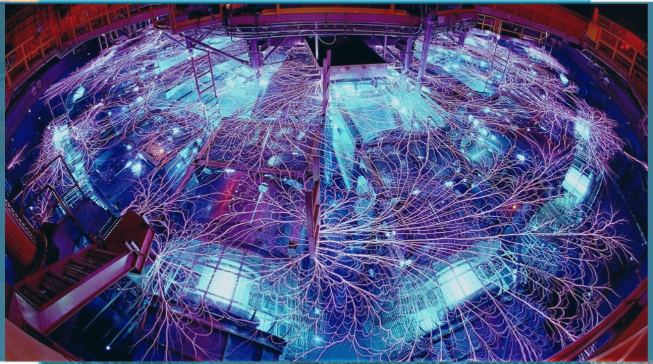
Modern Data Science & Extreme Physics: Making more of our data on the Z Machine & Beyond



Patrick F. Knapp

Sept 15, 2022

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SAND2022-12534 PE

I am representing a large group of talented individuals

W.E. Lewis, *M.E. Glinsky, M. A. Schaeuble, J.R. Fein, C. A. Jennings, E. C. Harding, S. B. Hansen, T. Nagayama, A. J. Harvey-Thompson, C. Tyler, M. R. Gomez, M. R. Weis, **P. F. Schmit, D. E. Ruiz, D. J. Ampleford, M. Geissel, M. Mangan, G.A. Chandler, G. Cooper, J.L. Brown, K. Blaha , S. Fields, S. A. Slutz, I.C. Smith, T. J. Awe, K. Beckwith, D. B. Sinars, M. Jones, G. A. Rochau, K. J. Peterson, T.R. Mattsson

R.G. Patel (1441), B.T. Klein (5681), K.A. Maupin (1463), A. Tran (1441), T. Moore (6754), E. Cyr (1442),

[1]V.R. Joseph, [1]C.F.J. Wu, [2]J. Gunning, [3]G. Vasey, B. [3]O’Shea, [4]M. Evans, [5]Shailaja Humane

[1]School of Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, GA
[2]CSIRO, Petroleum, Clayton, Victoria, Australia
[3]Department of Computational Mathematics, Science, and Engineering, East Lansing, MI
[4]Department of Physics and Astronomy, University of Rochester, Rochester, NY
[5]Nuclear Engineering & Radiological Sciences Department, University of Michigan, Ann Arbor, MI
*current location, BNZ Energy Inc., Santa Fe NM
**current location, Lawrence Livermore National Laboratory, Livermore CA

LABORATORY DIRECTED
RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

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[1]V.R

Our team is growing!
Center 1600’s first Maxwell fellow, Luke Stanek, will be participating
Multiple post-docs are also on the way
We are actively recruiting and seeking collaborations

Department of Physics and Astronomy, University of Rochester, Rochester, NY

[5]Nuclear Engineering & Radiological Sciences Department, University of Michigan, Ann Arbor, MI

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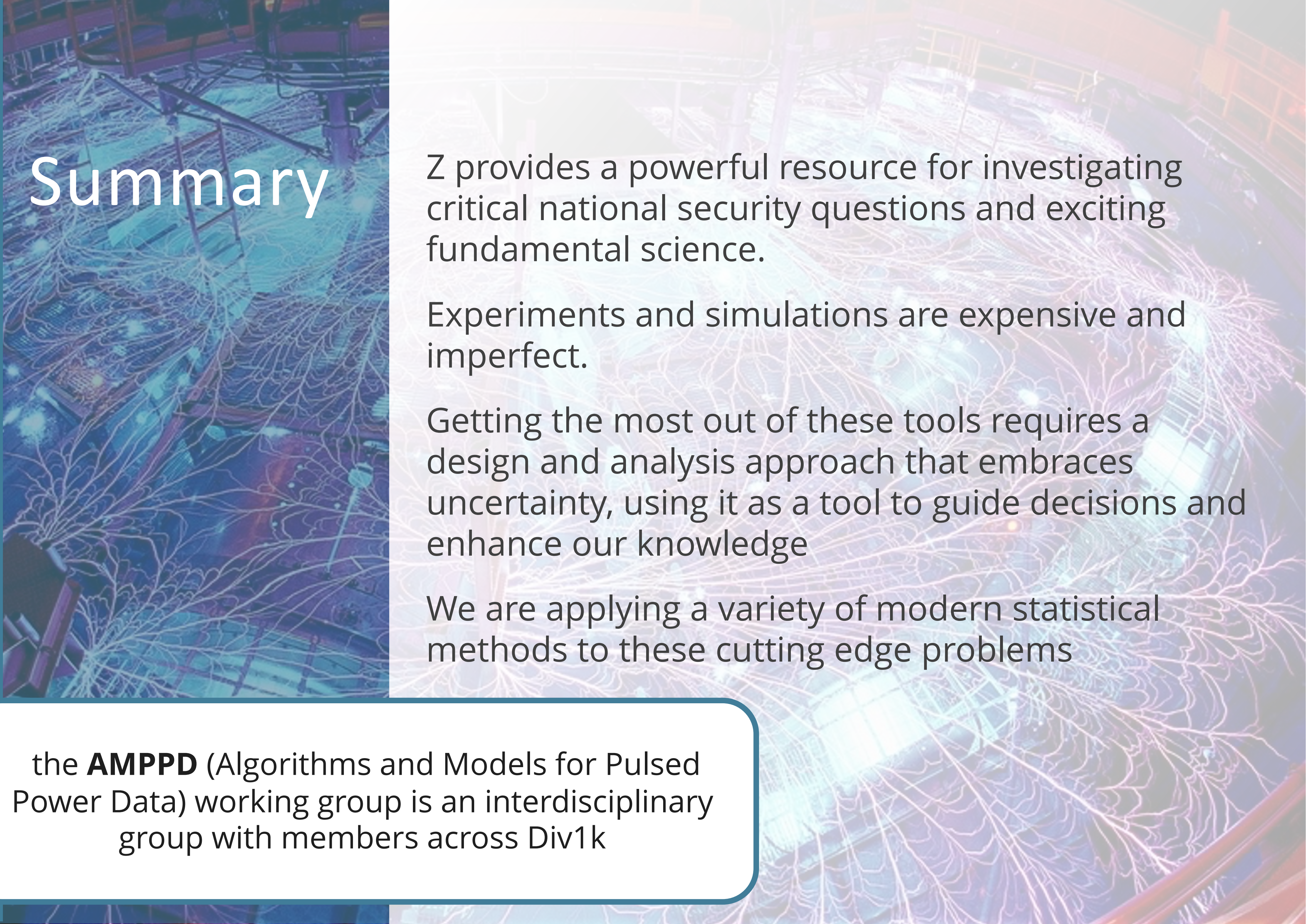


Summary

Z provides a powerful resource for investigating critical national security questions and exciting fundamental science.

Experiments and simulations are expensive and imperfect.

Getting the most out of these tools requires a design and analysis approach that embraces uncertainty, using it as a tool to guide decisions and enhance our knowledge

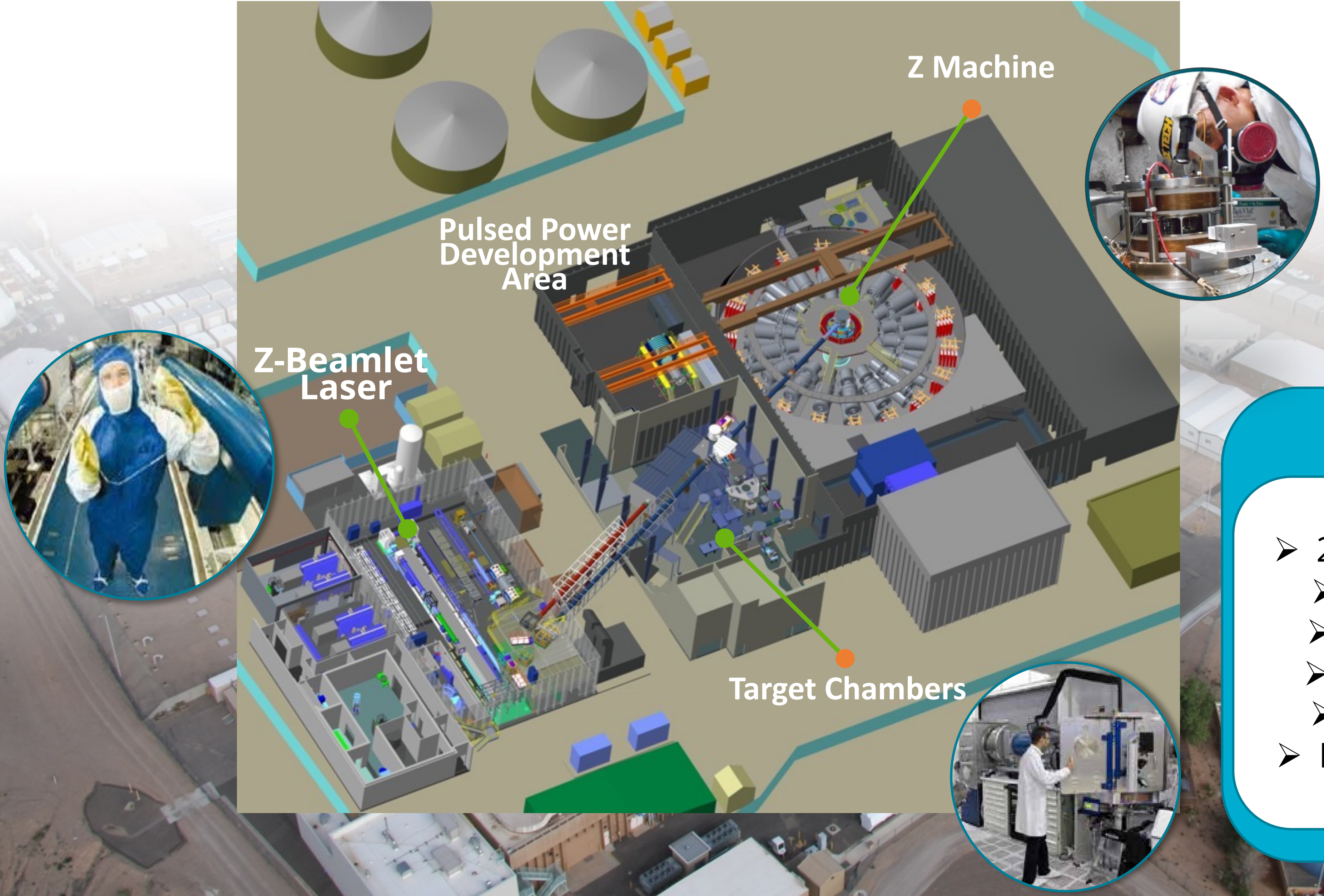
We are applying a variety of modern statistical methods to these cutting edge problems

the **AMPPD** (Algorithms and Models for Pulsed Power Data) working group is an interdisciplinary group with members across Div1k

Sandia's Z Pulsed Power Facility

The Earth's largest pulsed power machine

Sandia’s Z Pulsed Power Facility



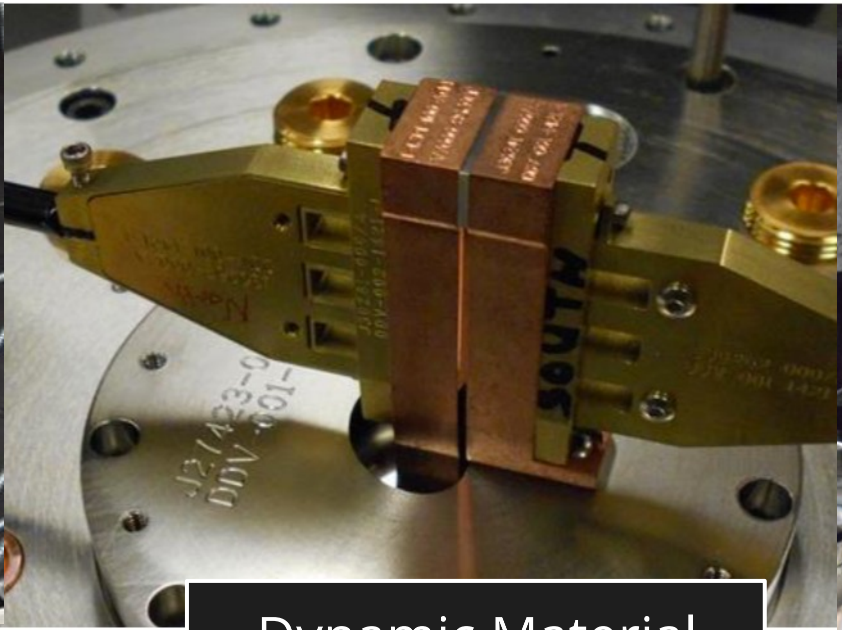
Capabilities

- ➢ 20 MA peak current
- ➢ 4 kJ, 1 TW laser
- ➢ 2 MJ’s soft x-ray
- ➢ kJ’s warm x-rays
- ➢ kJ’s fusion yield
- ➢ Mbar’s planar drive

