{24}	10	20

The Second Charged-Particle Transport Coefficient Comparison Workshop: comparing approaches for generating data

Approaches included:

computational expense

ms of cpu time

- Analytic models
- Average-atom models (AA)
- Models based on kinetic theory (KT)
- Molecular dynamics with a pre-computed potential (MD)
- Density-Functional Theory molecular dynamics (DFT-MD)

weeks of cpu time

The Second Charged-Particle Transport Coefficient Comparison Workshop: comparing approaches for generating data

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Analytic models

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Models based on kinetic theory (KT)

Molecular dynamics with a pre-computed potential (MD)

Density-Functional Theory molecular dynamics (DFT-MD)

weeks of cpu time

Transport coefficients from an average-atom model

electronic transport

The electron-ion collision rate is τ_{ei} generated from an average-atom model using the Ziman formalism.

Key inputs to the Ziman formalism:

- Mean-ionization state, Z^*
- Static structure factor, $S(k)$

$$\sigma^{\mathrm{DC}} = \frac{n_e e^2 \tau_{ei}}{m_e}$$

DC electrical conductivity

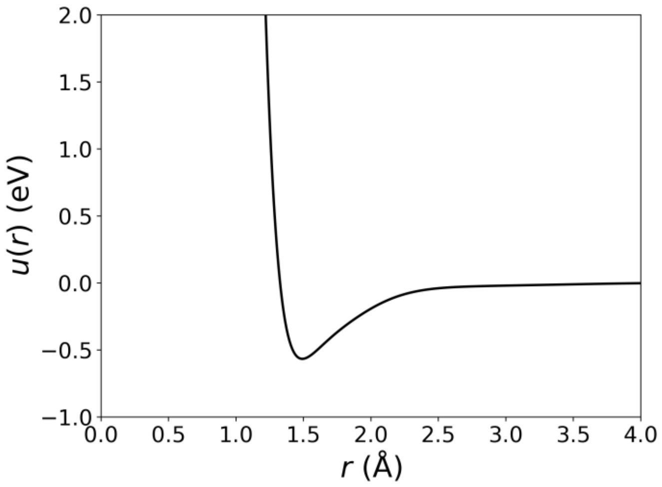
Variations in Z^* and $S(k)$ correspond to variations in *electronic* transport coefficients.

Reference:

- Sterne, P. A., et al. "Equation of state, occupation probabilities and conductivities in the average atom Purgatorio code." *HEDP* (2007)

ionic transport

$$u(k) = (Z^*)^2 u_C(k) + |u_{ei}|^2 \chi(k)$$



→ molecular dynamics code → transport coefficients

Variations in Z^* and $\chi(k)$ correspond to variations in *ionic* transport coefficients.

Reference:

- Stanek, Lucas J., et al. "Efficacy of the radial pair potential approximation for molecular dynamics simulations of dense plasmas." *PoP* (2021).

Results from multiple molecular dynamics runs can be used to estimate uncertainties

One way to compute transport coefficients from molecular dynamics is to use "Green-Kubo" relations.

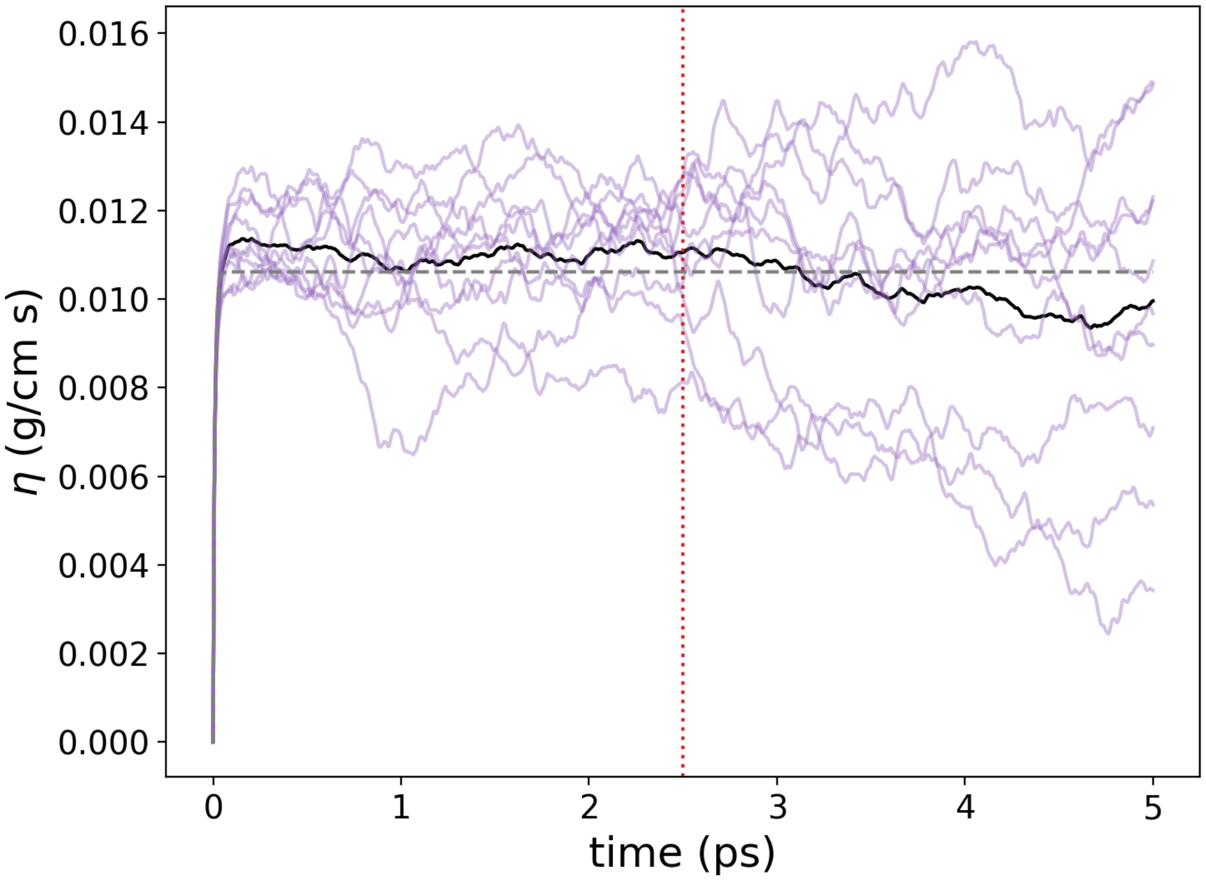
For the shear viscosity, the Green-Kubo relationship is

$$\eta = \frac{1}{V k_B T} \int_0^\infty dt \, \langle P_{\alpha\beta}(t) P_{\alpha\beta}(0) \rangle$$

Taking the value at 2.5 ps, and averaging across MD runs yields

$$\eta = 0.011 \pm 0.0221 (\mathrm{g/cm\text{-}s})$$

There exists uncertainty from:
1. choice of interaction potential (model) and,
2. statistical uncertainty from multiple MD runs.



References:
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- Stanek, Lucas J., et al. "Review of the second charged-particle transport coefficient code comparison workshop." *PoP* (2024).

