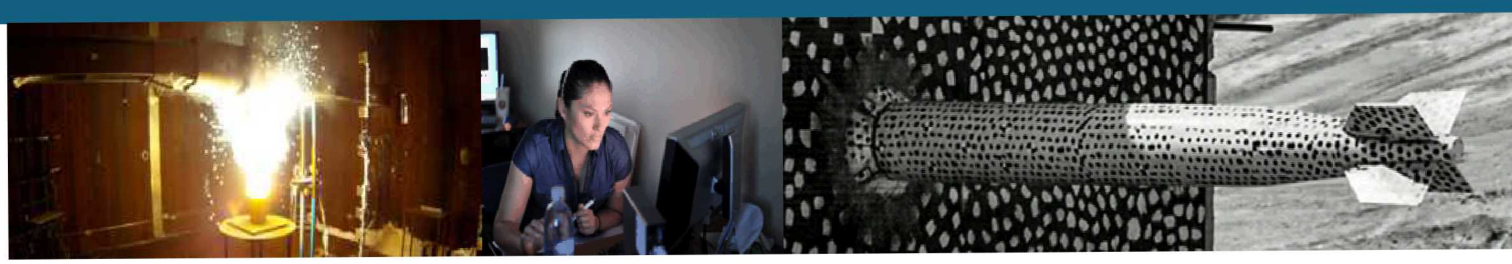
SAND2019-9498PE

$\bar{Z}$ Uncertainty Quantification for 1D Kinetic Simulations



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DOE CSGF

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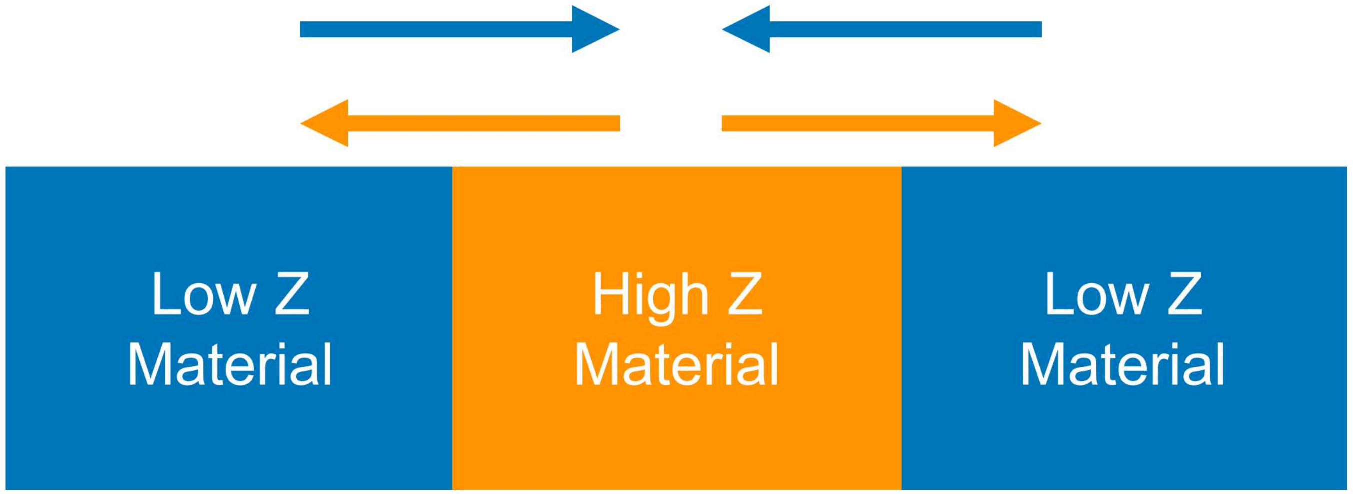
Overview

Simulations & analysis to compliment interface mixing experiments on the Z Machine

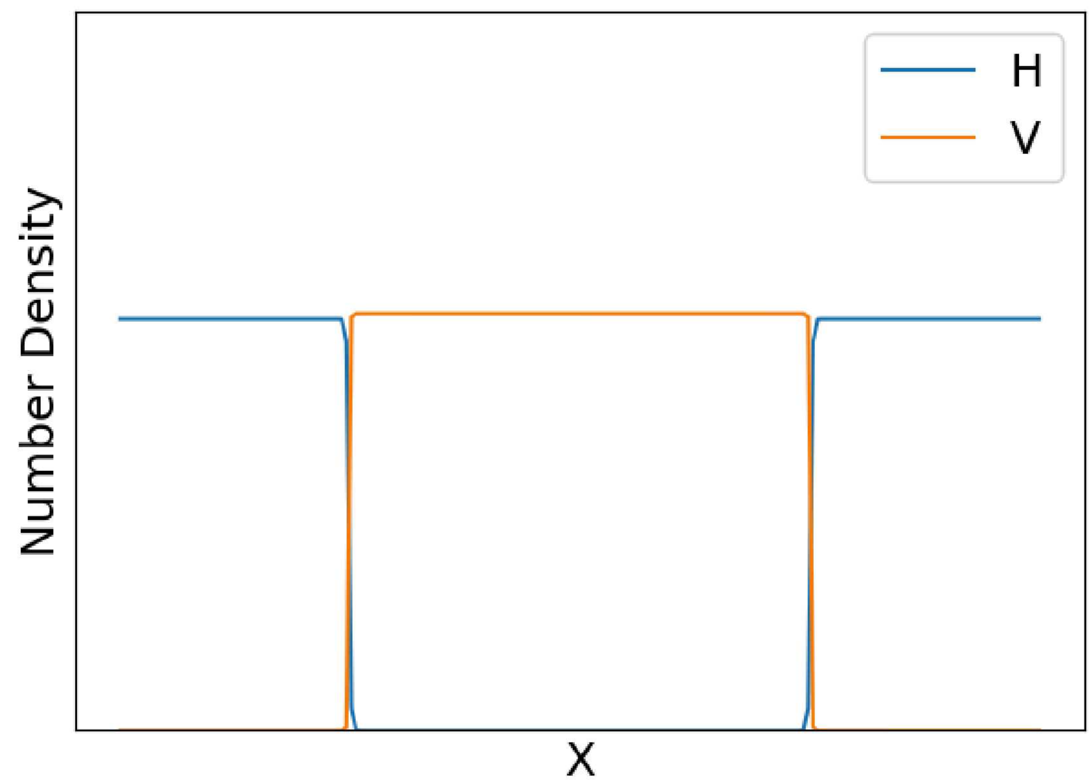
- Synthetic x-ray radiography to compare simulations to experiment
- Uncertainty quantification on $\overline{Z}$ models in 1D kinetic simulations (Haack et al. 2017b)