Precision tools for high energy density science

Radiation Science

- Weapon survivability
- Laboratory Astrophysics



Dynamic Material Properties

- Pu aging and manufacturing
- Planetary science

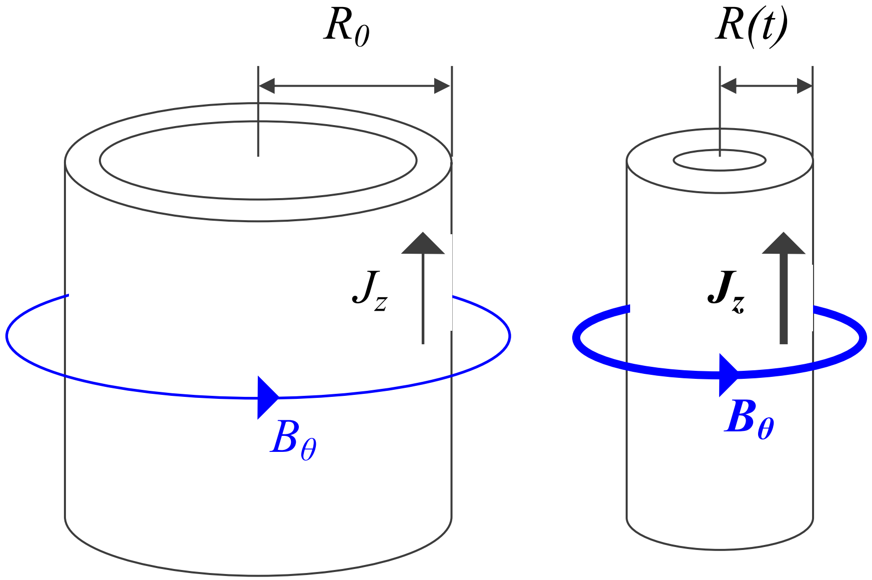
Inertial Confinement Fusion

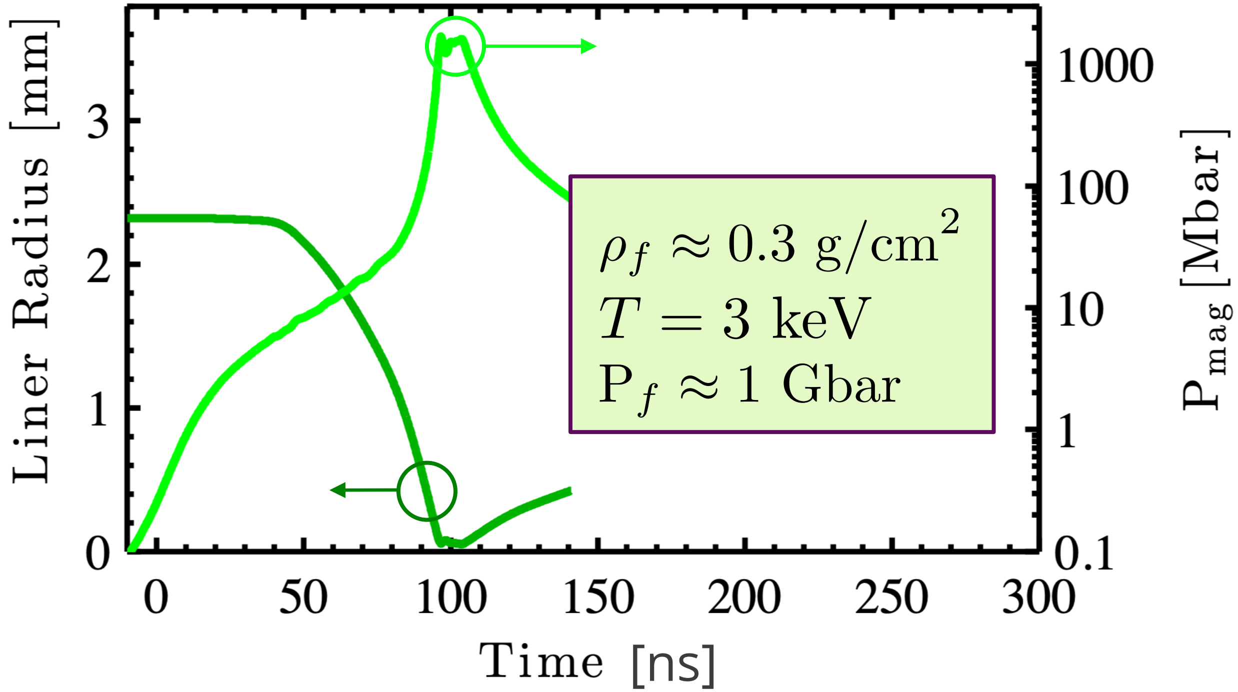
- Thermonuclear burn for NEP physics
- Basic fusion research

Magnetically-Driven Cylindrical Implosions are Efficient: Implosion Drive Pressure is Divergent!

$$P = \frac{B^2}{2\mu_o} = 140 \cdot \left(\frac{I_{[\mathrm{MA}]}/30}{R(t)_{[\mathrm{mm}]}} \right)^2 \quad [\mathrm{Mbar}]$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = \frac{\mathbf{J}\times\mathbf{B}}{c} - \nabla P$$





By varying the magnetic pressure pulse shape, liner dimensions, and duration of drive, Z can access a wide variety of end states

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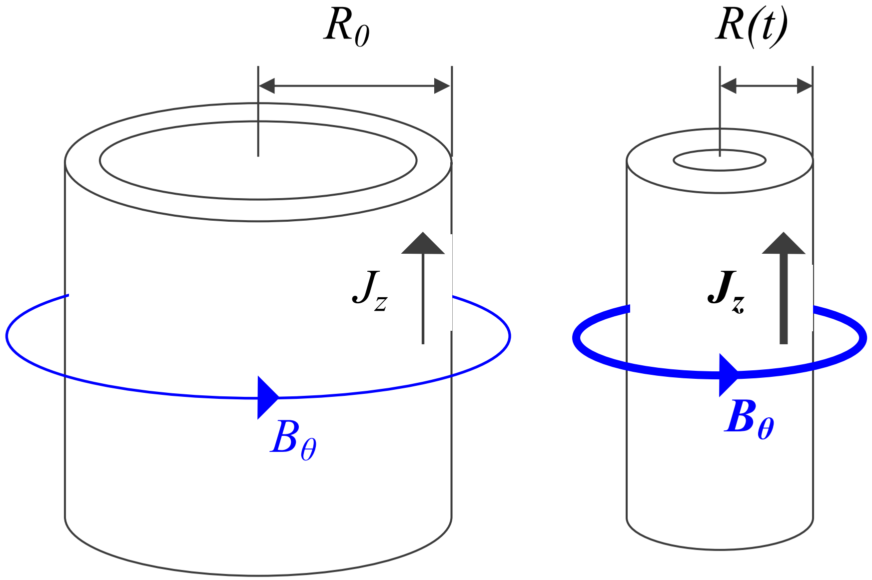

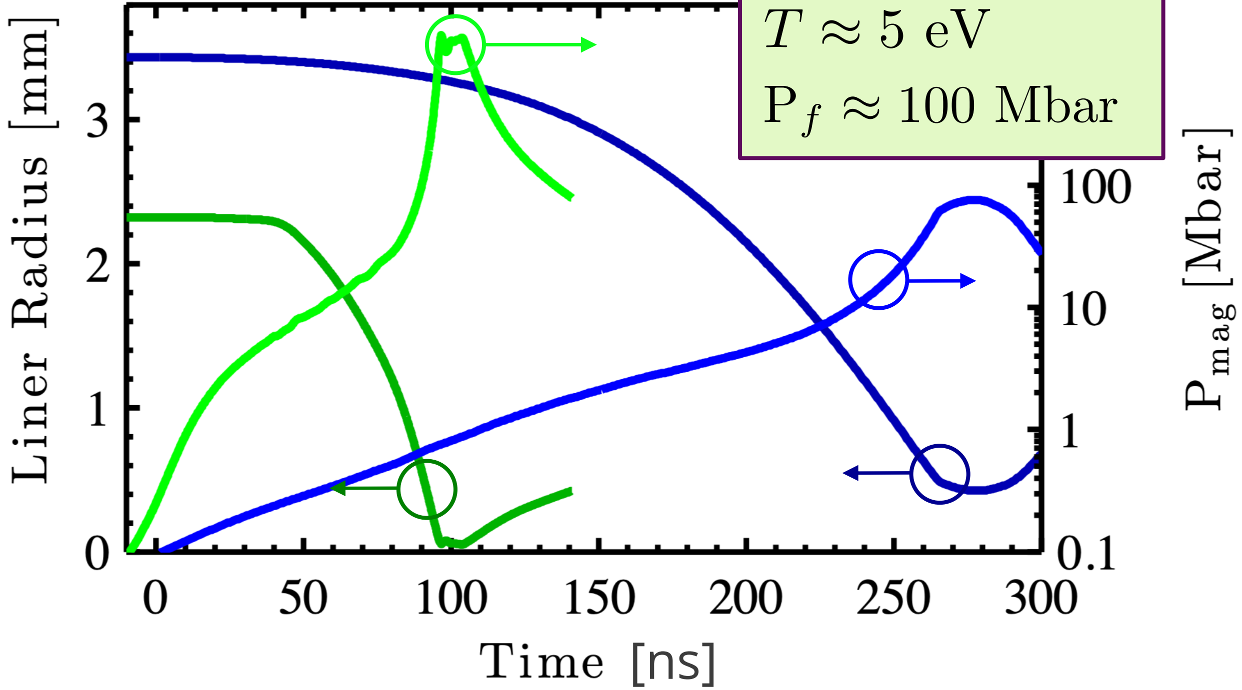

$\rho_f \approx 10\ \mathrm{g/cm}^2$
$T \approx 5\ \mathrm{eV}$
$\mathrm{P}_f \approx 100\ \mathrm{Mbar}$

By varying the magnetic pressure pulse shape, liner dimensions, and duration of drive, Z can access a wide variety of end states

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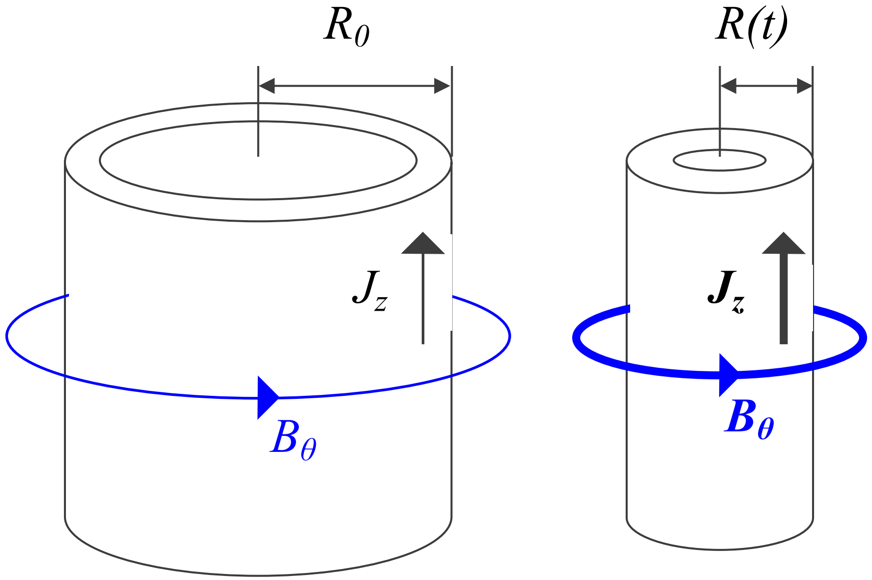
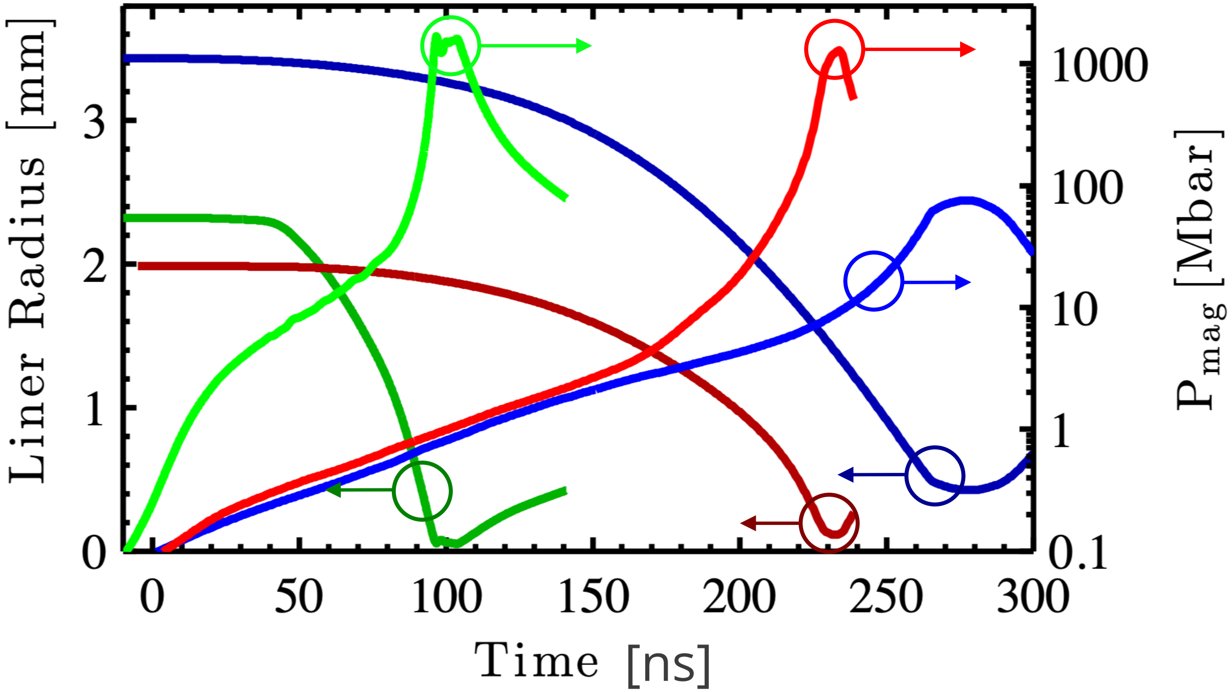
$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = \frac{\mathbf{J}\times\mathbf{B}}{c} - \nabla P$$