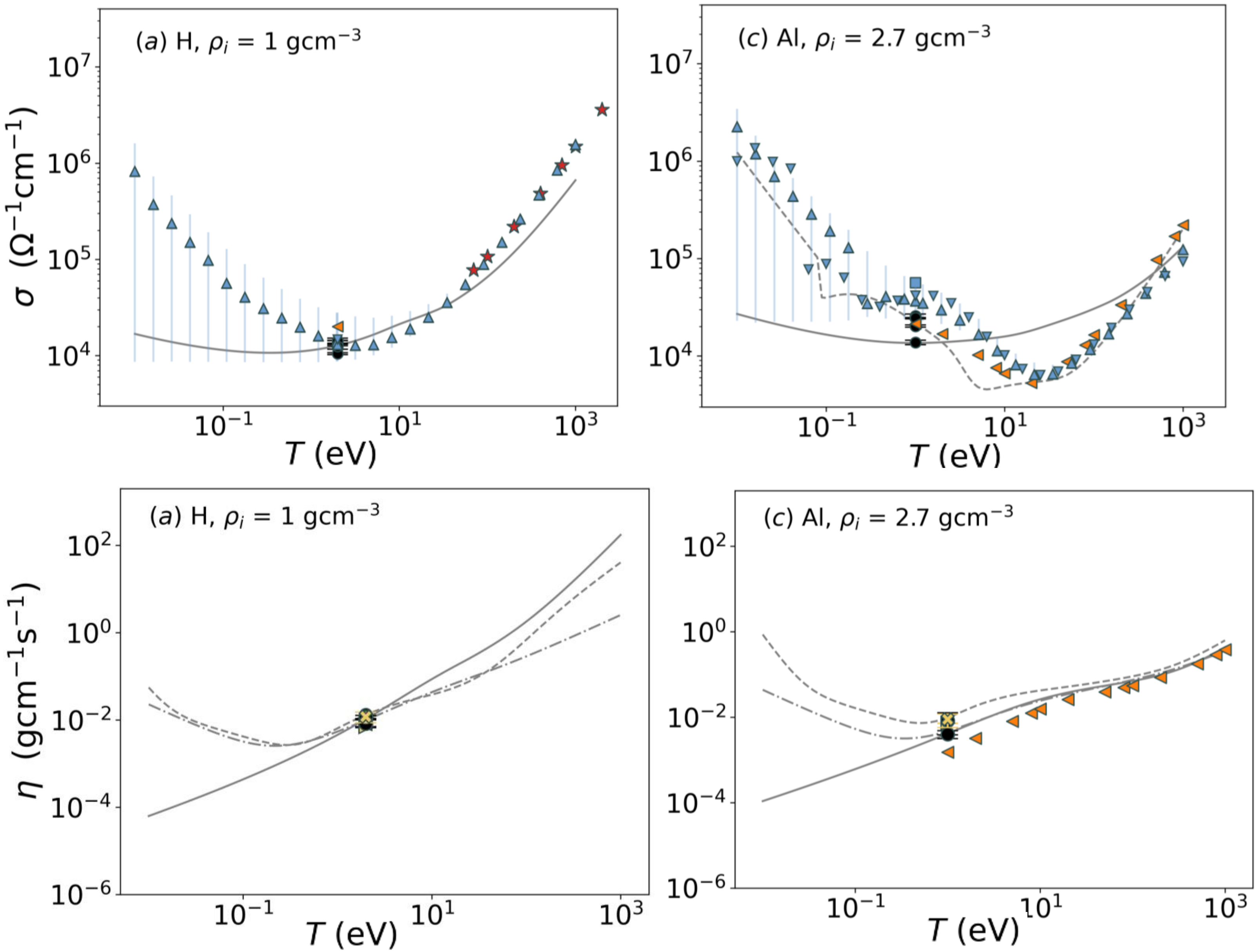
Comparisons of the transport coefficients from the workshop

Lines + star: analytic models

Points: simulation method (e.g, DFT-MD, KT, AA)

Lines: analytic models

Points: simulation method (e.g, DFT-MD, MD, KT)



Summary of the Second Charged-Particle Transport Coefficient Code Comparison Workshop

electron electrical conductivity

“...the difference was at worst **one order of magnitude between all models** and a **factor of two between similar models**.”

ion shear viscosity

“...the difference was at worst **one order of magnitude between all models** and a **factor of six between similar models**.”

for more on these findings, see the full article →

RESEARCH ARTICLE | MAY 02 2024

Review of the second charged-particle transport coefficient code comparison workshop

Special Collection: Charged-Particle Transport in High Energy Density Plasmas

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Outline

1. *Producing* transport coefficients accurately and rapidly;
2. *using* transport coefficients in hydrodynamic simulations.

Datasets of electrical conductivity are necessary closures for magnetohydrodynamic (MHD) simulations of experiments

Resistive MHD equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

continuity equation

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla P - \nabla \frac{B^2}{8\pi} + \frac{\mathbf{B} \cdot \nabla \mathbf{B}}{4\pi}$$

momentum equation

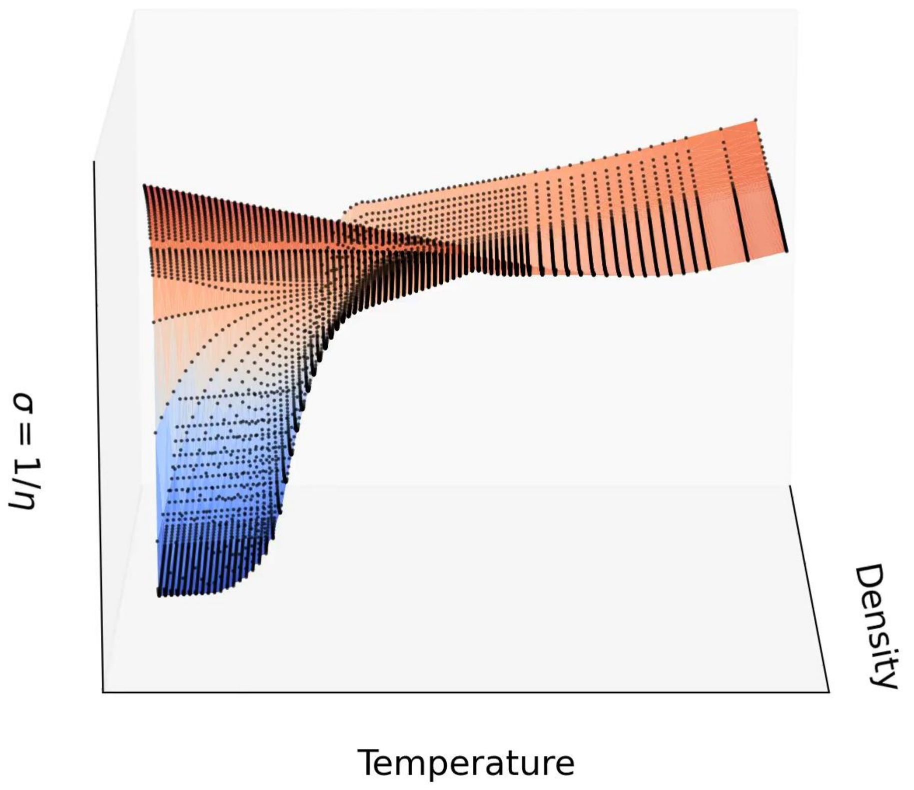
total pressure from an equation of state

$$\frac{\partial \mathbf{B}}{\partial t} = \frac{c^2}{\sigma 4\pi} \nabla^2 \mathbf{B} + \nabla \times (\mathbf{u} \times \mathbf{B})$$

induction equation

the DC electrical conductivity: I use the Lee-More-Desjarlais (LMD) model to produce this dataset.

I will now walk you through how I make a table like the one to the right.



Reference:

- Drake, R. Paul. "High-energy-density physics." *Physics Today* (2010)

Bayesian inference is an approach to estimate model parameters and include dataset uncertainties

Bayes' theorem:

$$P(\boldsymbol{\theta}|\sigma^{\mathrm{DC}}) = \frac{P(\sigma^{\mathrm{DC}}|\boldsymbol{\theta})P(\boldsymbol{\theta})}{P(\sigma^{\mathrm{DC}})}$$

Probability of data given model parameters (the likelihood distribution)

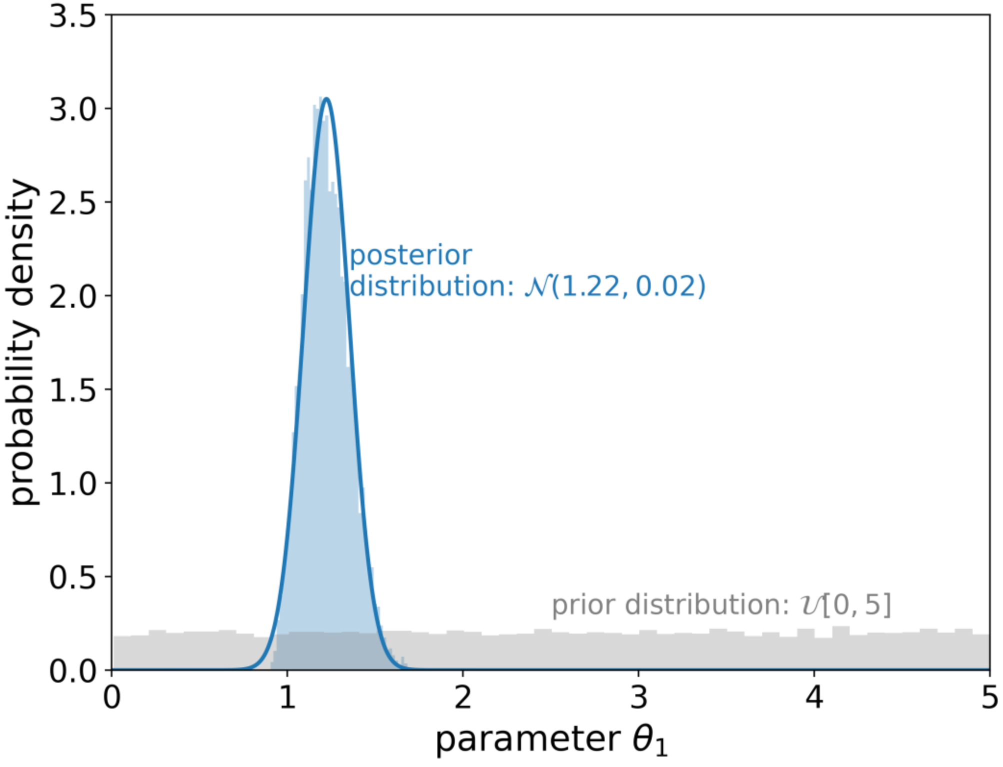
Prior knowledge of model parameters (the prior distribution)

Probability of model parameters given data (the posterior distribution)

Probability of a particular data value—a normalization factor.