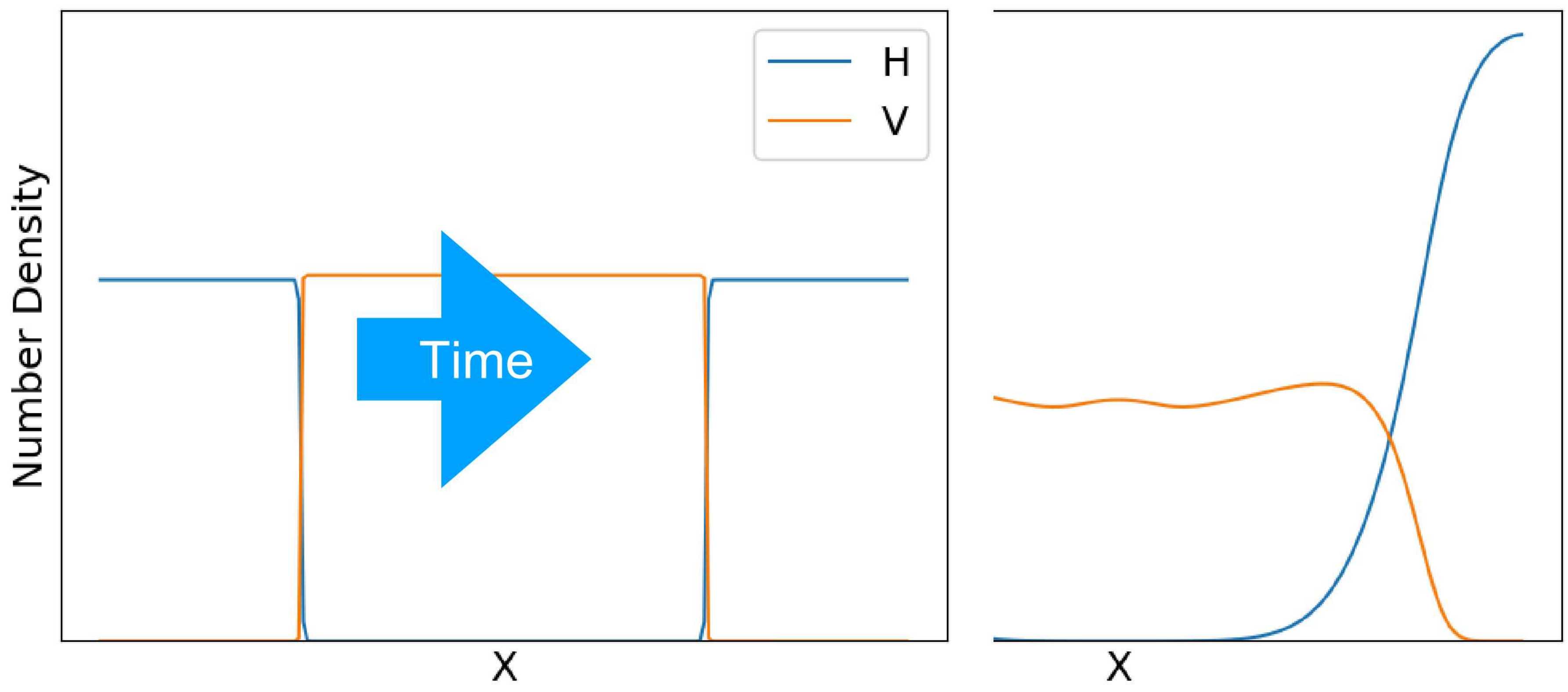
Interface Mixing

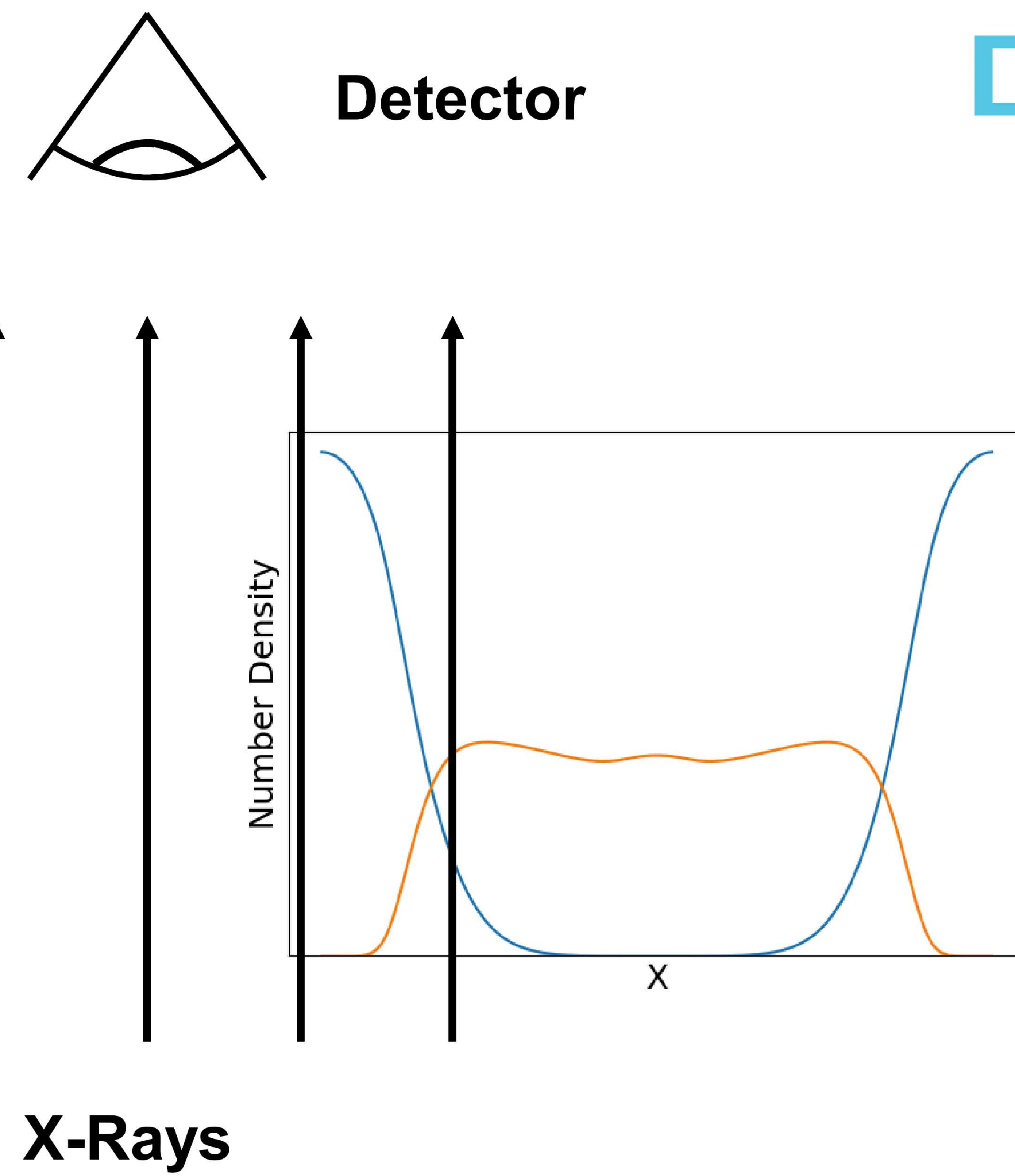


- Interface mixing decreases ICF yields
- Studies on the Z Machine with vanadium as our high-Z material, and plastic as our low