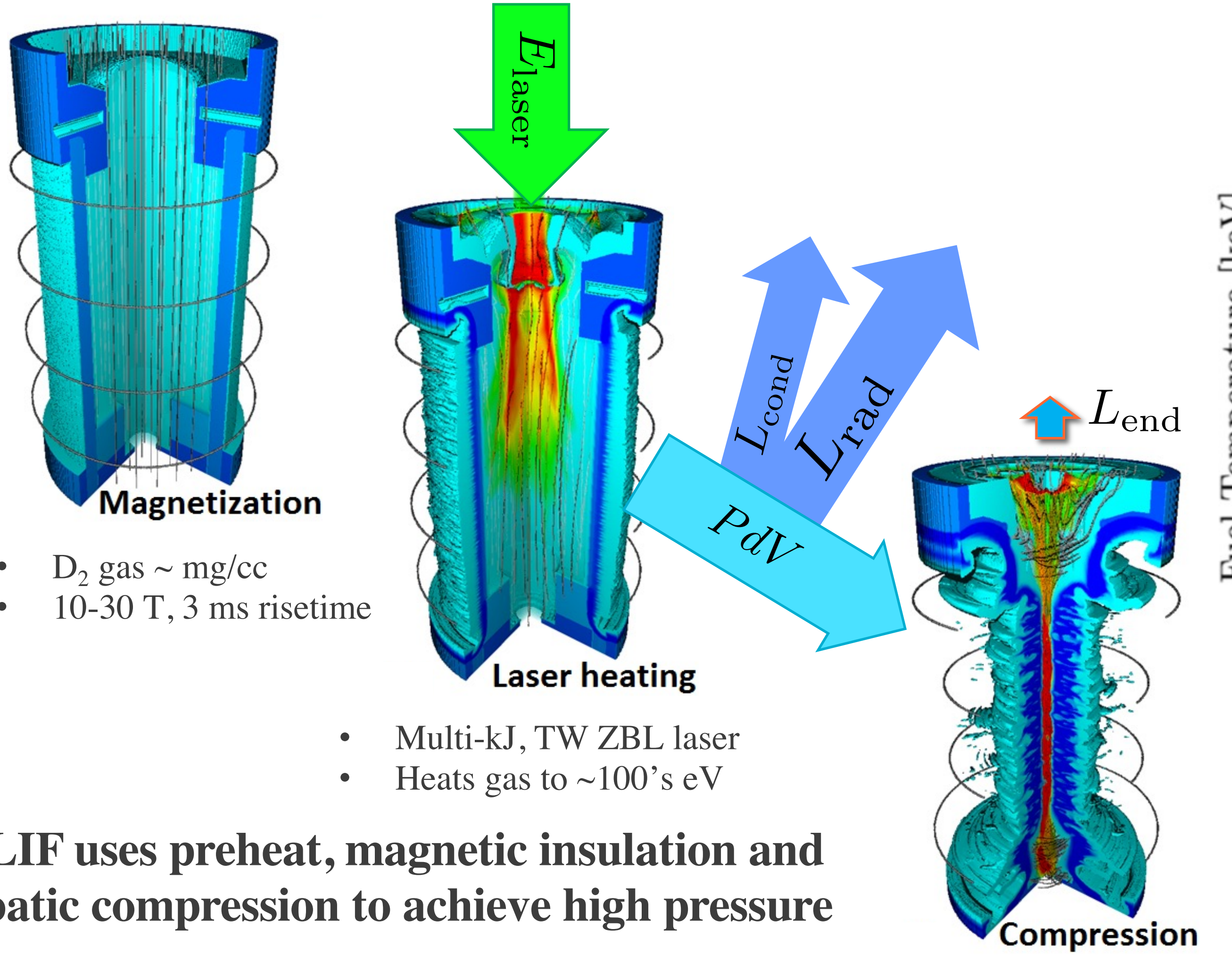
$\rho_f \approx 60\ \mathrm{g/cm^2}$
$T \approx 10\ \mathrm{eV}$
$\mathrm{P}_f \approx 2\ \mathrm{Gbar}$





By varying the magnetic pressure pulse shape, liner dimensions, and duration of drive, Z can access a wide variety of end states

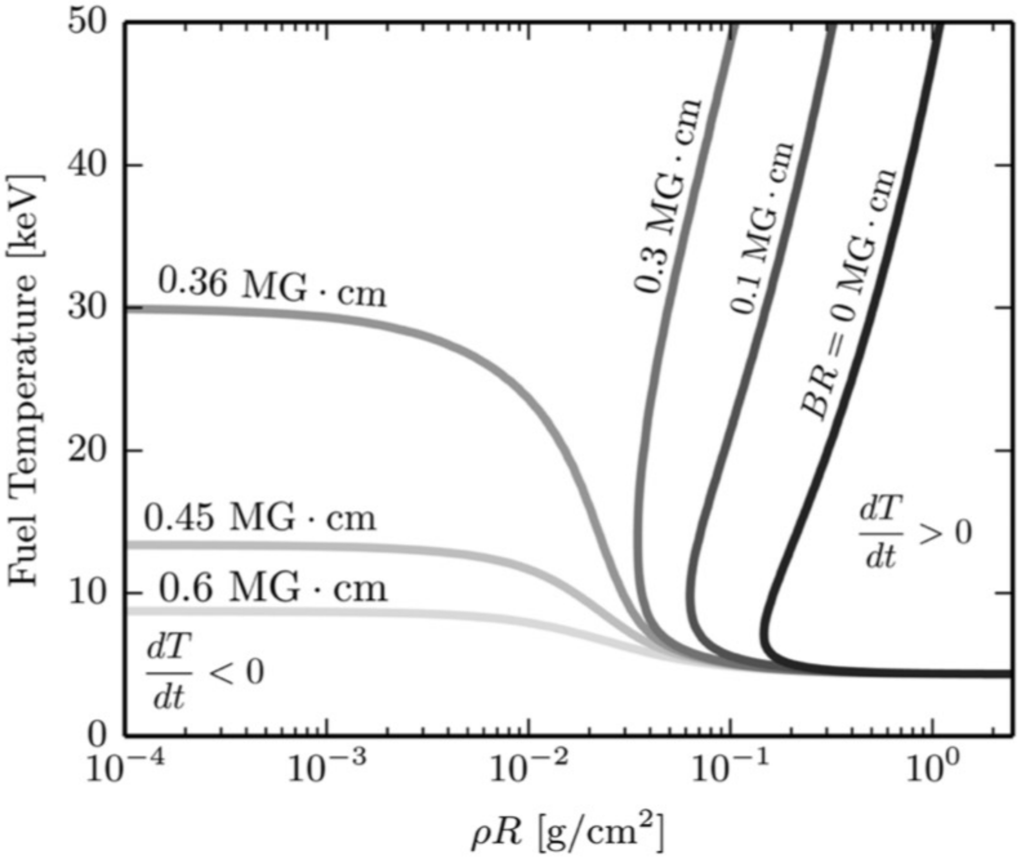
We are studying magnetic direct drive as a route to high fusion yield in the laboratory



- D_2 gas ~ mg/cc
- 10-30 T, 3 ms risetime

- Multi-kJ, TW ZBL laser
- Heats gas to ~100’s eV

MagLIF uses preheat, magnetic insulation and adiabatic compression to achieve high pressure



Slutz et al., Phys. Plasmas 17, 056303 (2010), S. A. Slutz. and R.A. Vesey, PRL **108**, 025003 (2012)

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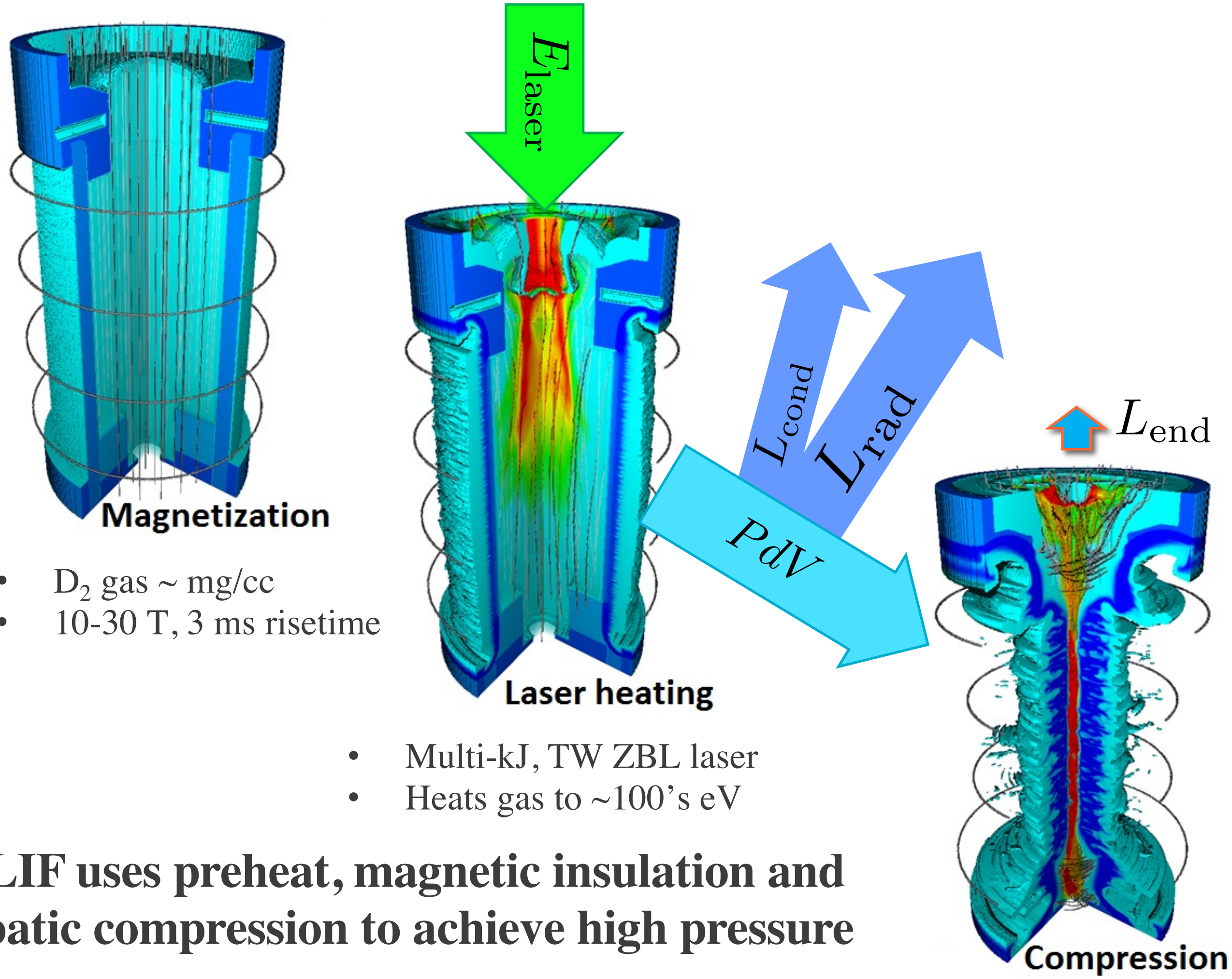