Bayesian inference determines the parameters of the Lee-More-Desjarlais model to estimate the electrical conductivity.

Bayes' theorem reduces a "guess" distribution, to an "optimized" distribution.

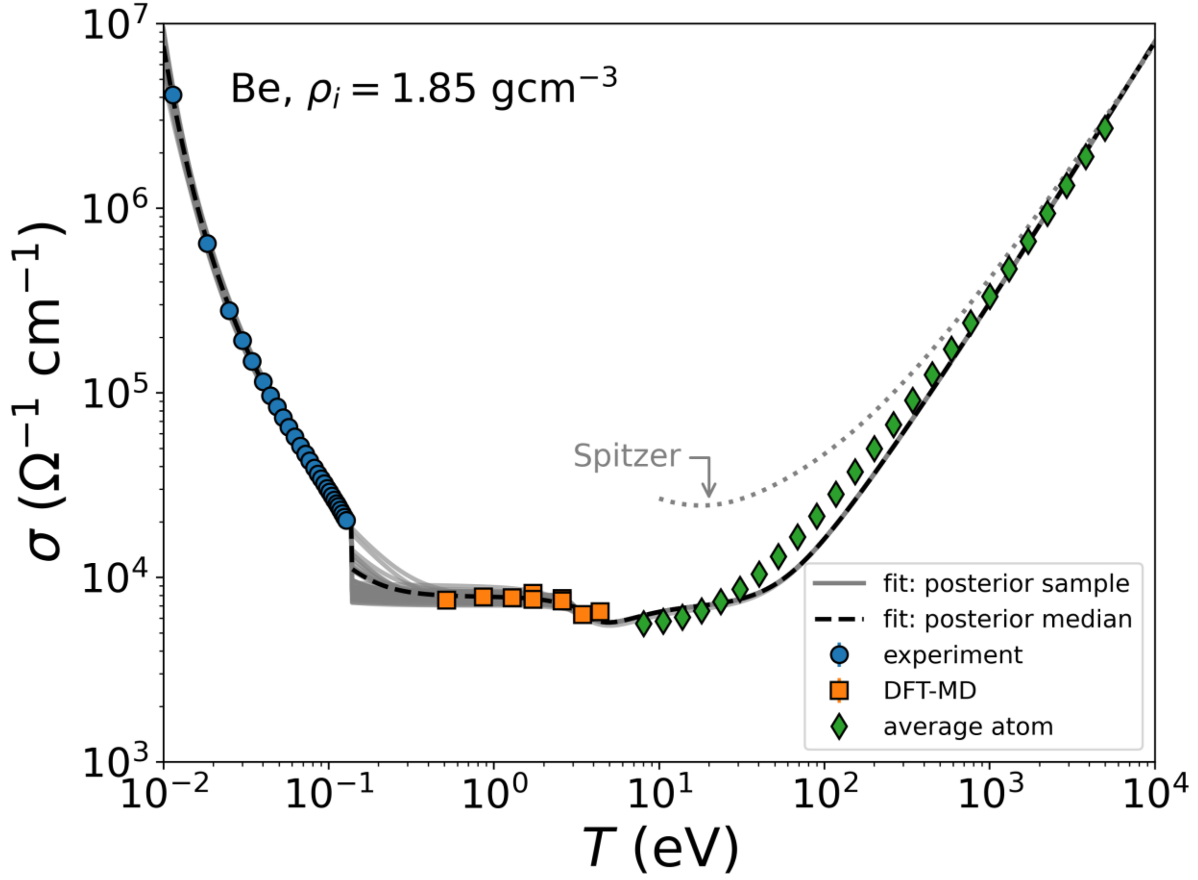


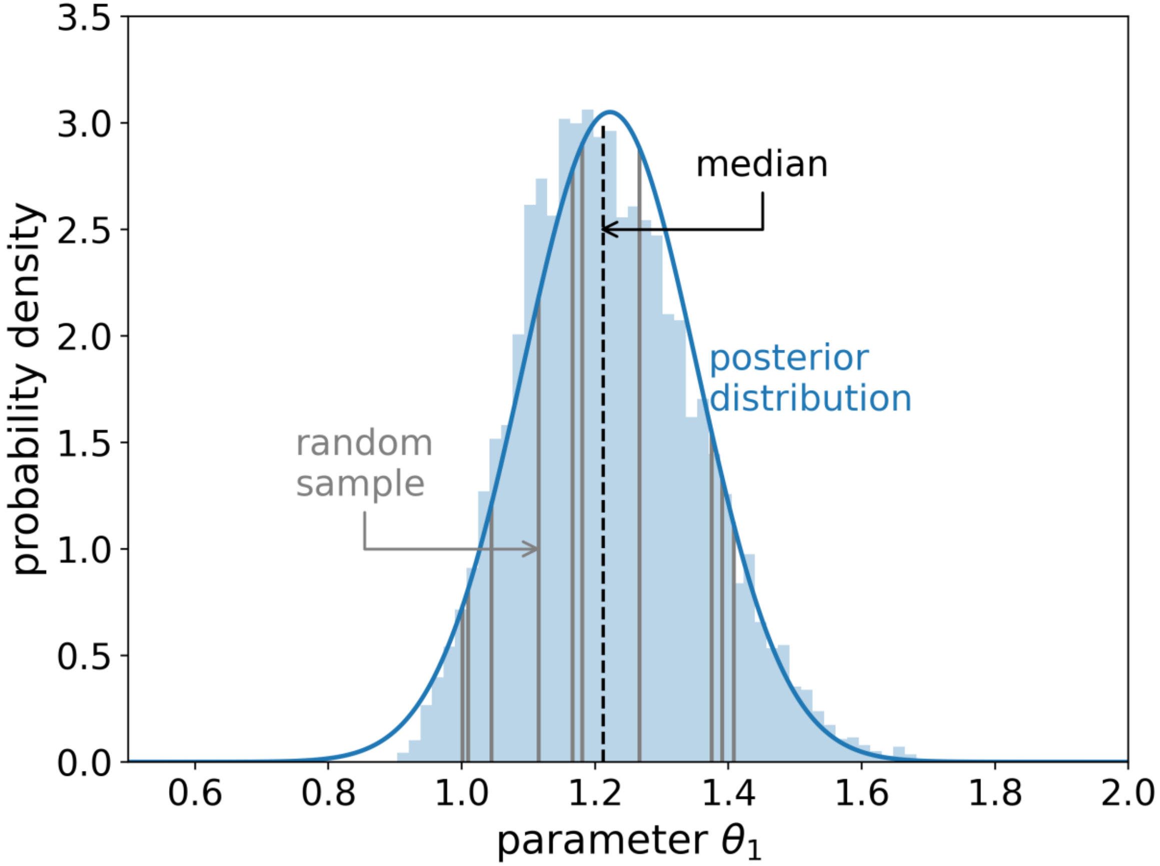
Sampling the posterior distribution produces an ensemble of models.

References:

- Lee, Yim T., and R. M. More. "An electron conductivity model for dense plasmas." *The Physics of fluids* 2 (1984)
- Desjarlais, Michael P. "Practical improvements to the Lee-More conductivity near the metal-insulator transition." *Contributions to Plasma Physics* (2001)