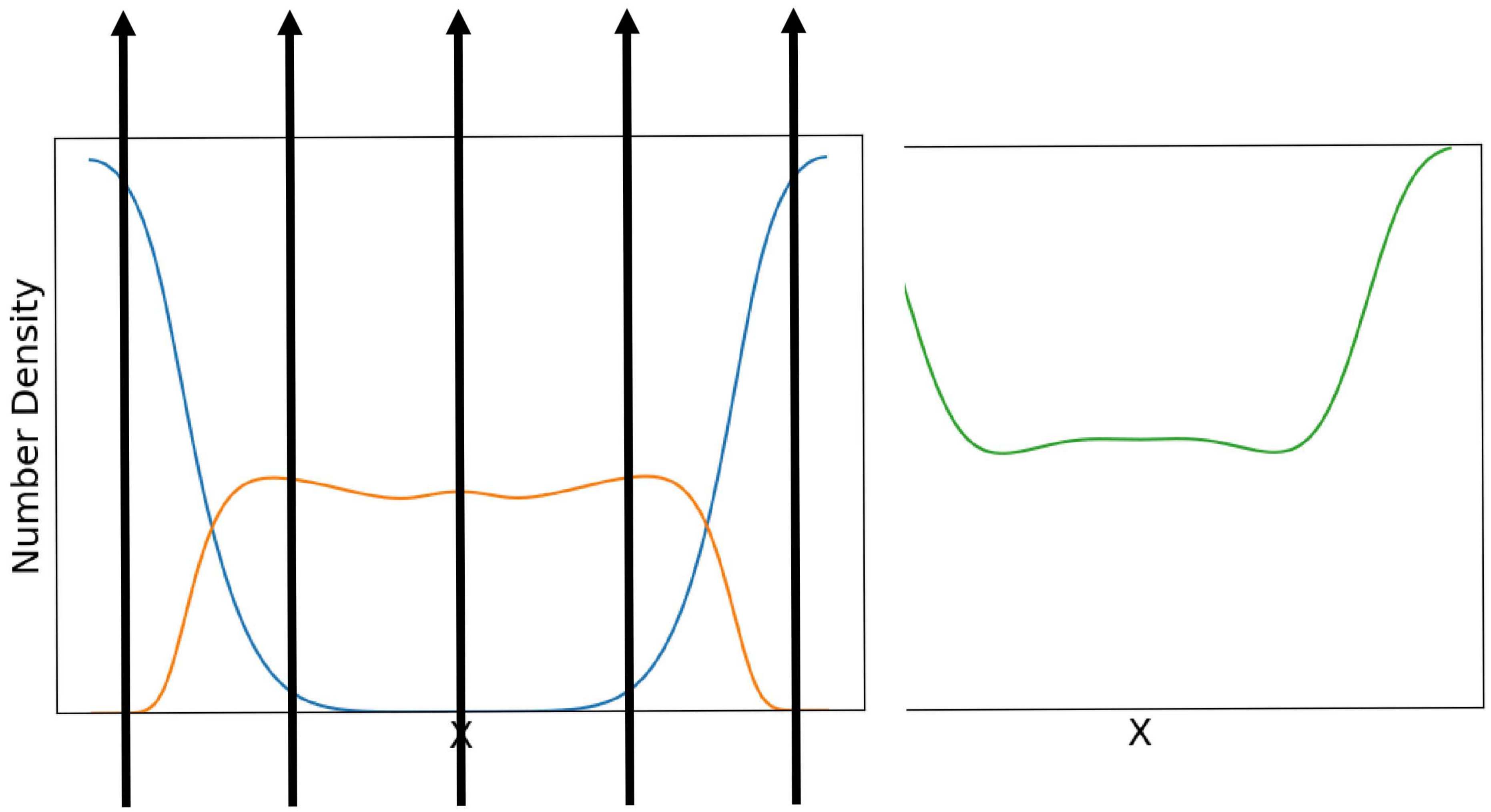
1D Kinetic Simulation

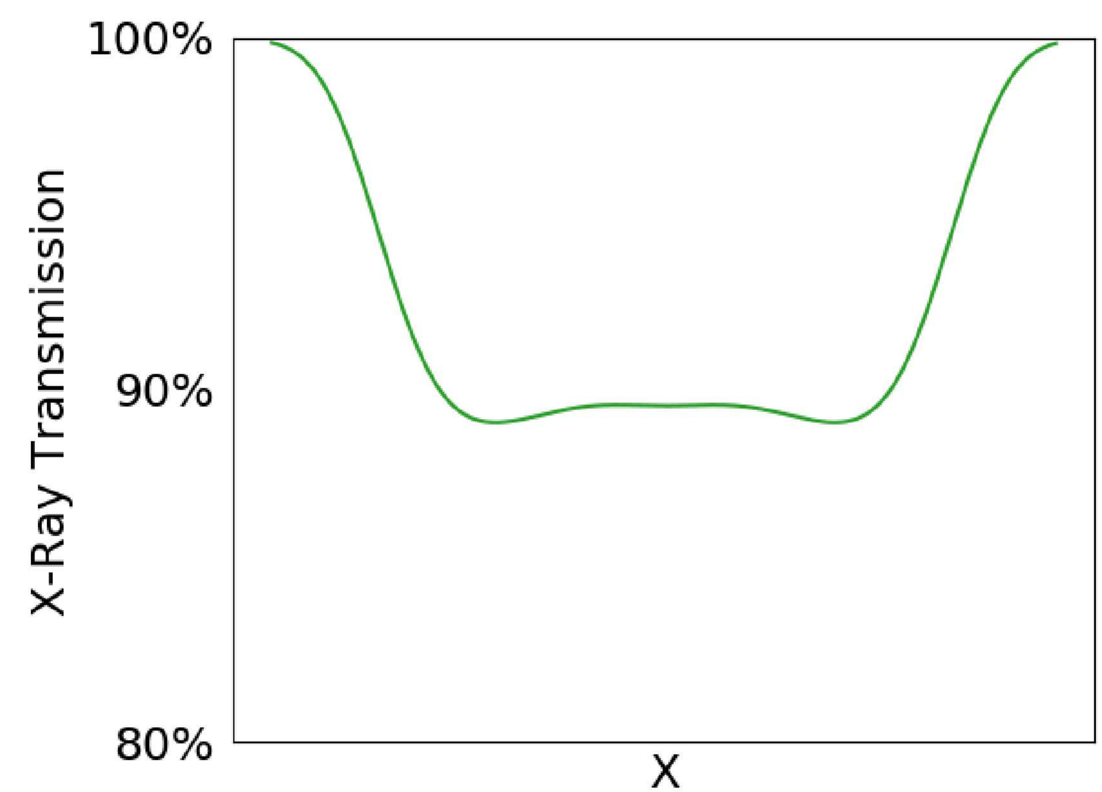


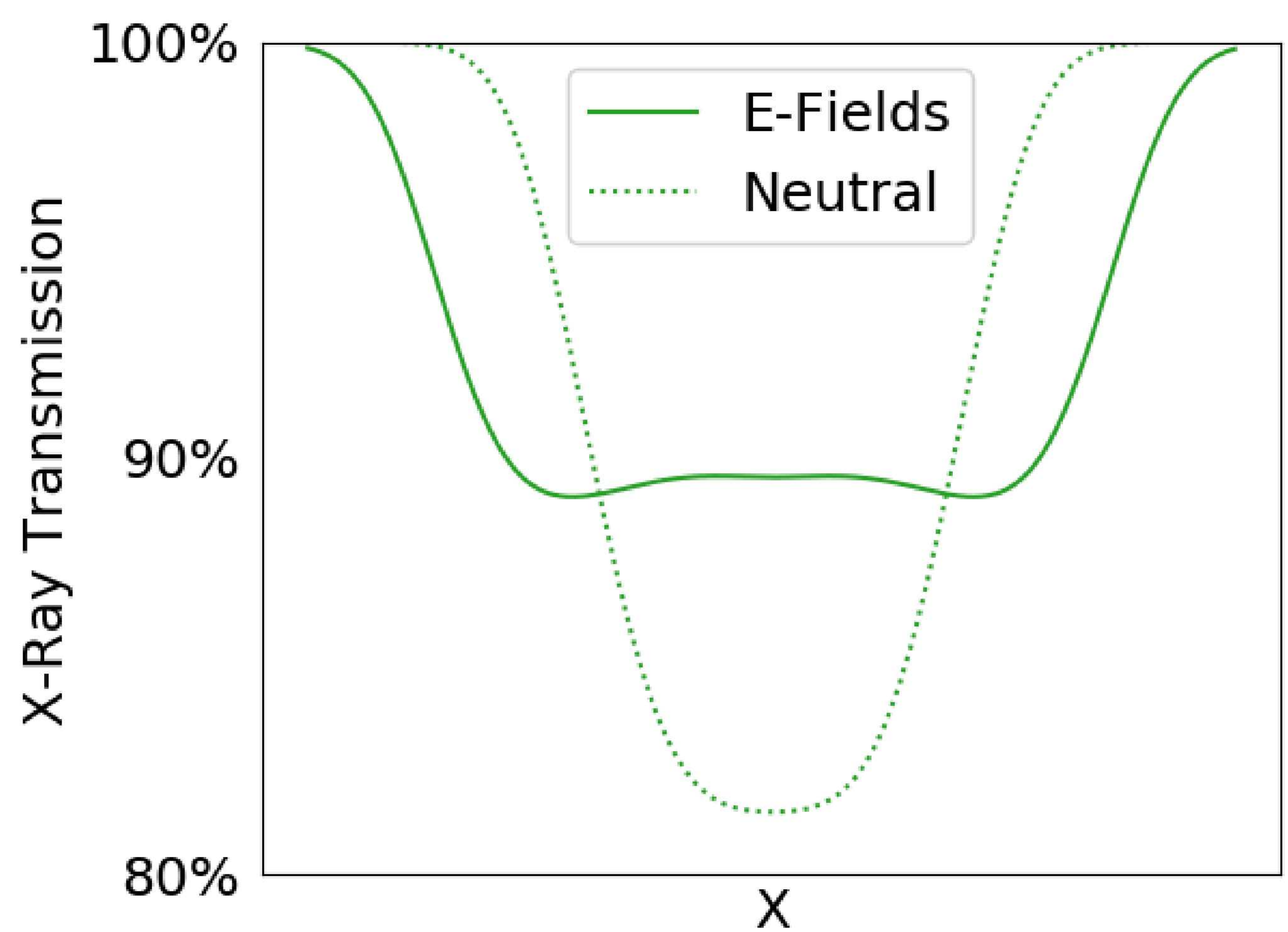

H
V
Number Density
Time
X
X


Detector
Number Density
X
X-Rays

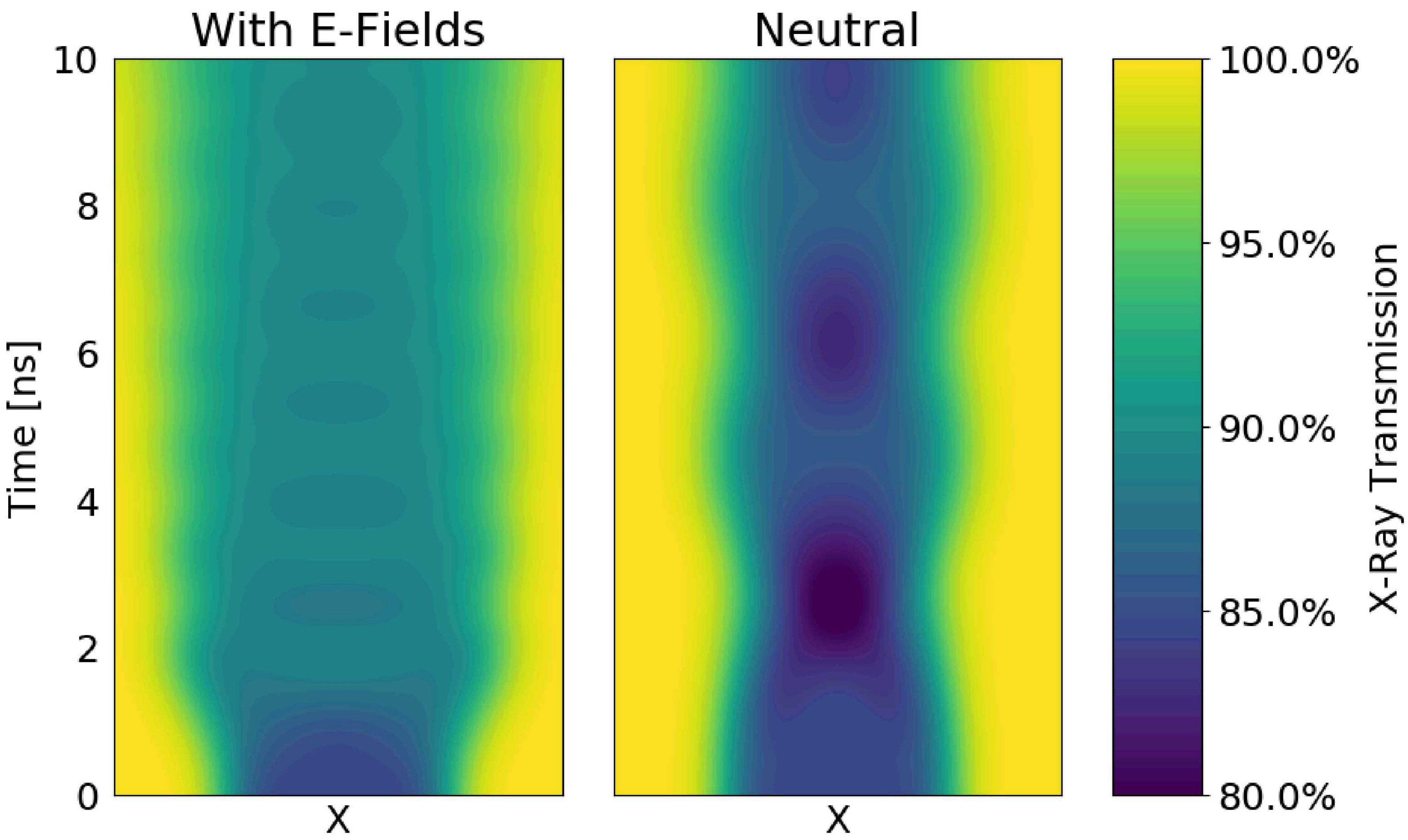