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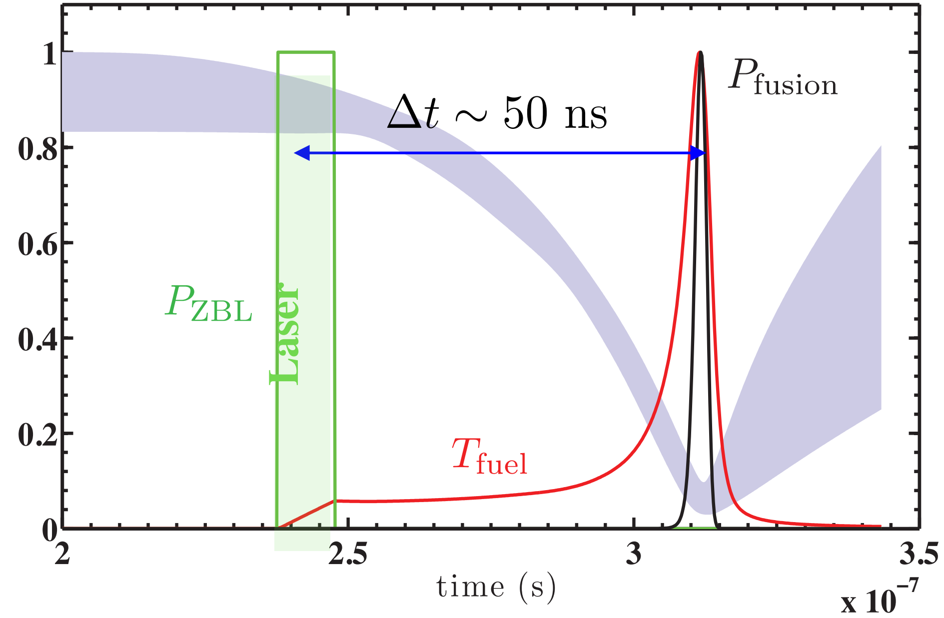
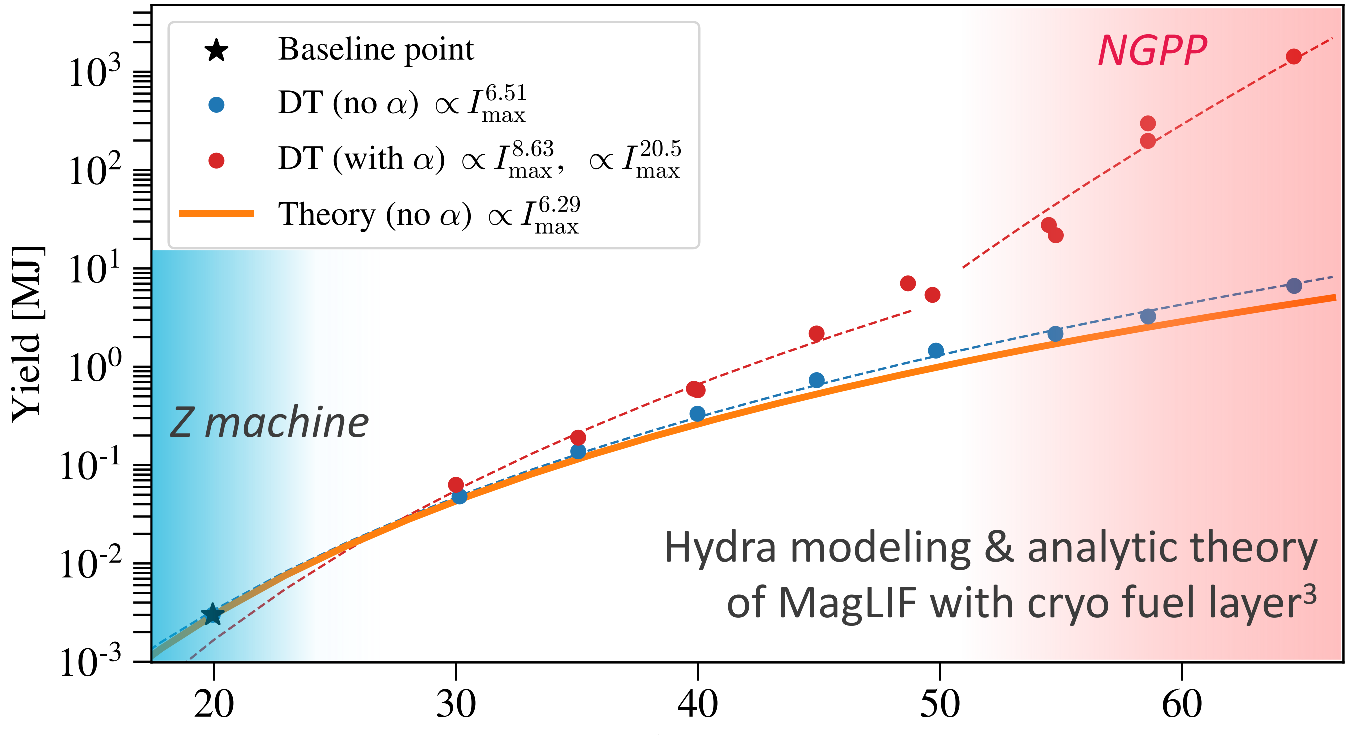


- B-field confines fusion products with low fuel ρR
- Magnetic insulation keeps fuel hot
- Laser heating allows high pressures with the lower implosion velocities
- Calculations show scaling to high yield and gain

Slutz et al., Phys. Plasmas 17, 056303 (2010), S. A. Slutz. and R.A. Vesey, PRL **108**, 025003 (2012)

At larger driver scale this concept has the potential to produce > 10 MJ's of fusion yield for stockpile stewardship

MagLIF can reach 100 MJ yields at reasonable facility scales



Hydra modeling & analytic theory of MagLIF with cryo fuel layer[3]

- Achieving high yield will require scaling up to a larger driver (NGPP)
- Both numerically optimized[1] and analytically scaled[2] approaches show potential for 10's of MJ of yield
- In order to scale up with confidence we require a detailed understanding of our current state as well as our uncertainties

---

[1] S.A. Slutz *et al.*, Phys. Plasmas (2018), [2] P.F. Schmit and D.E. Ruiz., Phys. Plasmas (2020),
[3] S.A. Slutz and R.A. Vesey, PRL (2012)

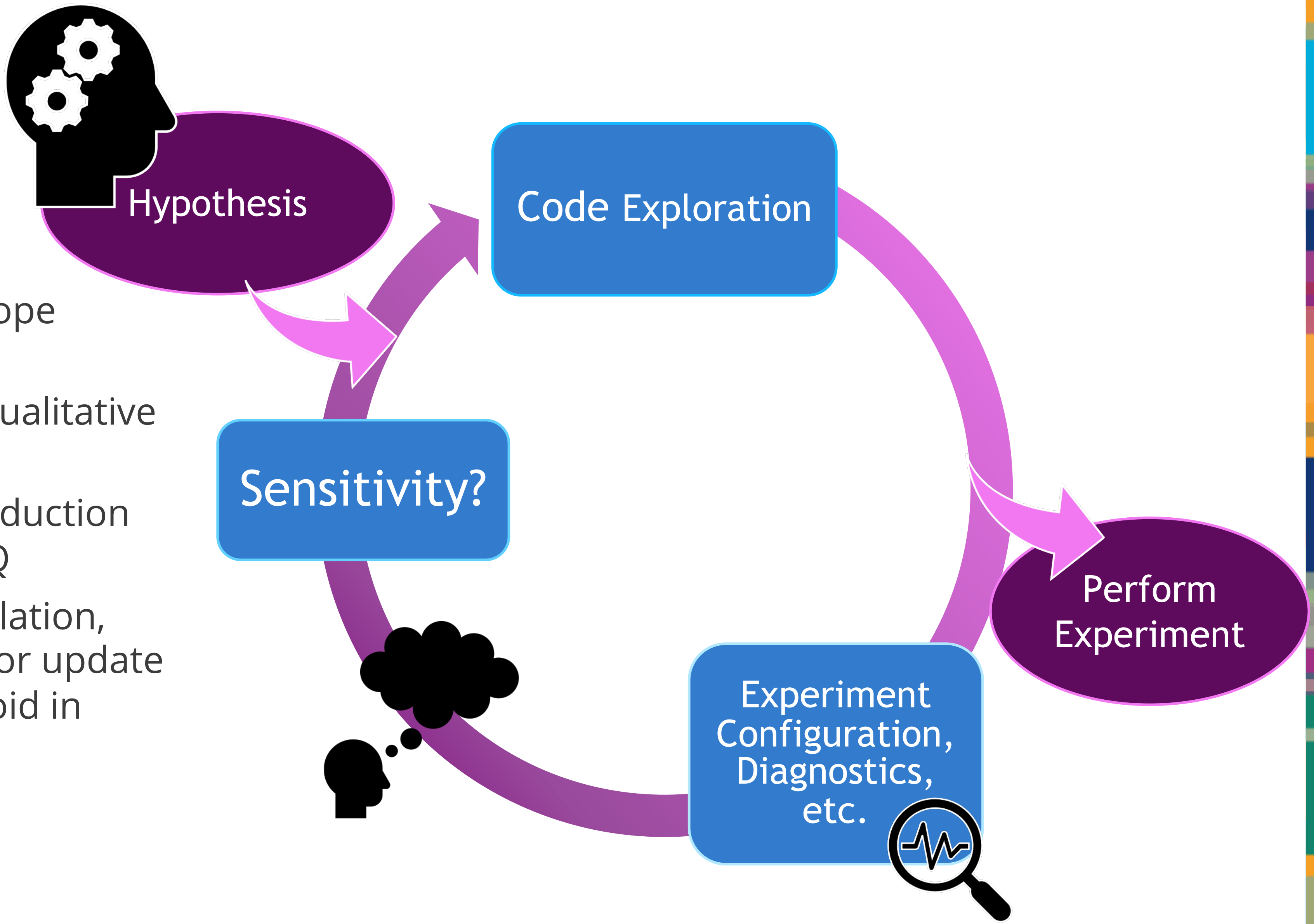
Vision

- Improve our ability to extract important information with quantified uncertainties from complex experiments using Bayesian inference and data assimilation
- Leverage these statistical models to drive optimization of instrumental and experimental configurations to maximize the utility of our experiments
- Use these capabilities to drive tactical and strategic investment decisions using quantifiable metrics

Our goal is to to advance our understanding of HED and ICF systems utilizing a seamless integration of theory, modeling, and experiment

How do we traditionally do experiment design, data analysis, and integration with theory?

- Small model explorations to scope hypotheses
- Design experiments for large/qualitative changes
- Labor intensive manual data reduction and analysis with little or no UQ
- Compare reduced data to simulation, adjust modeling practices and/or update mental map of ”dragons” to avoid in parameter space

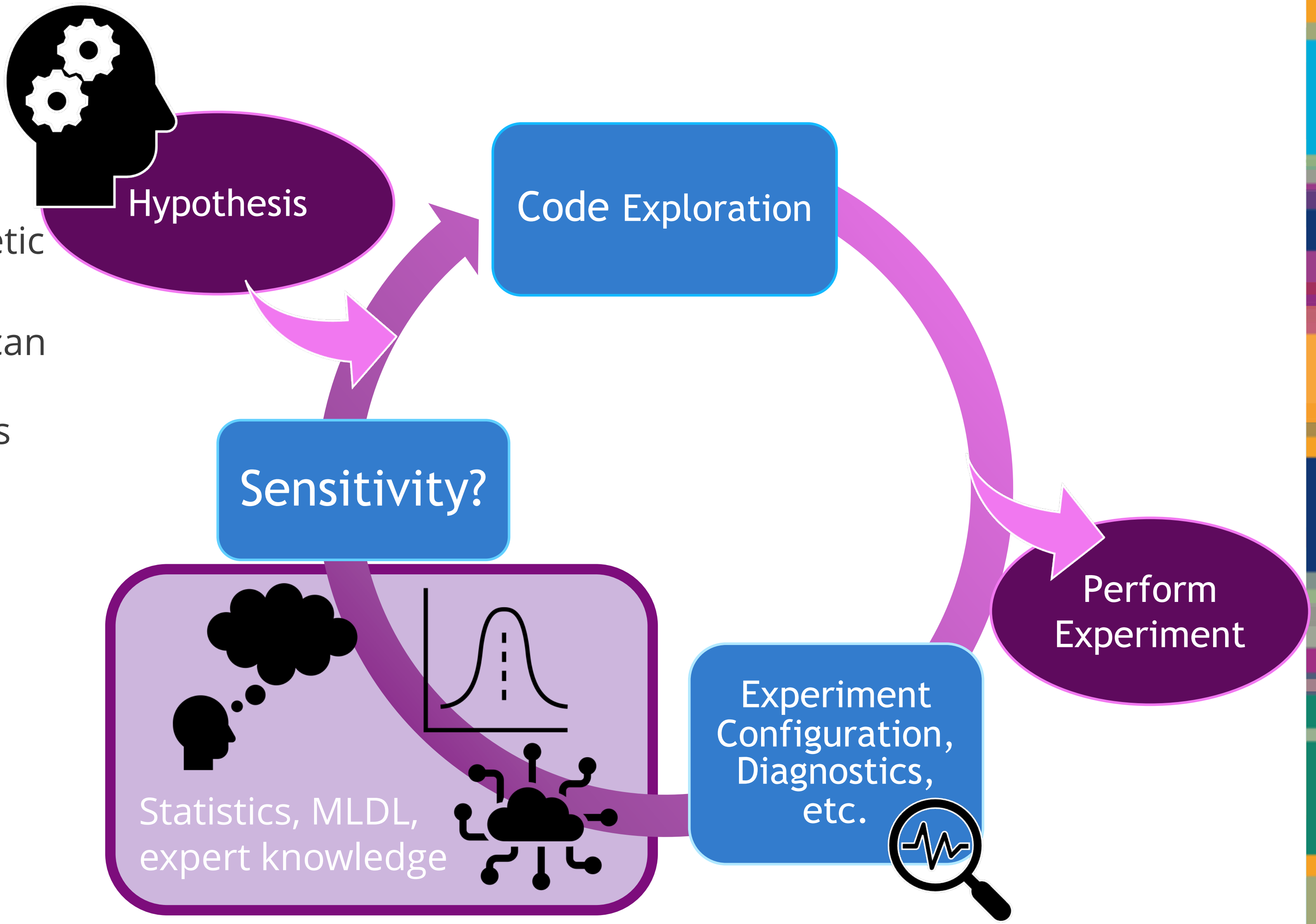


https://cee-gitlab.sandia.gov/amppd

Our goal is to to advance our understanding of HED systems utilizing a seamless integration of theory, modeling, and experiment

How do we want to approach these tasks?