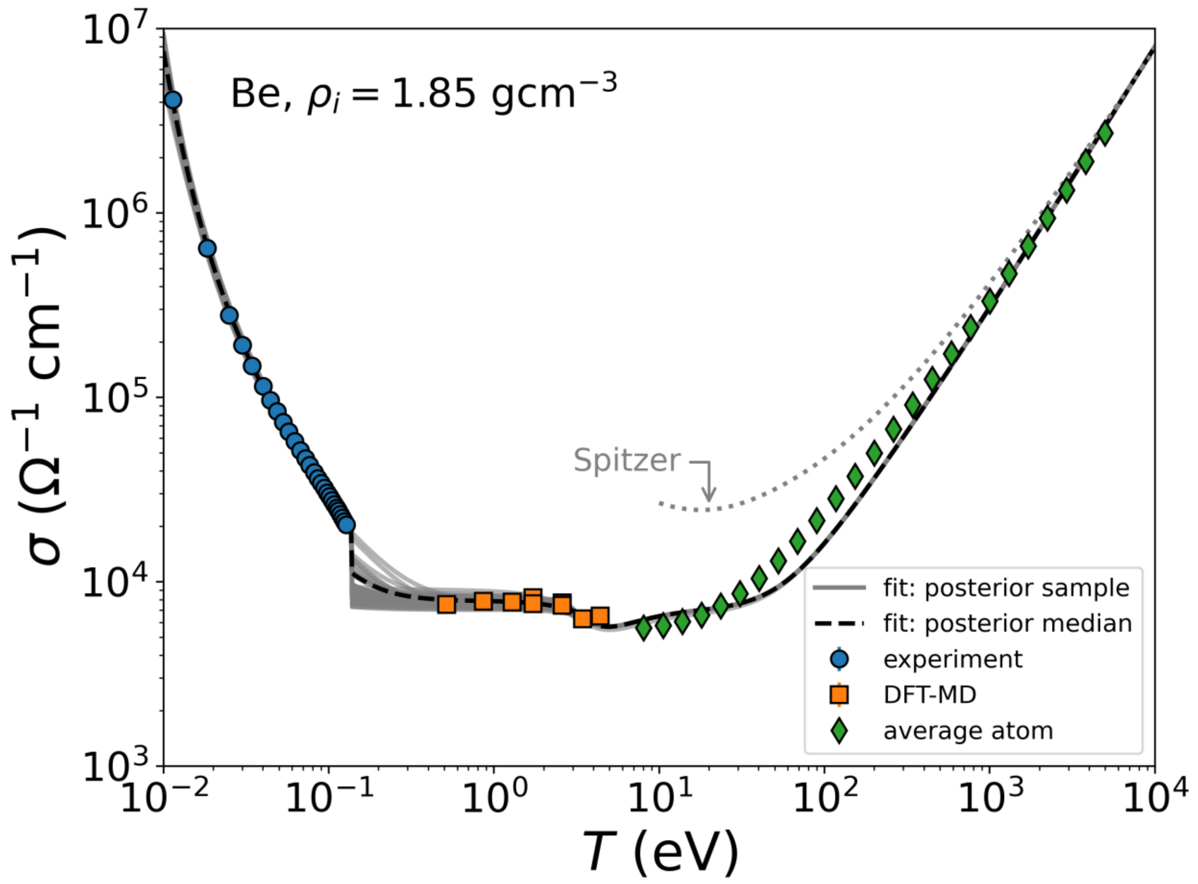
Fitting a parameterized electrical conductivity model produces a wide-ranging "look-up" table

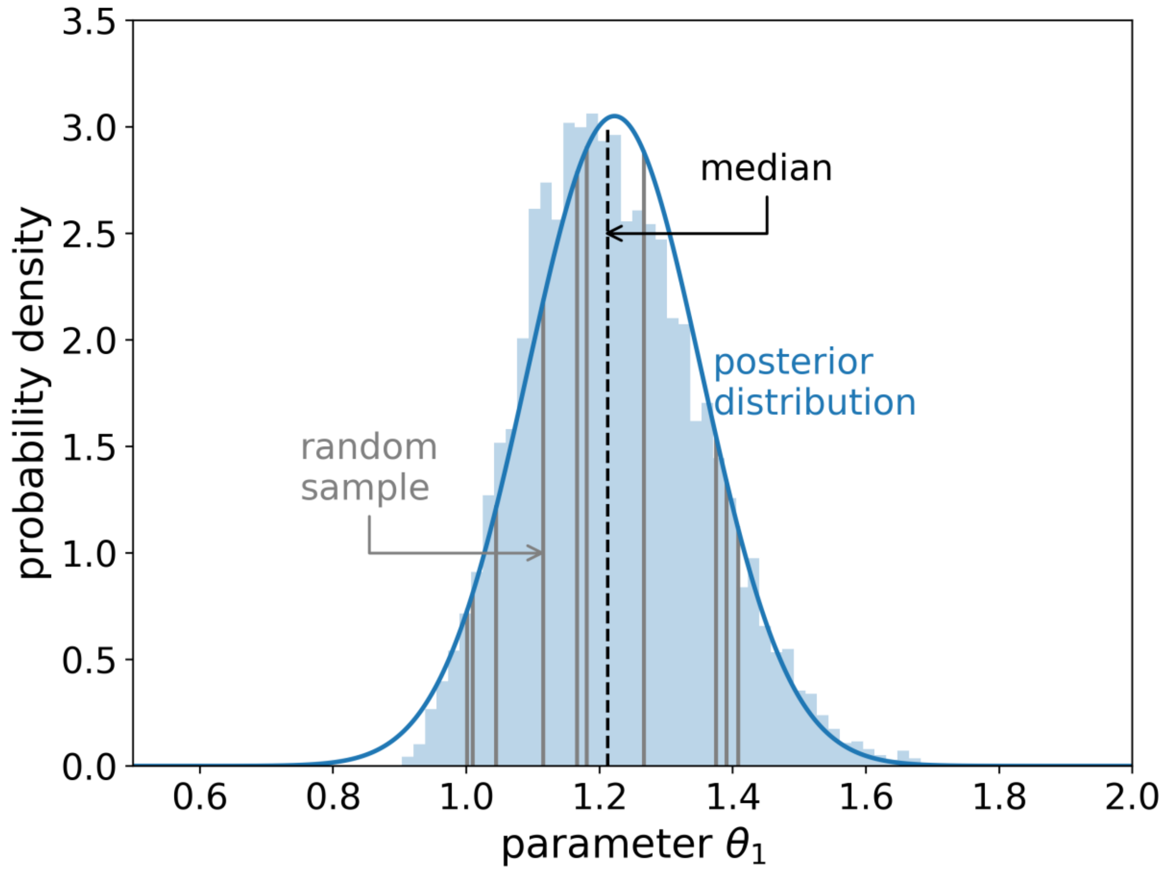




Here, we assume a 10% uncertainty on all data.

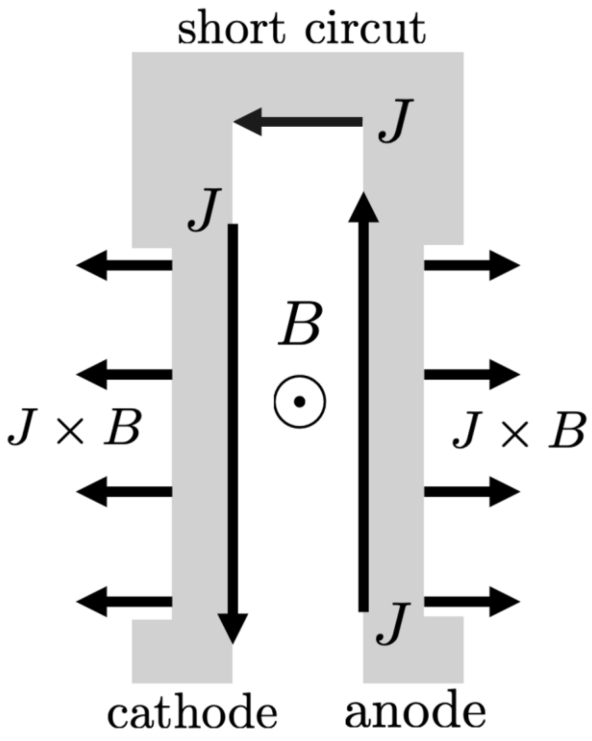
Fitting a parameterized electrical conductivity model produces a wide-ranging "look-up" table





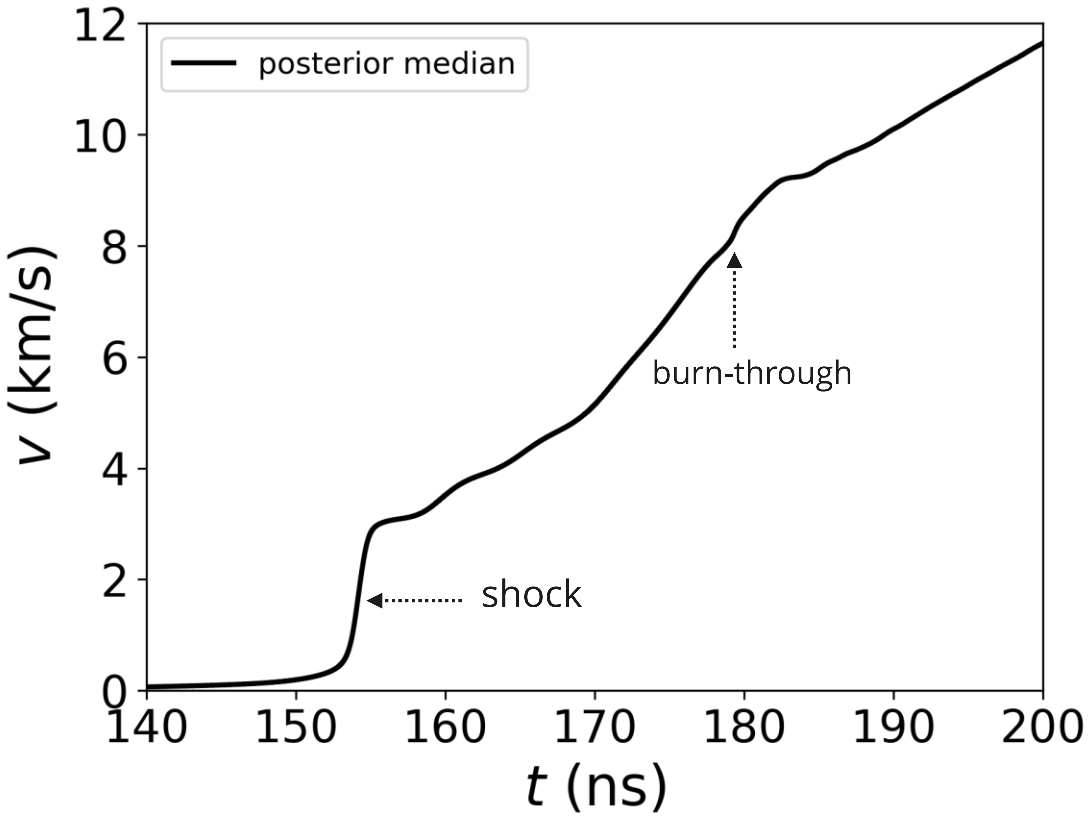
The automated fitting procedure is carried out at different values of density to produce a table that varies with temperature and density.