Synthetic X-Ray Radiography



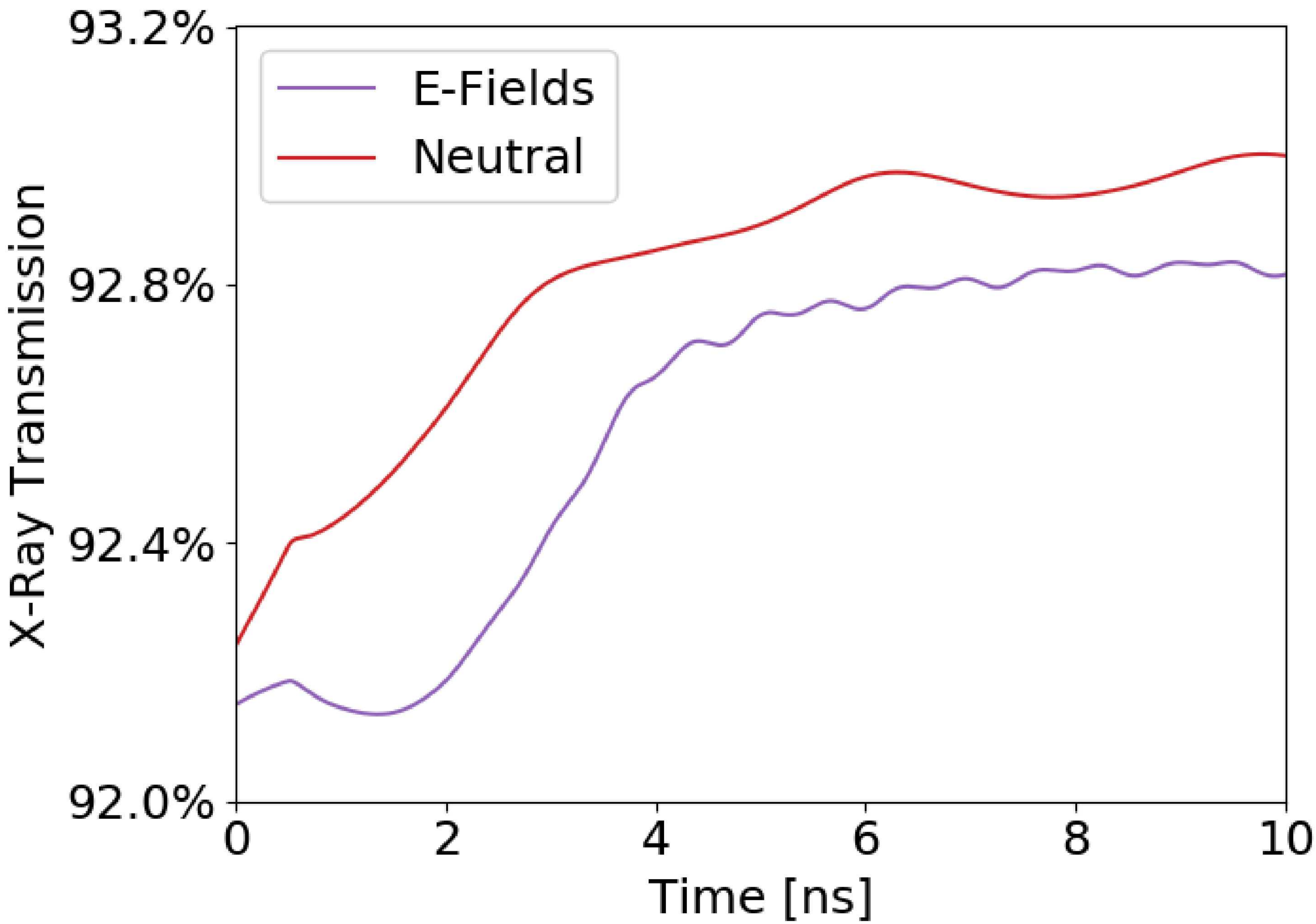

100%
90%
80%
X-Ray Transmission
X


100%
90%
80%
X-Ray Transmission
X
E-Fields
Neutral

Radiography Space-Time



Radiography Light Curves



Flexible Radiography

- Design philosophy: one analysis tool for multiple simulation types
- Works with our 2D rad-hydro sims as well
- Built on yt (yt-project.org) for uniform interface to different outputs
- Extensible to new geometries and codes

Connection to Ionization

- Showed electric fields affect simulation evolution
- These are shaped by free electrons & ions
- Free electrons & ions are created through ionization
- Our ionization model should affect sim evolution
- But by how much?
  And can we detect it? (model discrimination)
- Uncertainty quantification (UQ)

What is $\bar{Z}$?