- Ensemble simulations w/ synthetic diagnostics for sensitivities
- Quantified uncertainties so we can place requirements on experiments and measurements
- Automated data processing and integration with UQ
- Design experiments for model calibration and discrimination from the outset



Hypothesis

Code Exploration

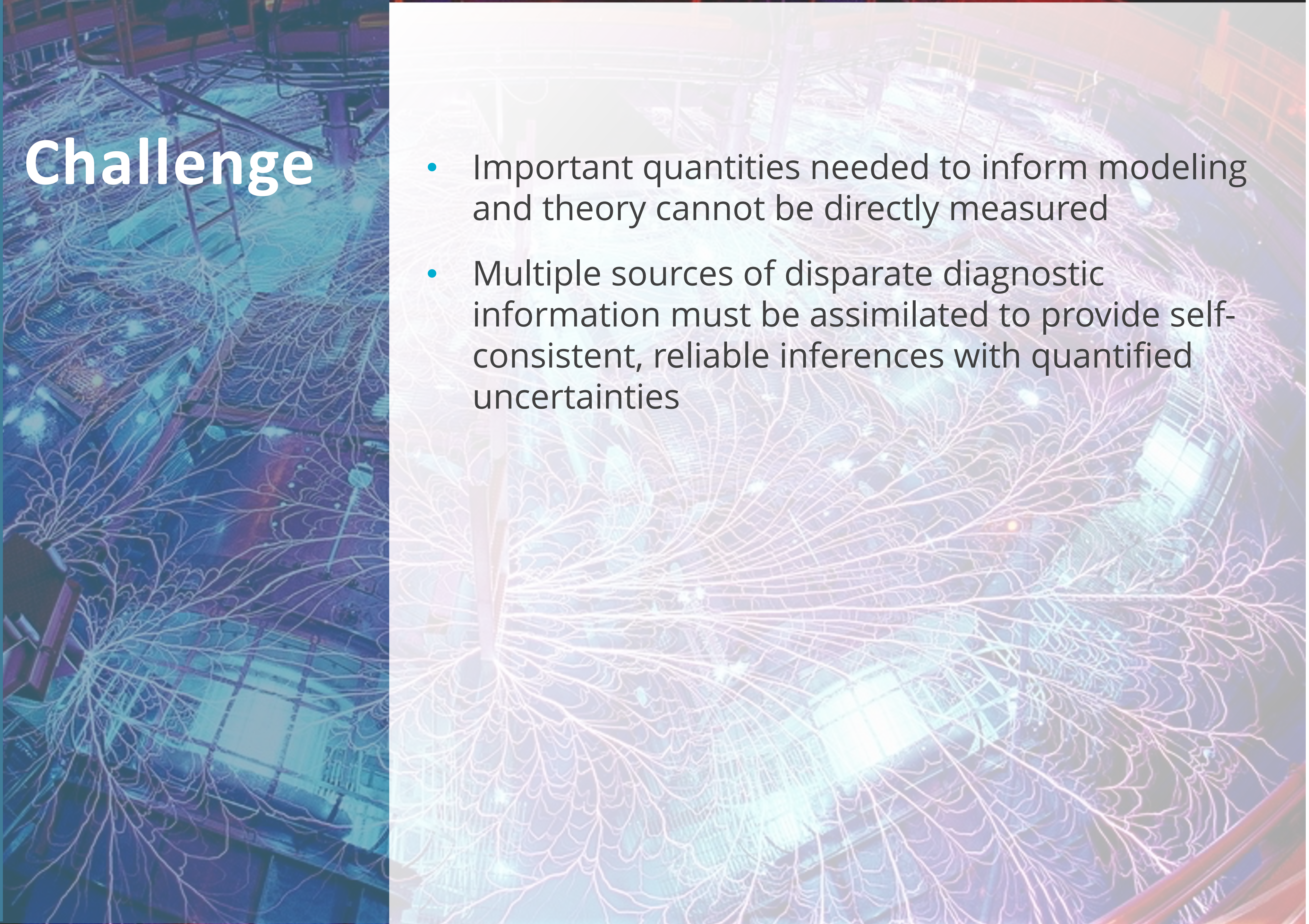
Perform Experiment

Experiment Configuration, Diagnostics, etc.

Sensitivity?

Statistics, MLDL, expert knowledge

https://cee-gitlab.sandia.gov/amppd



Challenge

- Important quantities needed to inform modeling and theory cannot be directly measured
- Multiple sources of disparate diagnostic information must be assimilated to provide self-consistent, reliable inferences with quantified uncertainties

In order to understand our proximity to and progress towards ignition we must infer key quantities from experiments

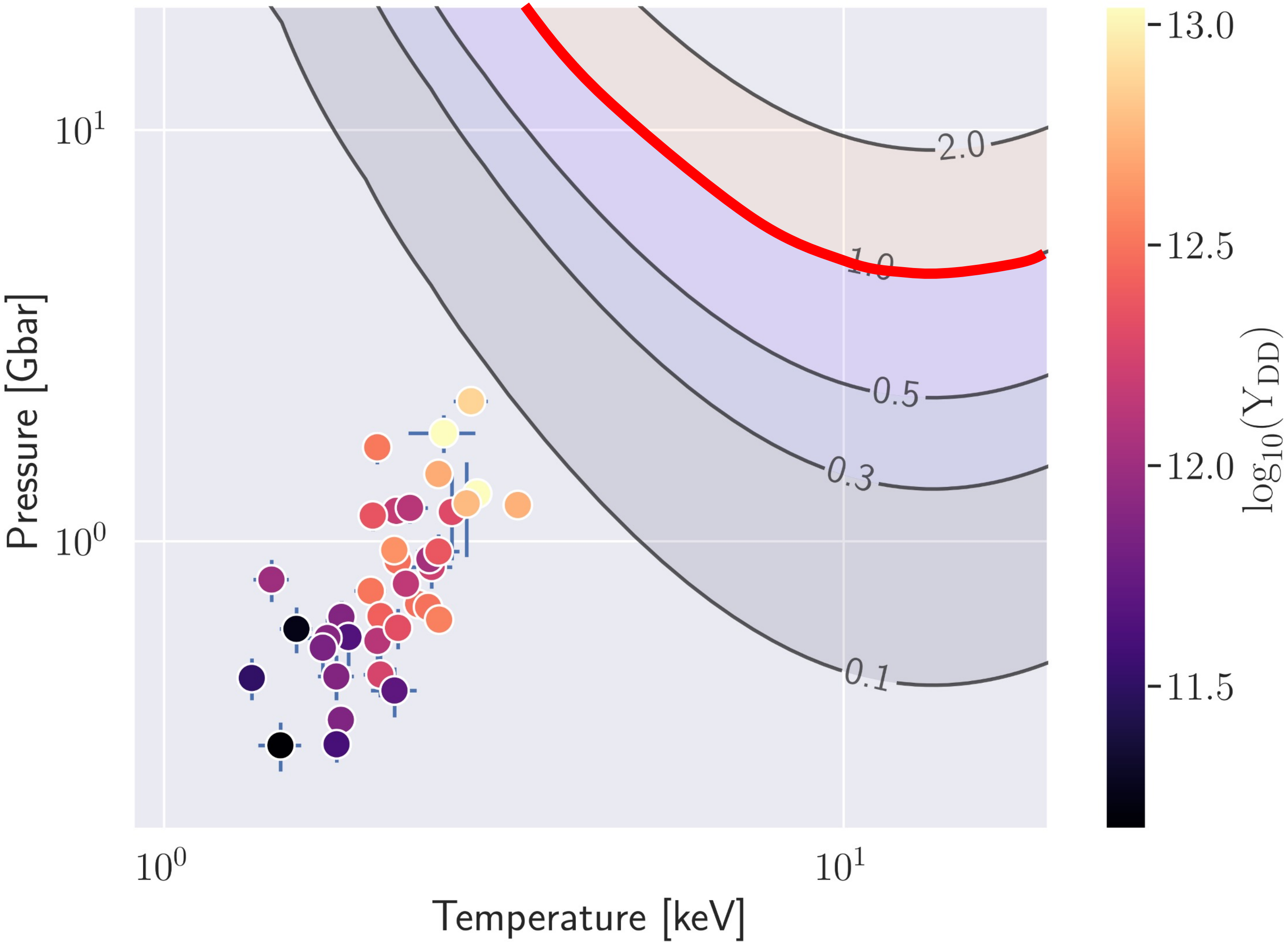
$$\chi = \frac{\varepsilon_\alpha}{24} P_{\mathrm{HS}} \tau_{\mathrm{E}} \frac{\langle \sigma v \rangle_{\mathrm{DT}}}{T^2}$$

Fuel pressure and energy confinement time cannot be directly measured

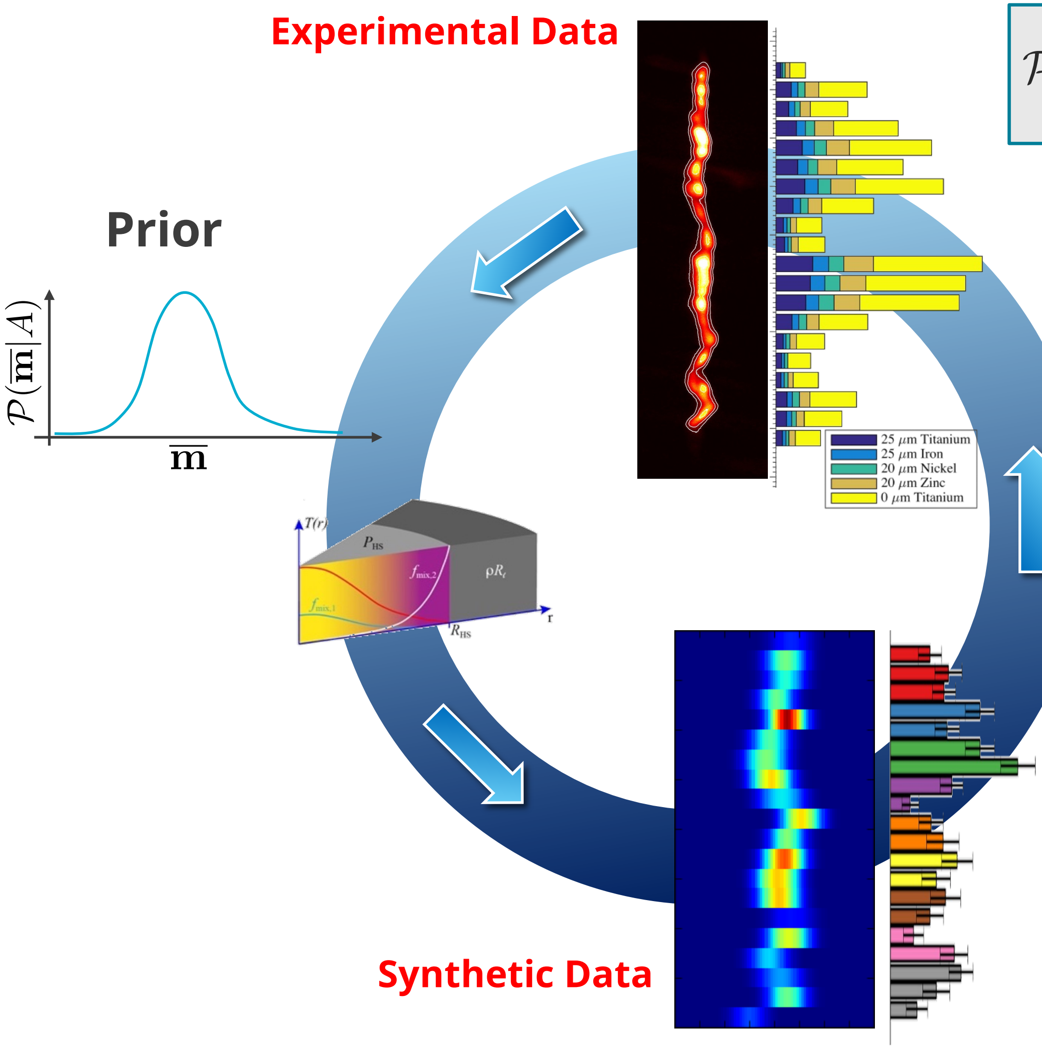
Typically make separate inferences from multiple nuclear and x-ray diagnostics and combine them