An exemplar problem of a magnetically-launched flyer plate/return-current can enables an uncertainty analysis



Current generated by the Z machine accelerates a piece of material outward; its velocity informs us of potential current losses.

MHD simulation

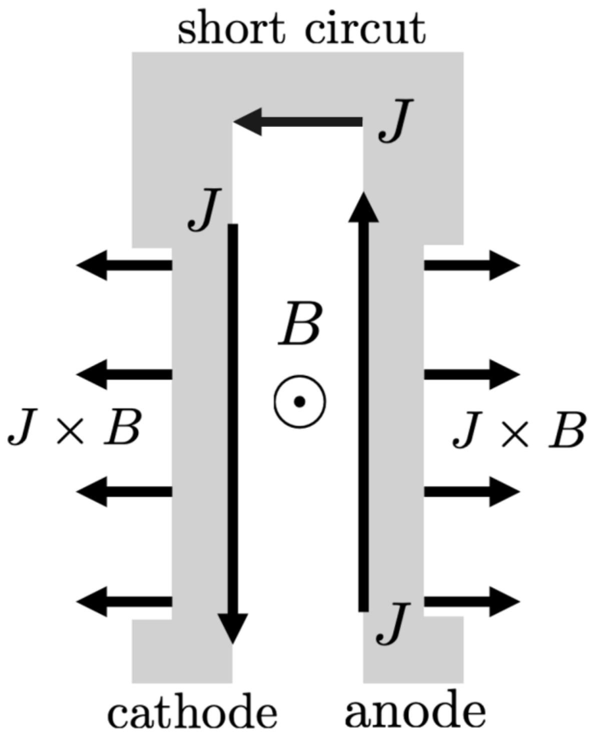


Features like a shock or magnetic field burn-through help assess our simulation efficacy when compared to experiments.

References:

- Cochrane, K. R., et al. "Magnetically launched flyer plate technique for probing electrical conductivity of compressed copper." *JAP* (2016).
- Porwitzky, A., et al. "Determining the electrical conductivity of metals using the 2 MA Thor pulsed power driver." *RSI* (2021).

An exemplar problem of a magnetically-launched flyer plate/return-current can enables an uncertainty analysis



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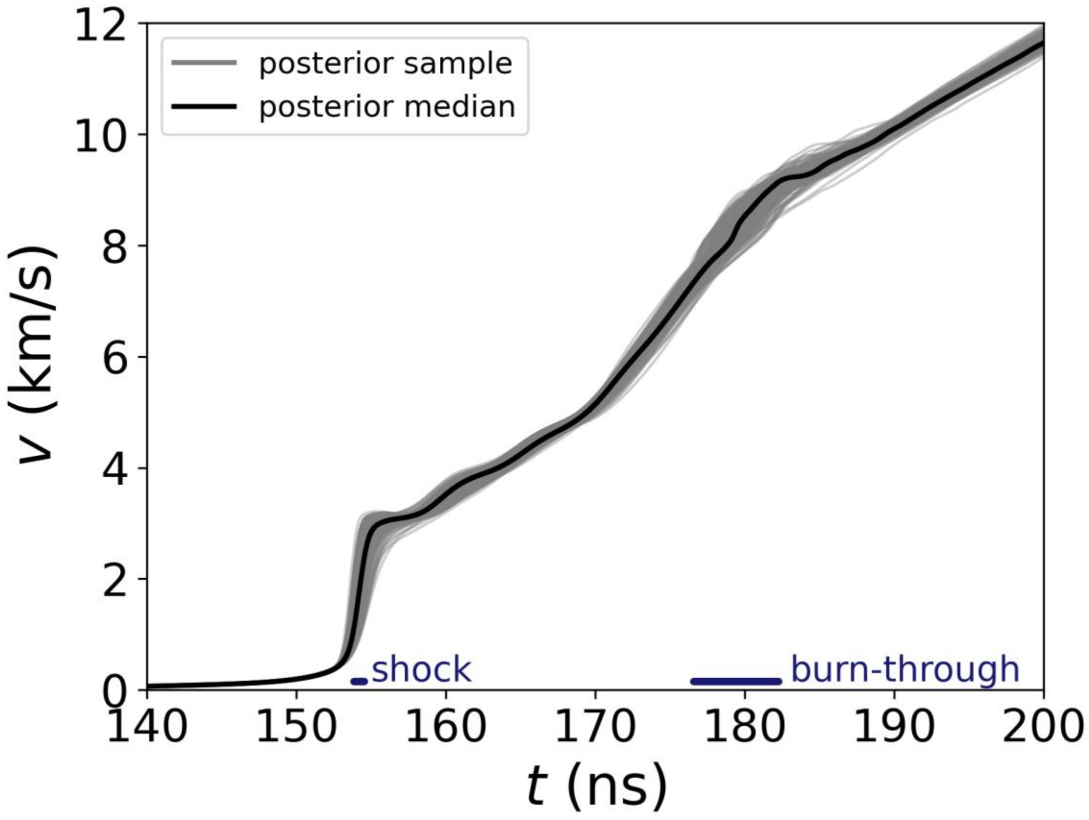
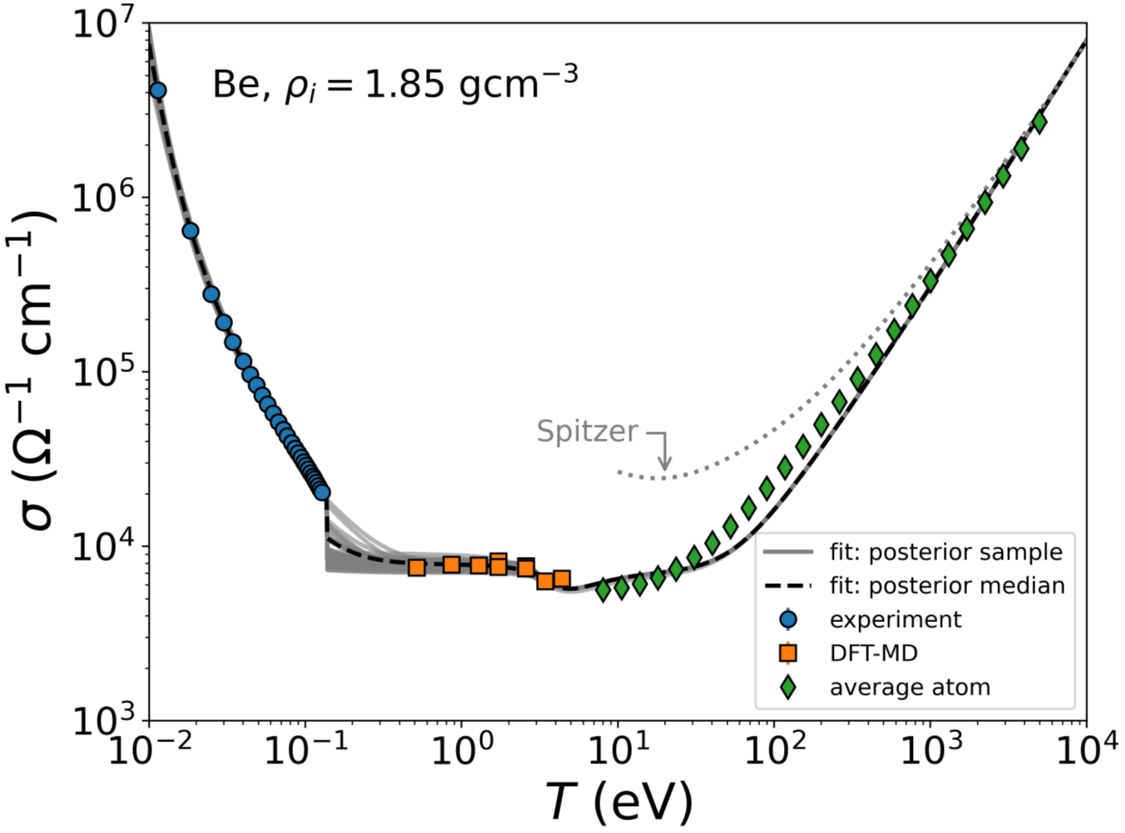
MHD simulation →