The mean ionization state (mean charge Z) of a collection of atoms

There is no one agreed-upon definition or theoretical framework

- Average atom models (spheres of plasma around one nucleus)
  - Thomas Fermi is a simple example
  - More in Murillo et al. 2013
- Phenomenological models
  - Saha equation (balances free energy in ideal gases)
  - Lee-More-Dejarlais* (electrical conductivity)

UQ on $\bar{Z}$

- $\bar{Z}(n, T_e)$ currently a Thomas Fermi average atom model for *each* species
- Replace vanadium's model with tabulated $\bar{Z}(n, T_e)$
- Vary these tables in a sensible, known way to see impact on x-ray radiography

Table Generation

- Sandia has tools originally designed for UQ on EOS models
- These tools also support a Lee-More-Desjarlais (LMD) electrical conductivity model, from which one can back out $\bar{Z}$
- The methodology:
  - Fit LMD to some data to give us a starting set of parameters
  - Use MCMC to populate Bayesian posterior for the fit parameters
  - Generate tables by sampling the posterior

Why use Bayesian Inference

We want to fit a model to some data.

We could just optimize for the "best" fit…

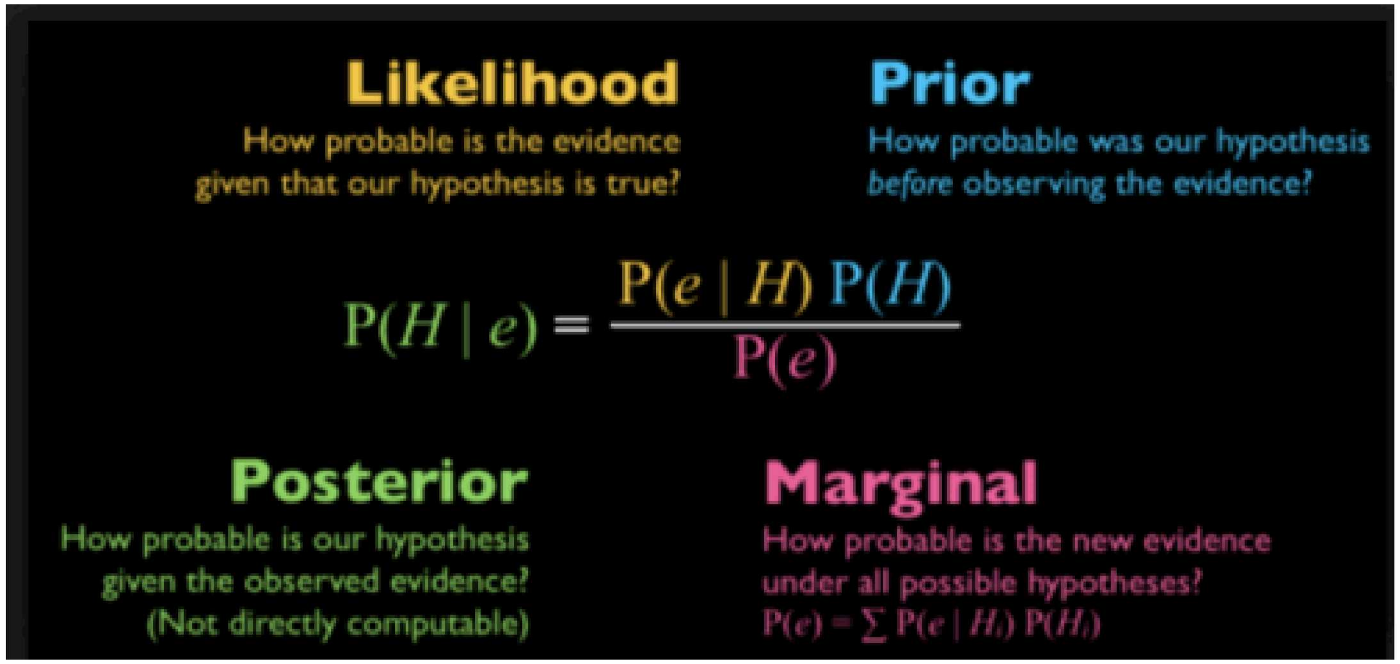
…but there's almost certainly a distribution of parameters that all provide acceptable fits, so we assign an uncertainty.

How we conceptualize this uncertainty is important.

Not using Bayes, these uncertainties might be confidence intervals.

But with a Bayesian approach, parameter uncertainties are drawn from the **parameters' probability distribution, which we can then sample.**