Prone to bias since it is not possible to enforce consistency

Does not allow for addition of new information as it becomes available



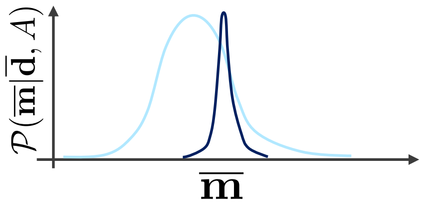
Bayesian Data Assimilation allows us to find the solution that *simultaneous* matches all observables



Bayes' Theorem

$$\mathcal{P}(\overline{\mathbf{m}}|\overline{\mathbf{d}}, A) = \frac{\mathcal{P}(\overline{\mathbf{d}}|\overline{\mathbf{m}}, A)\mathcal{P}(\overline{\mathbf{m}}|A)}{\mathcal{P}(\overline{\mathbf{d}}|A)}$$

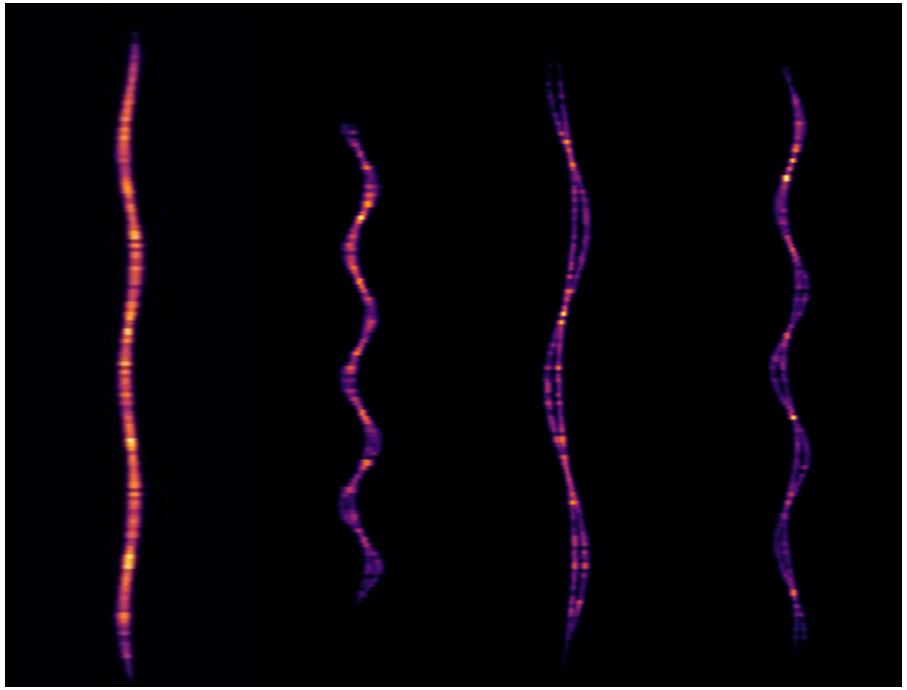
Posterior

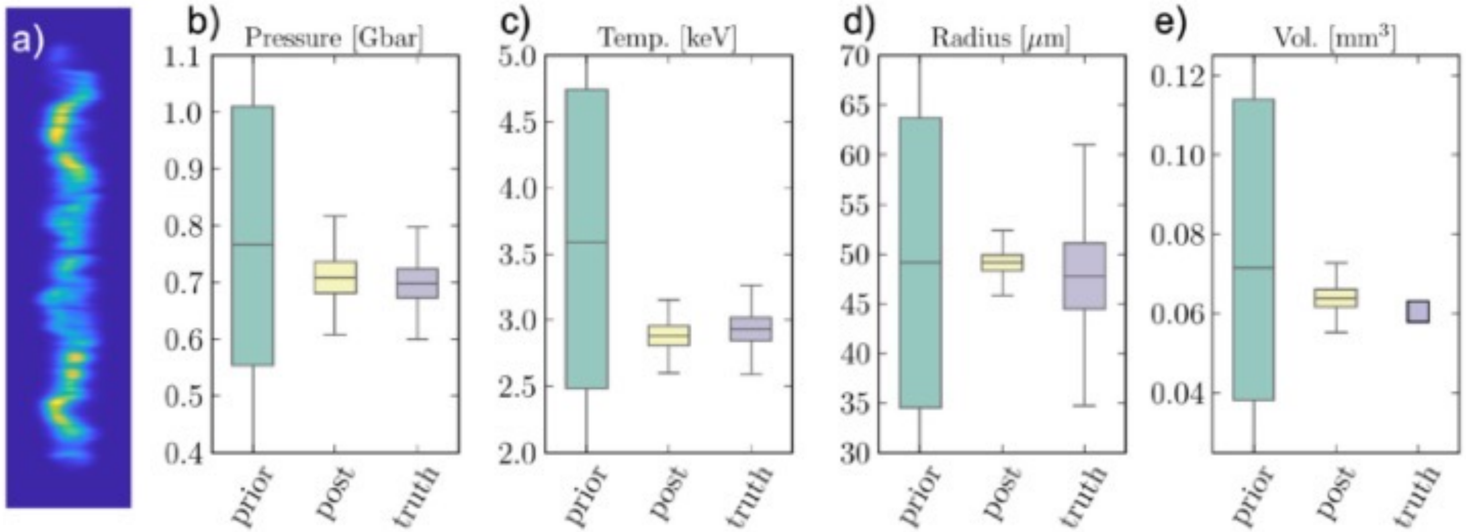


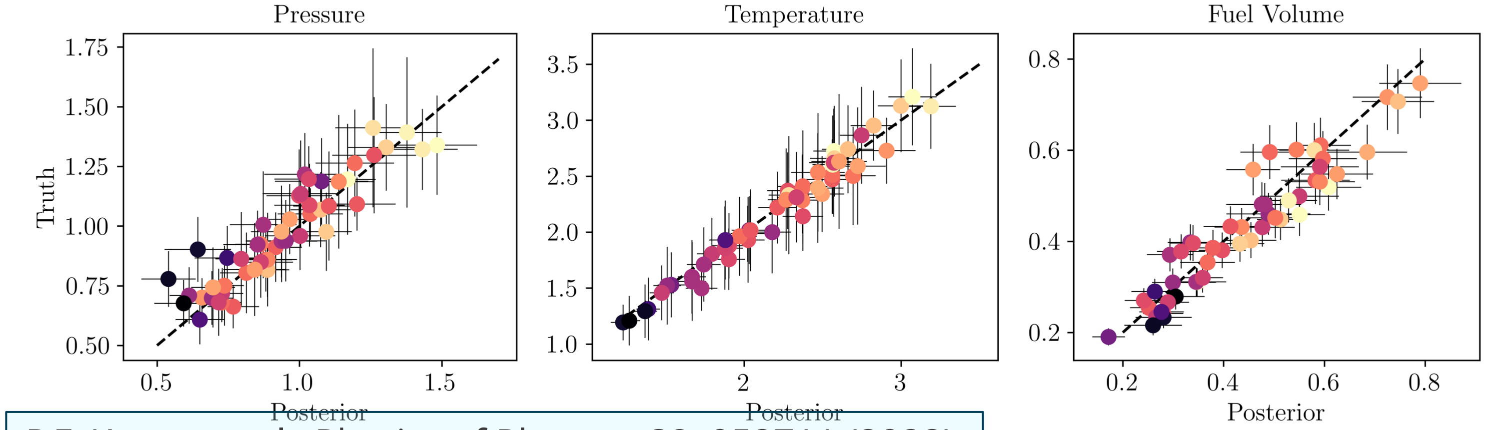
- Using a forward model of the plasma and diagnostics allows us to self-consistently reproduce all observables
- Prior distributions on model parameters allow us to regularize the solution
- The solution is not a point estimate, but a distribution of model parameters
- The distribution provides insights into uncertainties, correlations, sensitivities, and more

P.F. Knapp et al., Physics of Plasmas **29**, 052711 (2022)

Extensive validation was conducted using an idealized model database and 3D MHD simulation data



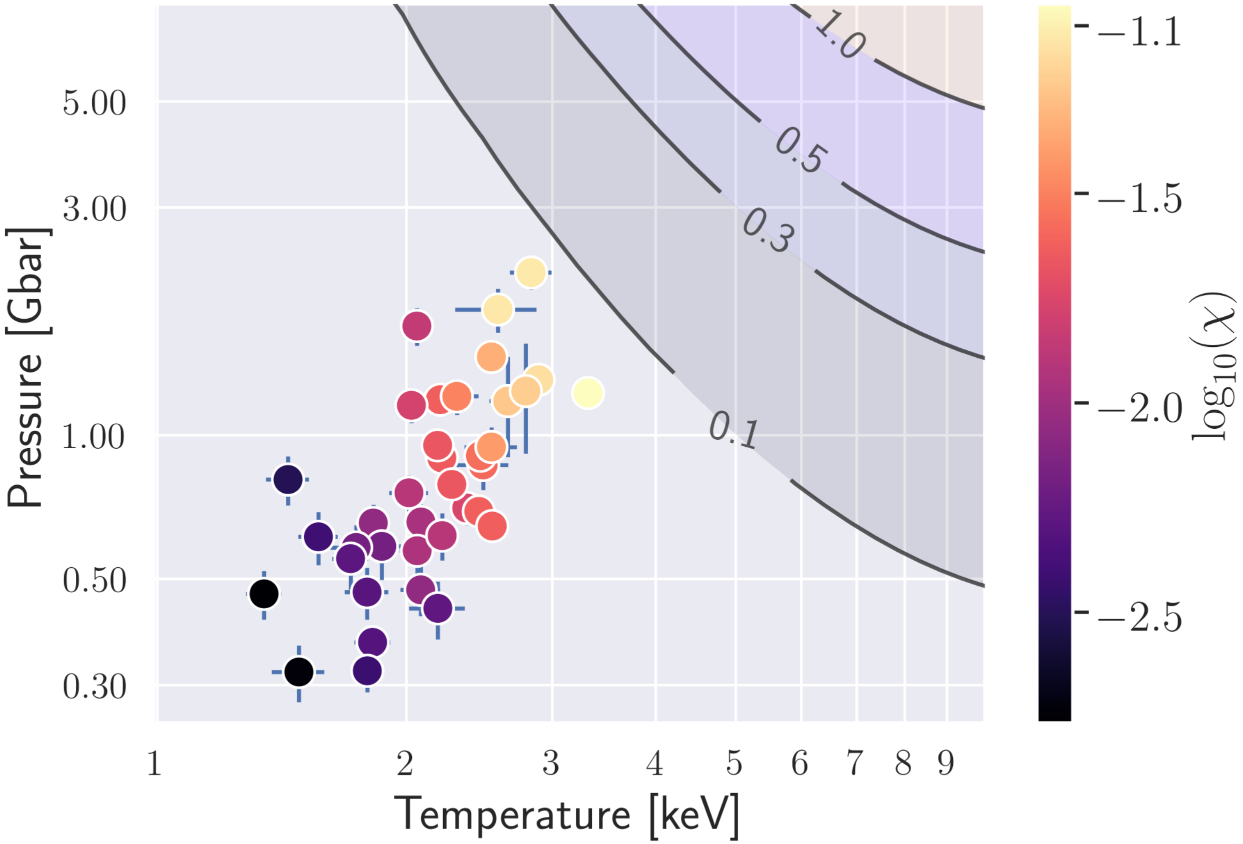




Despite significant 3D structure and simplifications in our inference model, we are able to infer unbiased quantities from experimental data

P.F. Knapp et al., Physics of Plasmas **29**, 052711 (2022)

This capability is used to analyze experimental data in order to understand our progress towards self-heating