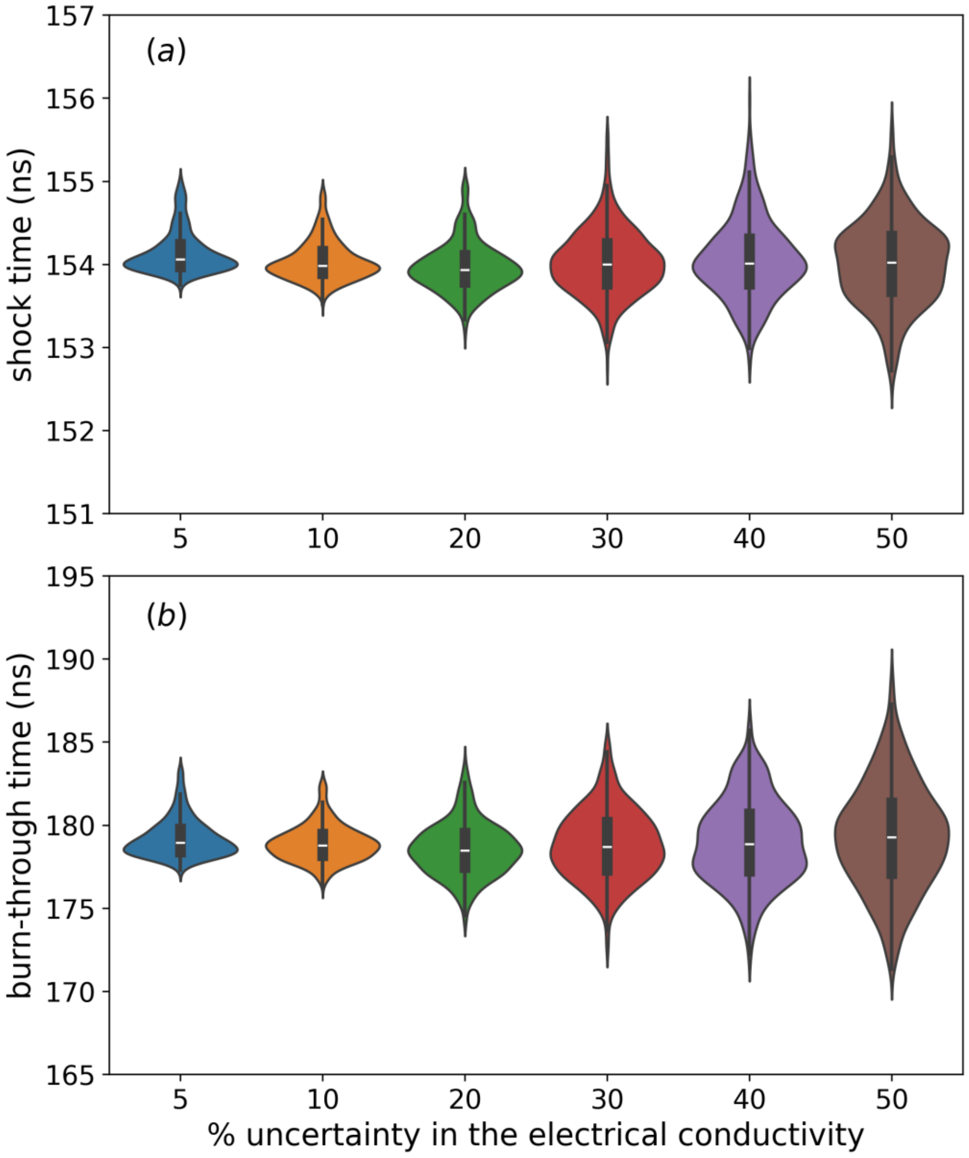


500 MHD simulation with different conductivity datasets reveal the sensitivity of the material's velocity to the conductivity.

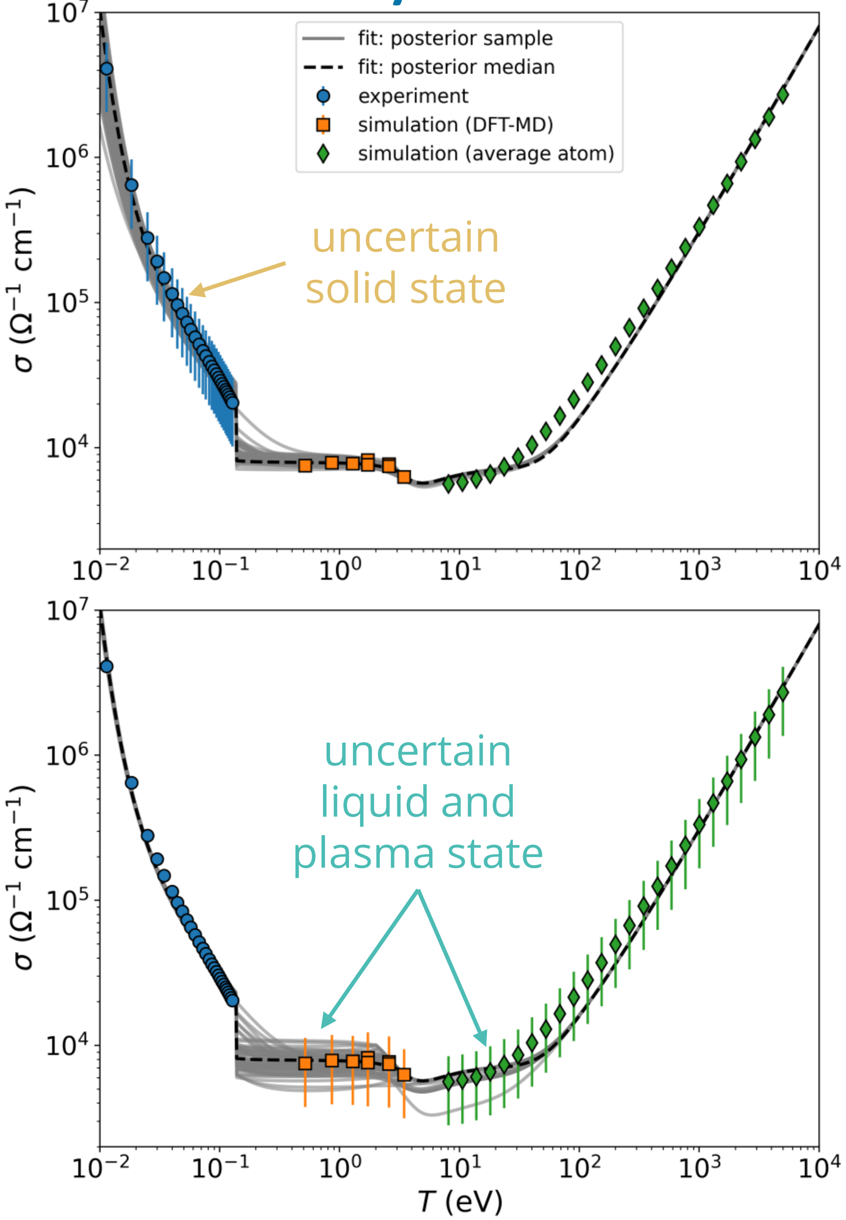
Shock and burn-through times become more uncertain with larger uncertainty in the electrical conductivity data