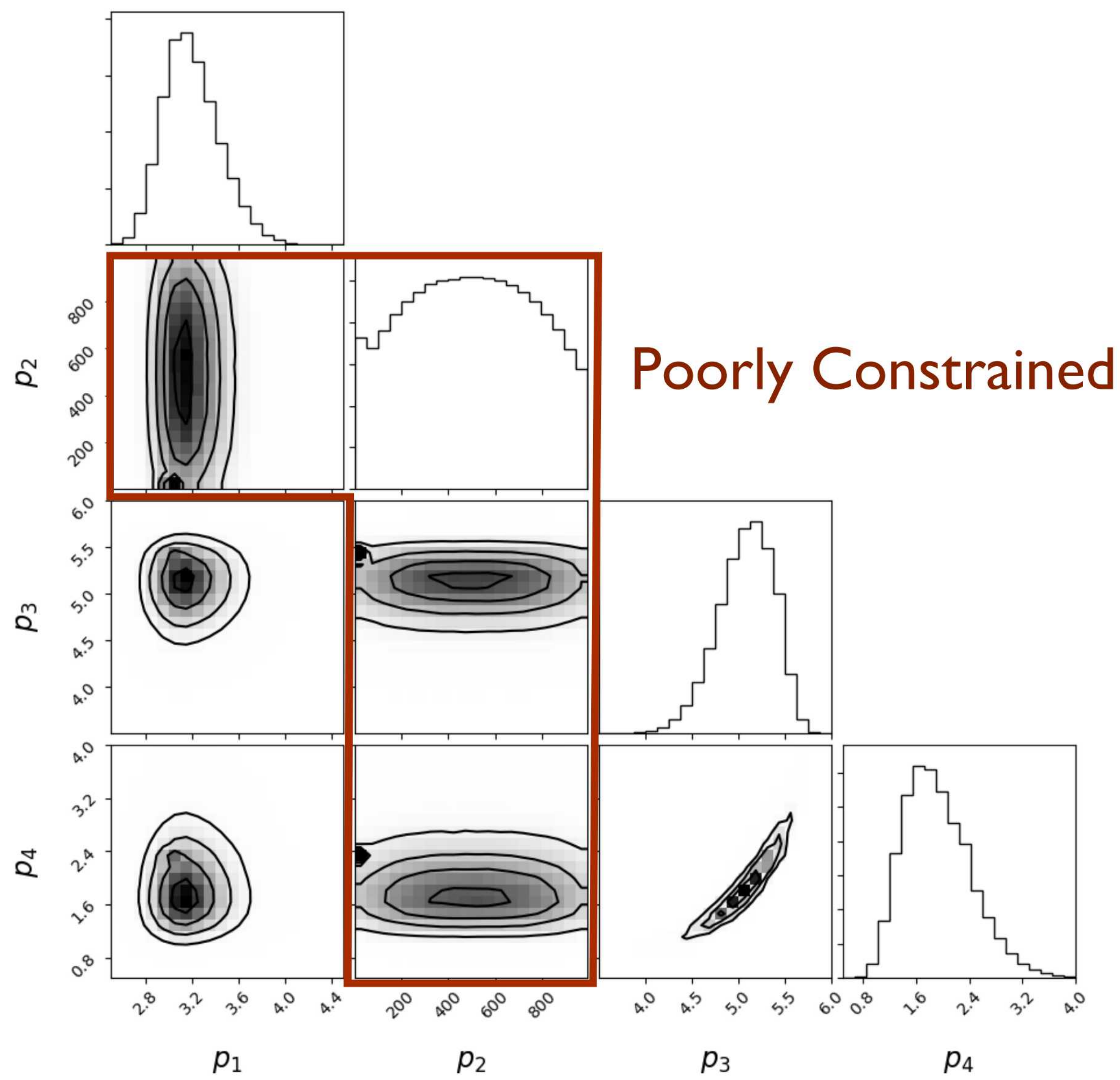
Bayes's Theorem



https://medium.com/@mark.rethana/bayesian-statistics-and-naive-bayes-classifier-33b735ad7b16

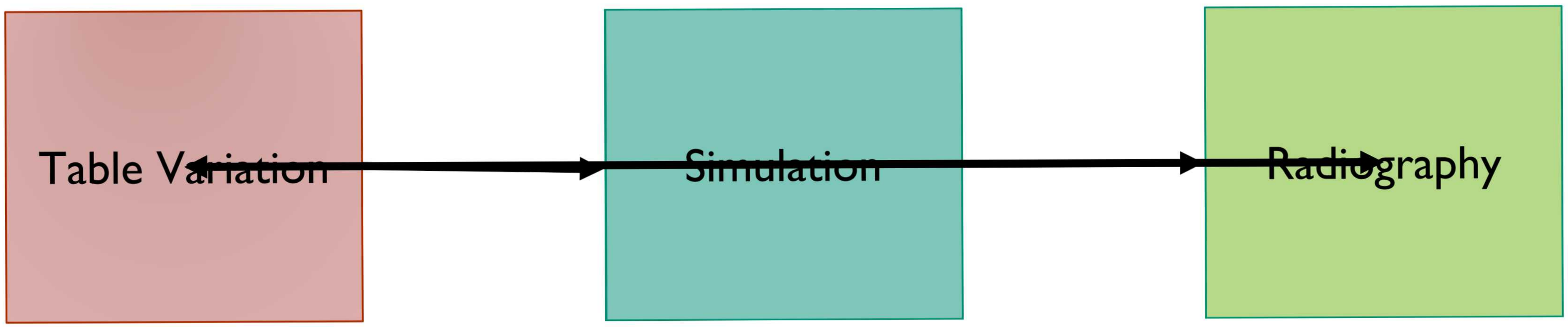
- Here, H is the LMD model with a given set of parameters.
- Priors can enforce physicality, such as bounds on parameters.
- The likelihood captures the difference between the data and the model, while also considering data uncertainties.
- The marginal is just a normalization & is practically impossible to compute, so it is often ignored in practice.
- The posterior tells us how likely H is the appropriate underlying model for the data we observe (parameter probability distribution).

More on the Posterior



- Posteriors are often high-dimensional
  - Visualized with "corner plots" like above, showing marginal & joint distributions for the model parameters
- Sample parameters from the posterior distribution as a systematic way of varying our model

Workflow



Uncertainty Quantification

Project Status

- As you might have guessed, the synthetic radiography is working
- 1D kinetic code has been modified to support $\bar{Z}$ tables alongside TF
- Currently fitting LMD & populating posterior
- Simulations will be run after I leave
- Then, paper(s)!

Other Applications

- Radiography tools can be used to assess various questions of model discrimination
  - Current synthetic radiography for Z Machine modeling is slow (too much detail) and GUI-based
  - My tools are also designed to work with multiple simulation types
  - *Caveat:*
    yt's current support for un- and semi-structured is minimal, limiting the flexibility of the radiography (i.e., can't do off-axis ray tracing)
- UQ workflow not restricted to $\bar{Z}$ from LMD or even $\bar{Z}$ at all