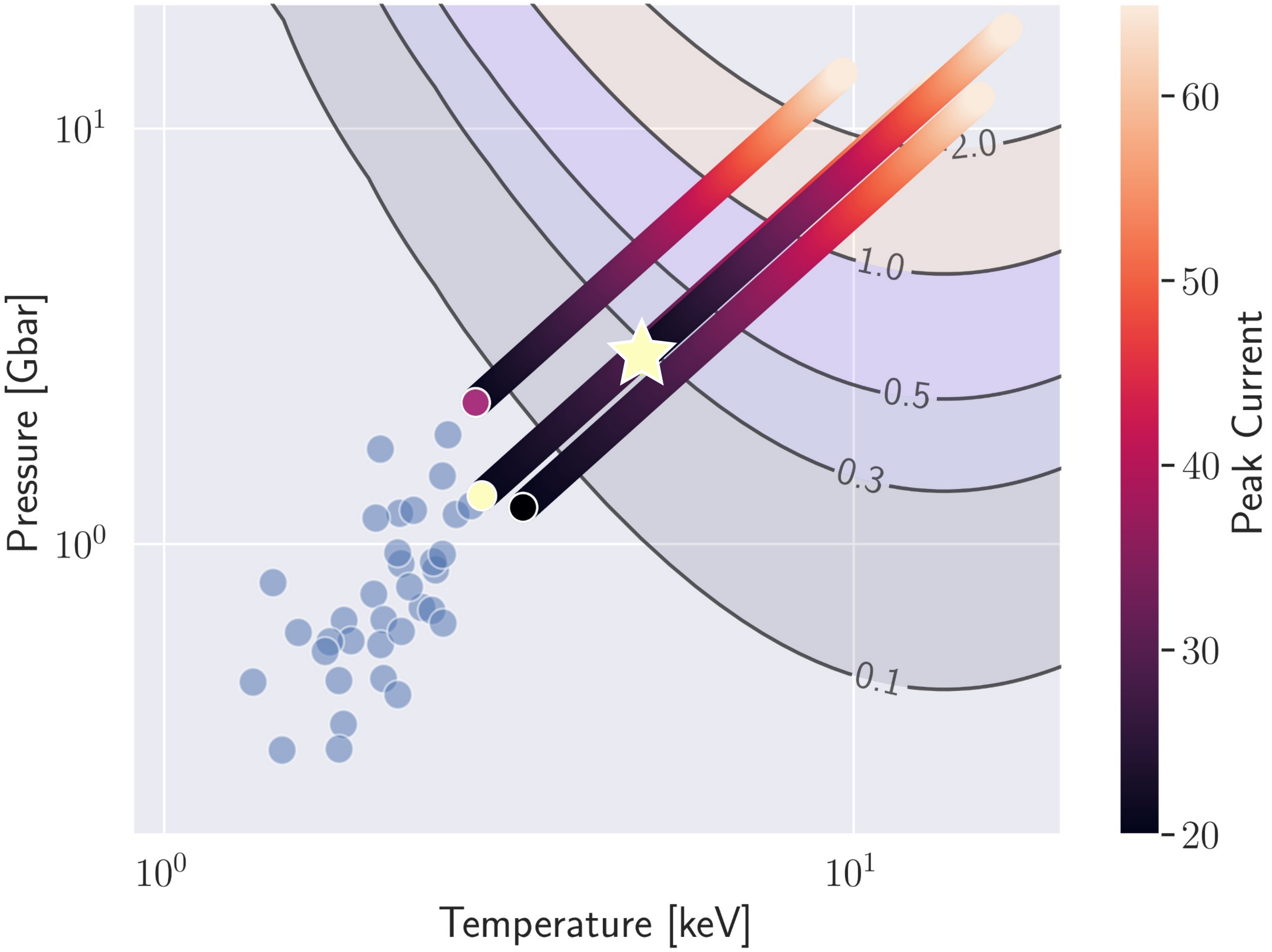
We analyzed a database of 36 MagLIF experiments dating back to 2015

Includes a wide range of neutron yields, preheat configurations, initial magnetic field strengths, fill densities, etc.

$$\chi = \frac{\varepsilon_\alpha}{24} P_{\mathrm{HS}} \tau_{\mathrm{E}} \frac{\langle \sigma v \rangle_{\mathrm{DT}}}{T^2}$$

P.F. Knapp et al., Physics of Plasmas **29**, 052711 (2022)

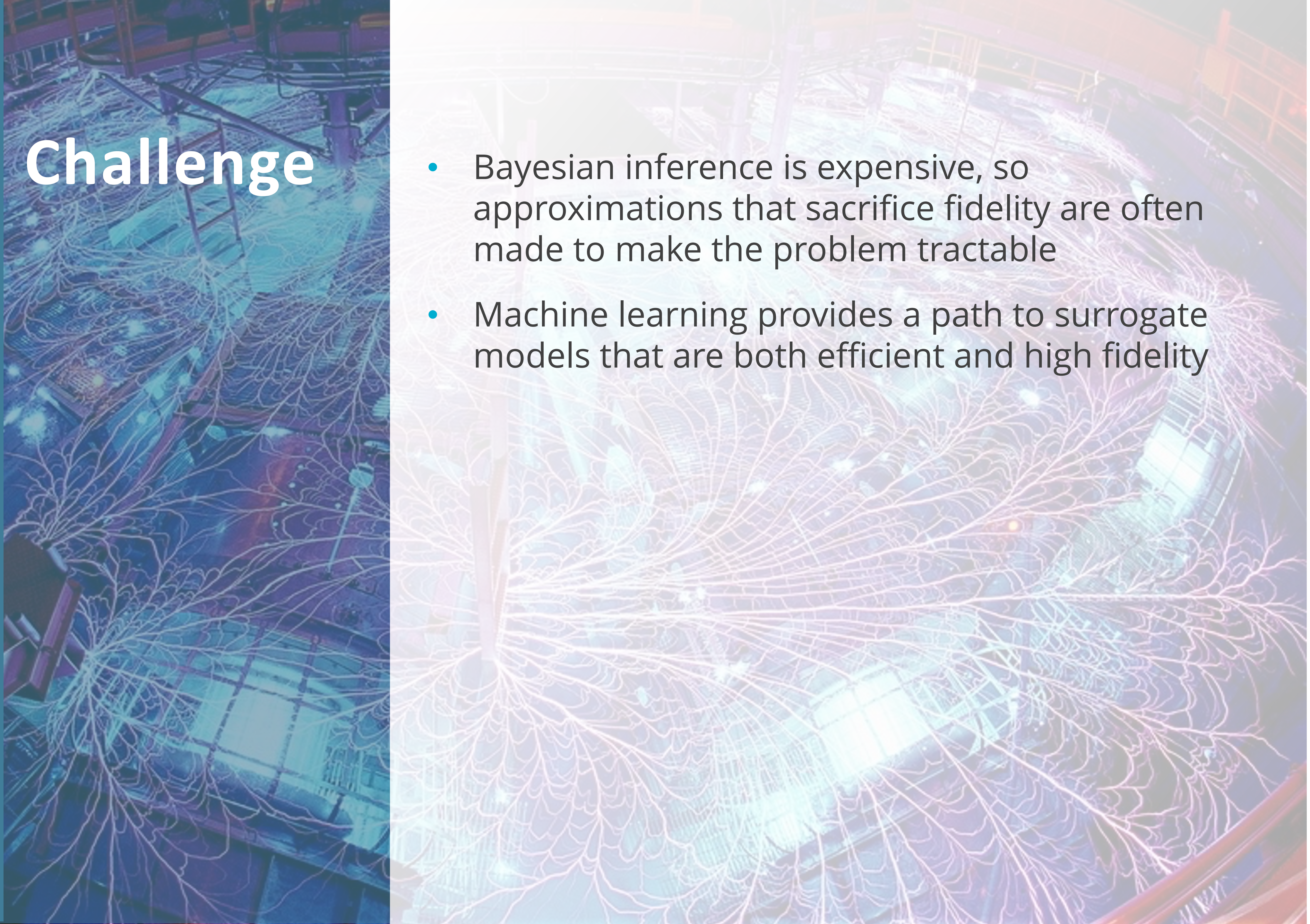
Multiple *existing* data points show the ability to scale to self-heating at realizable drive current



Shot	Y_{DD} [10^{13}]	$\chi_{no\text{-}\alpha}$=1	$Y_{no\text{-}\alpha}$=1 MJ	Y_α [MJ]
z3179	0.5	40 MA	49 MA	6-10
z3236	1.1	38 MA	44 MA	5-9
z3576	0.7	45 MA	62 MA	5-10
*Opt.	21	28 MA	41 MA	3-4.2

- The optimized target exceed $Y_{no\text{-}\alpha}$=1 MJ at the lowest drive current
- Yield amplification due to α-heating is 3-4x
- At 60 MA this target produces >40 MJ

P.F. Knapp et al., Physics of Plasmas **29**, 052711 (2022)
P.F. Schmit and D.E. Ruiz., Phys. Plasmas **27**, 062707 (2020)
S.A. Slutz, et al., Physics of Plasmas **23**, 022702 (2016)

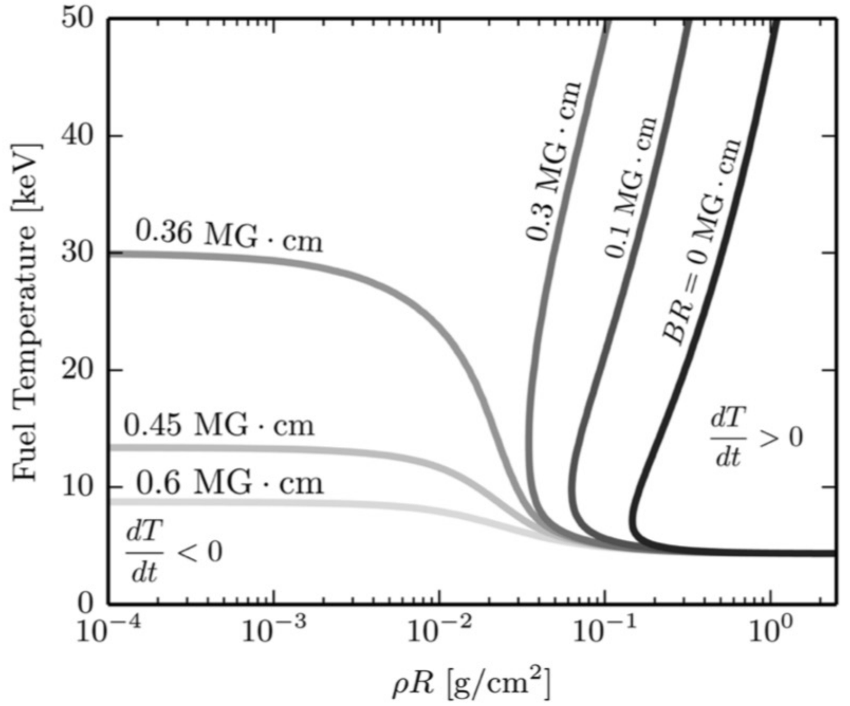


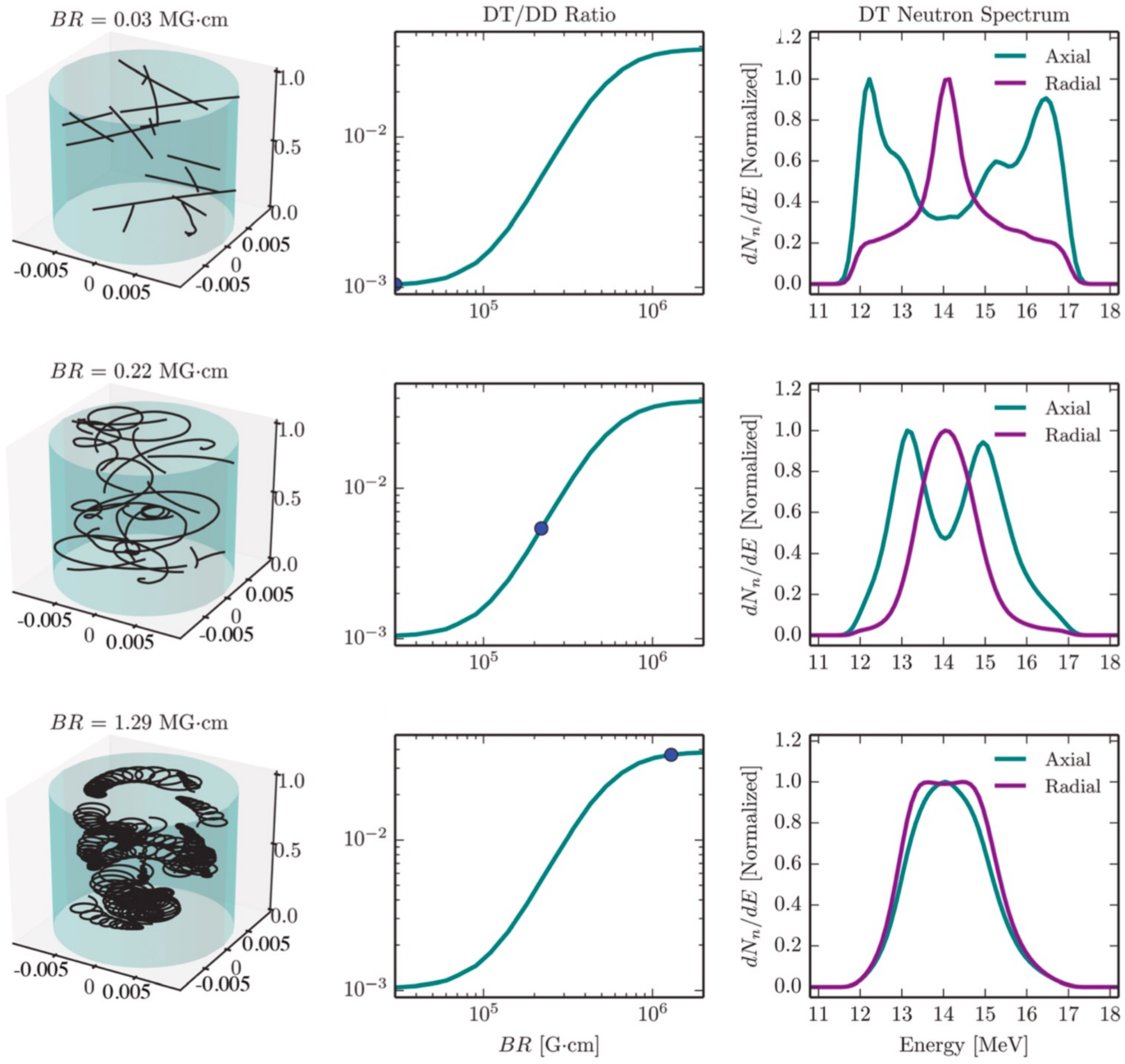
Challenge

- Bayesian inference is expensive, so approximations that sacrifice fidelity are often made to make the problem tractable
- Machine learning provides a path to surrogate models that are both efficient and high fidelity