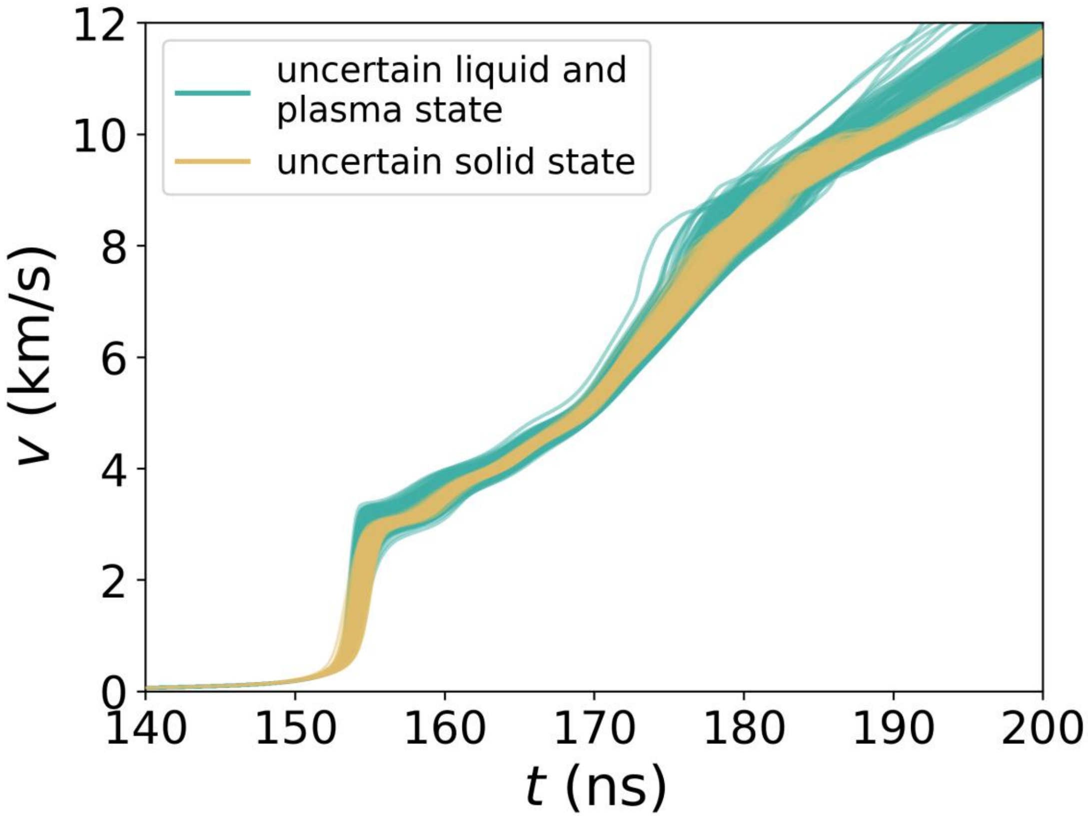


These fits assumed a 10% uncertainty on the data; varying that assumption shows the impact on the shock and burn-through times.



The Bayesian inference framework pinpoints where new conductivity data are maximally impactful





Greater uncertainty in the liquid and plasma state correspond to larger variations in the velocity of the flyer plate.

Better sampling approach: the Morris-Mitchell criterion

The Morris-Mitchell Criterion

Number of datasets you want to create for a MHD code (e.g., 10)

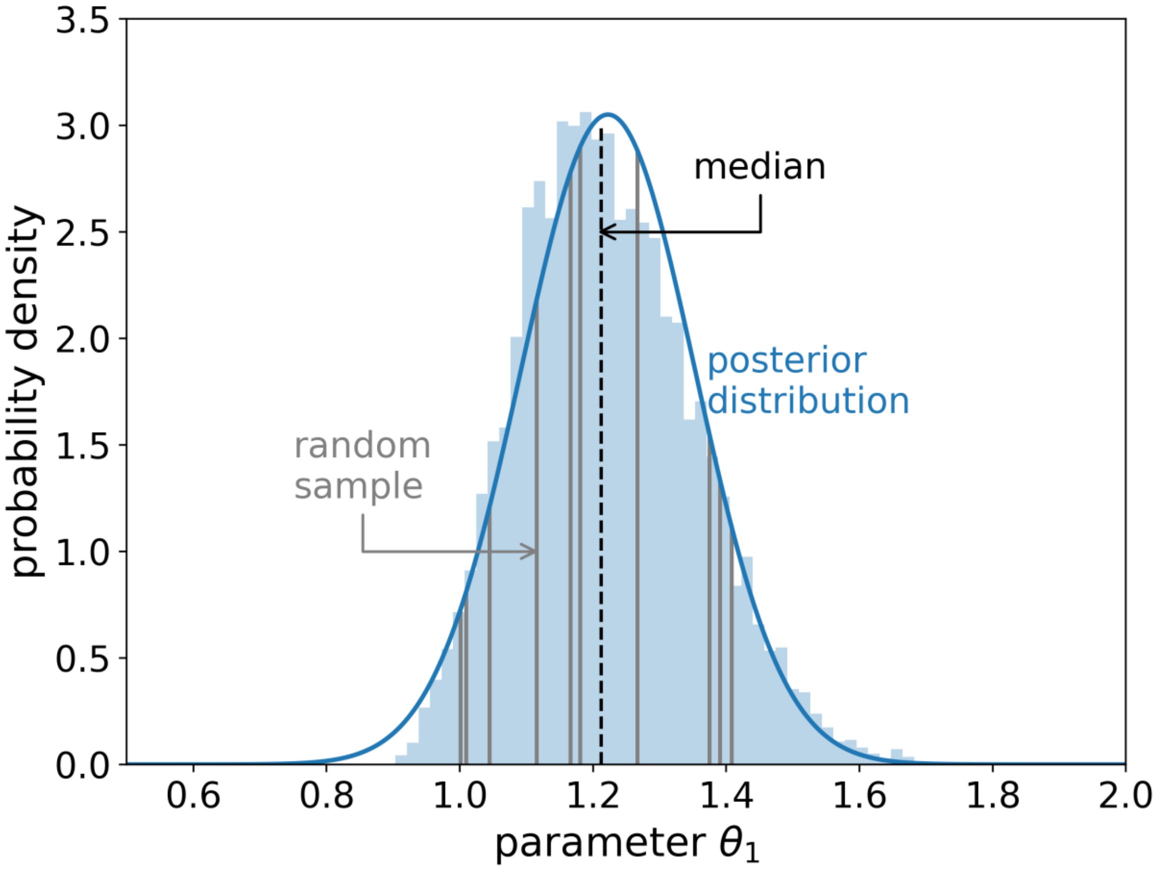
$$\phi = \left[\sum_{j=1}^{M} d(\boldsymbol{\theta}_j, \boldsymbol{\theta}_{j-1})^{-q}\right]^{1/q} \quad q \in \mathbb{Z}^+$$

Euclidean distance

$\boldsymbol{\theta}_j$ j-th set of conductivity model parameters.

$$\phi^{\text{opt}} = \min\{\phi_1, \phi_2, \cdots, \phi_k\}$$

number of datasets of size M



Reference:

- Morris, Max D., and Toby J. Mitchell. "Exploratory designs for computational experiments." *Journal of statistical planning and inference* (1995)

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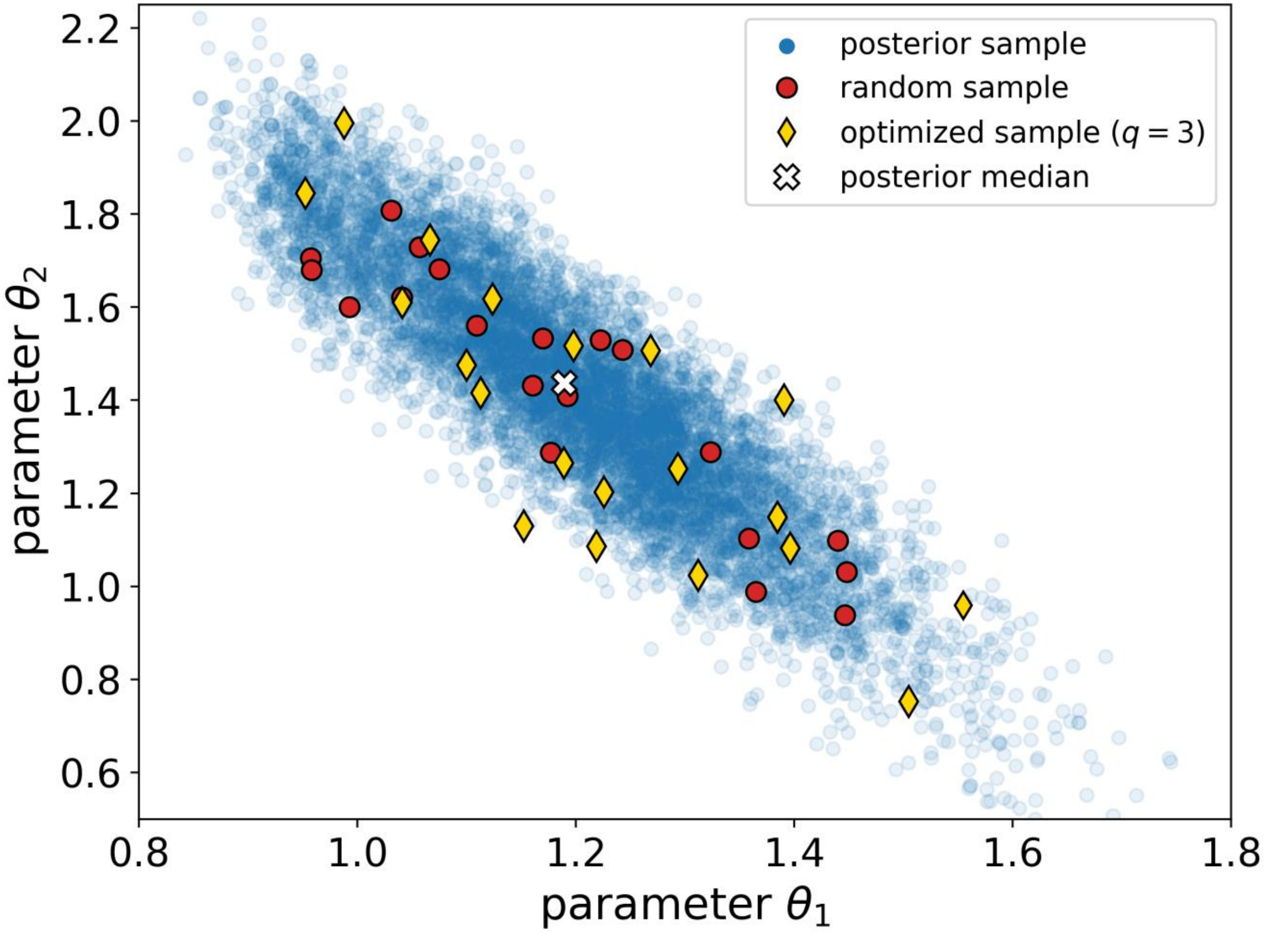
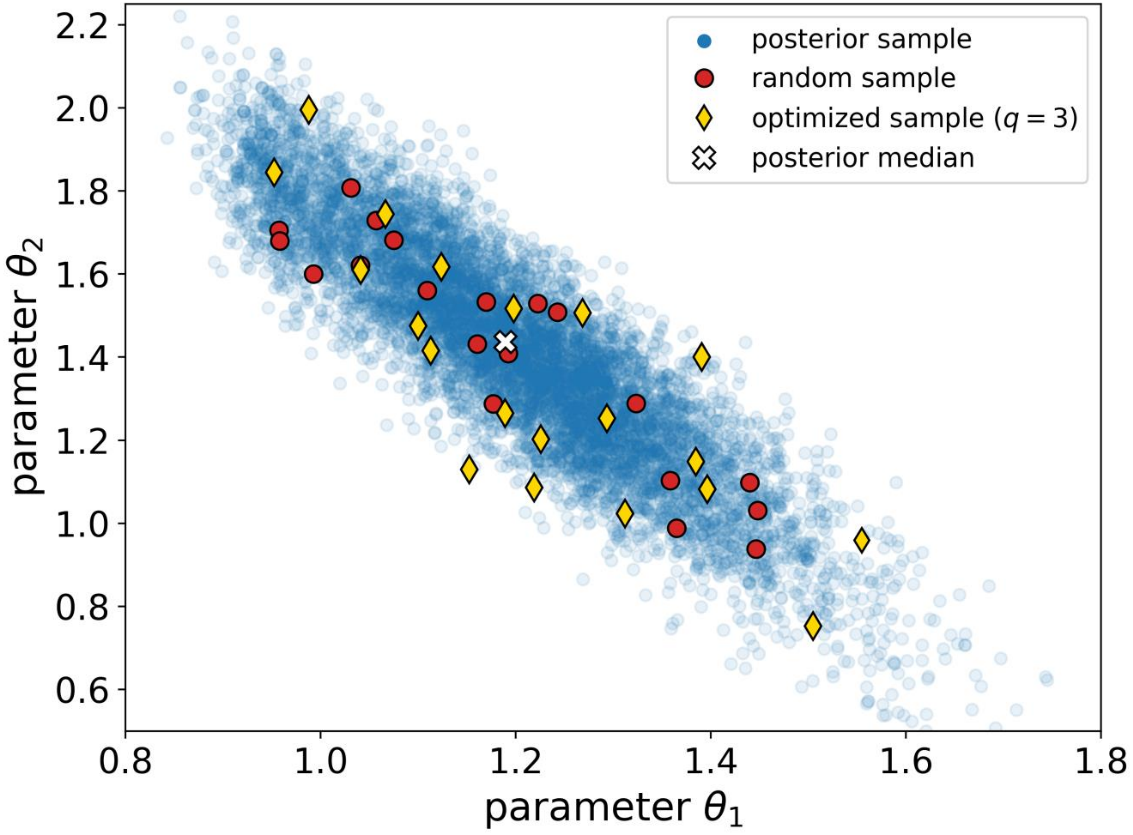
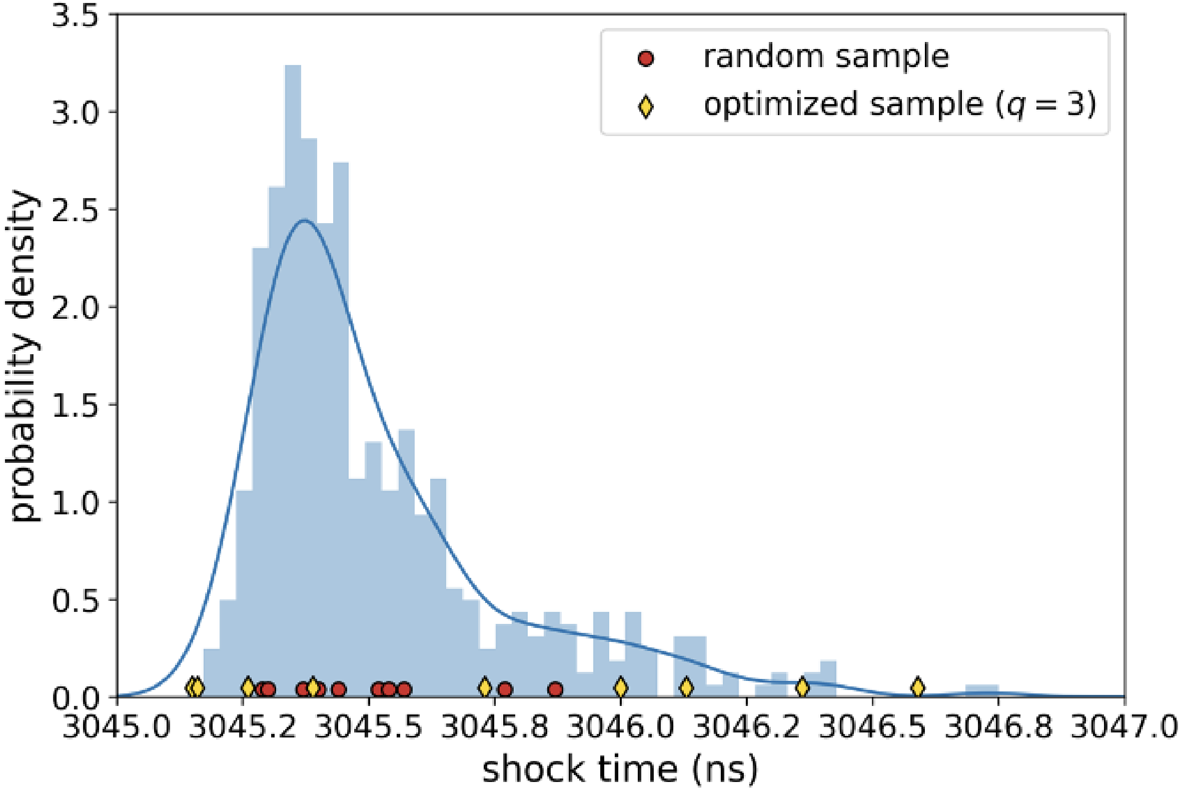


Using an improved sampling approach, the statistics of the full distribution are better approximated with a few samples



conductivity model parameters

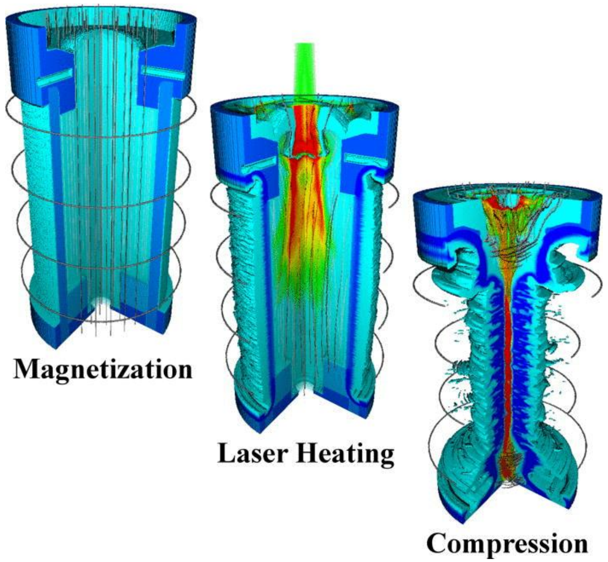


MHD shock time

Summary and Outlook

1. Bayesian inference allows for a sensitivity analysis of MHD simulations.
2. The automated framework highlights the high-impact regions to collect new data: the liquid and plasma state.
3. Transport coefficient data need to be reported with uncertainty.

Next Steps: uncertainty quantification on integrated simulations (e.g., MagLIF).



MagLIF includes:

- The elements Be, D, and T,
- magnetized transport coefficients,
- laser preheat,
- and more.