Another critical performance metric is the fuel magnetization during fusion burn

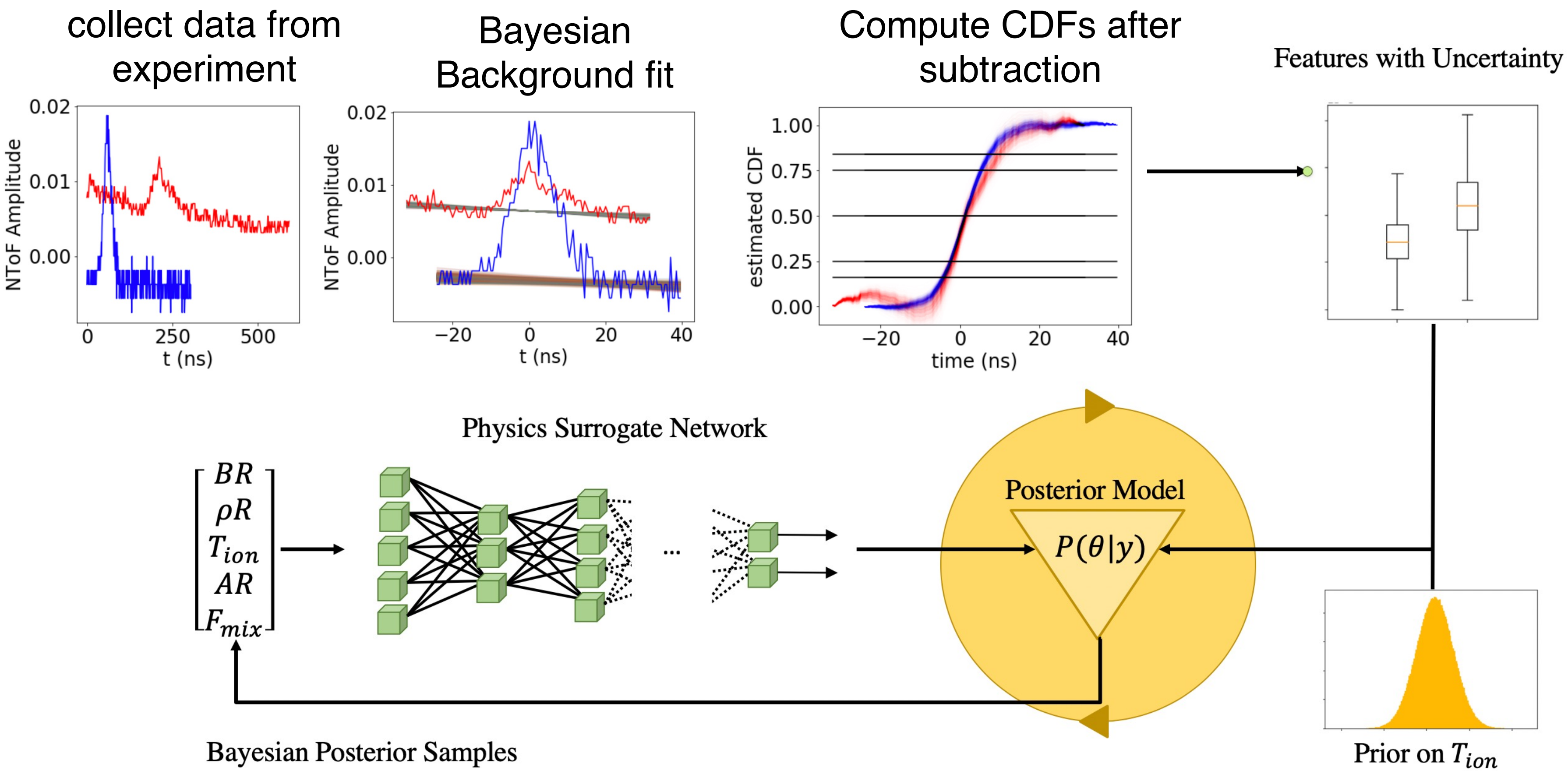
$$\begin{aligned}\text{Primary}: D + D &\rightarrow \begin{cases} n + {}^3\text{He} & 2.45\ \text{MeV} \\ p + T, & 1.01\ \text{MeV} \end{cases} \\ \text{Secondary}: D + T &\rightarrow n + \alpha\,. \quad 11.8\text{–}17.1\ \text{MeV}\end{aligned}$$





P.F. Schmit, et al. PRL 113, 155004 (2014)
P.F. Knapp et al., Physics of Plasmas **22**, 056312 (2015)

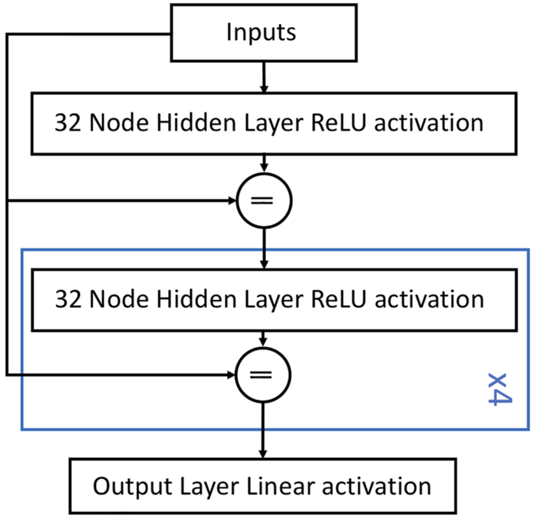
Experimental data exhibit significant noise which should be captured in uncertainty of features extracted.

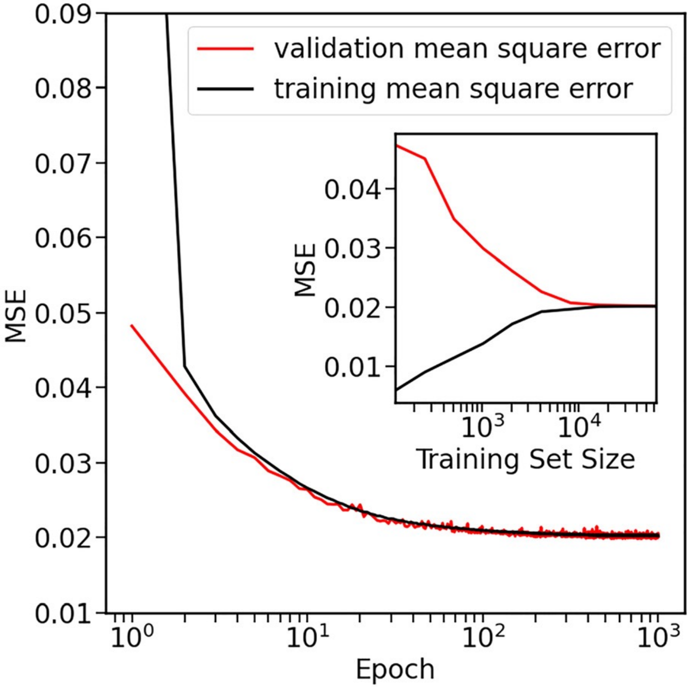


- An expensive physics model is the basis of BR inference[2,3]
  - 1 Evaluation in ~10-100 CPU hours
- We created a deep-learned surrogate of this model
  - 1 Evaluation in ~1 ms on a laptop
- MCMC requires ~10k model evaluations

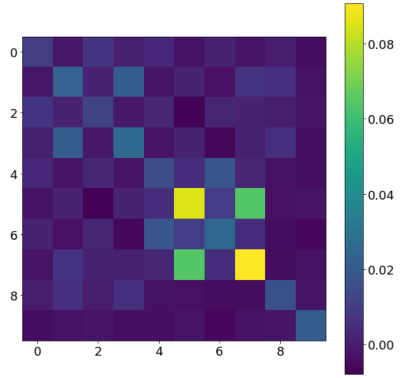
W.E. Lewis et al., Phys. Plasmas 28, 092701 (2021)

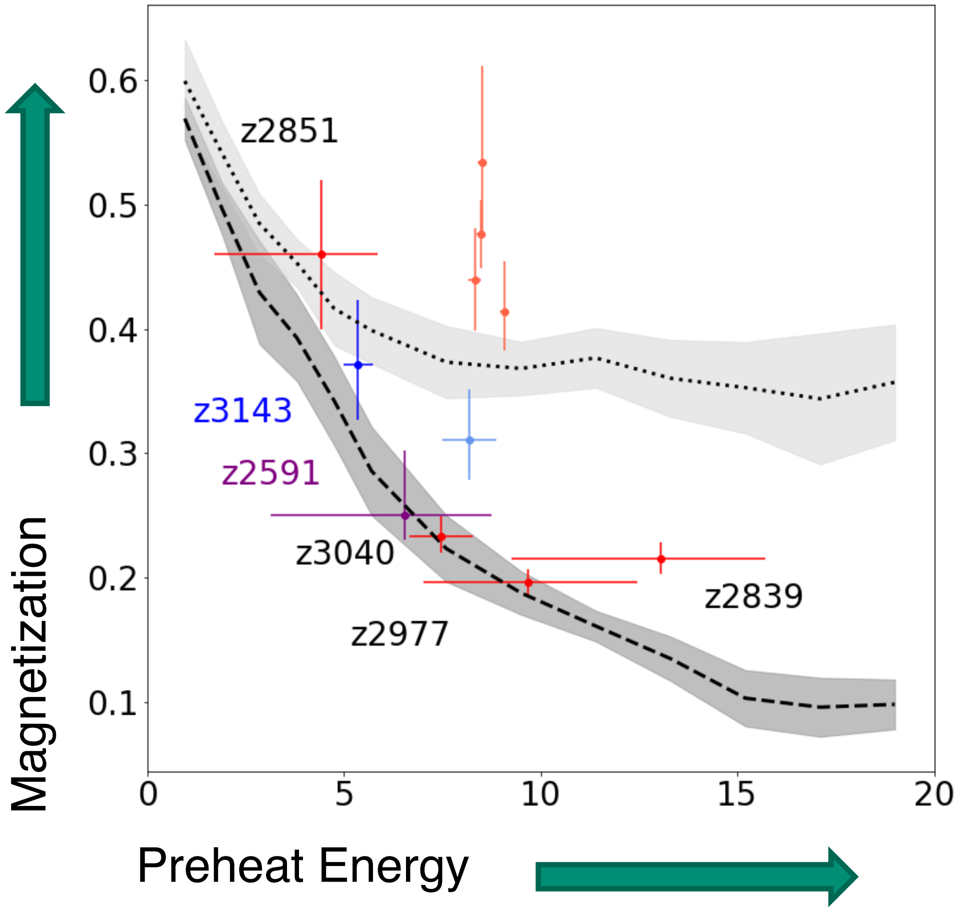
The surrogate uncertainty is quantified using the out-of-sample error and incorporated into the inference





Estimate OOS covariance from performance on data not seen during training (~ 2k validation and ~14k training)

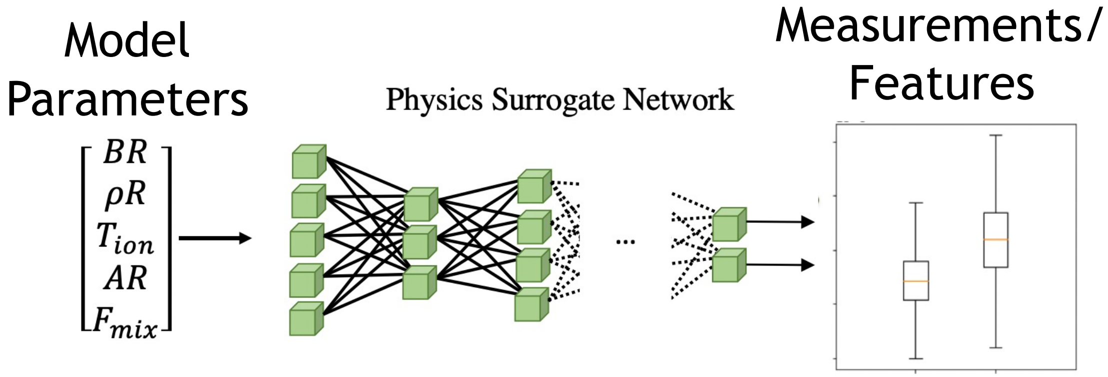




W.E. Lewis et al., Phys. Plasmas 28, 092701 (2021)

We have had some success in applying input/ouput surrogate models and are exploring new tools to improve their performance

Deep Neural Network (DNN)

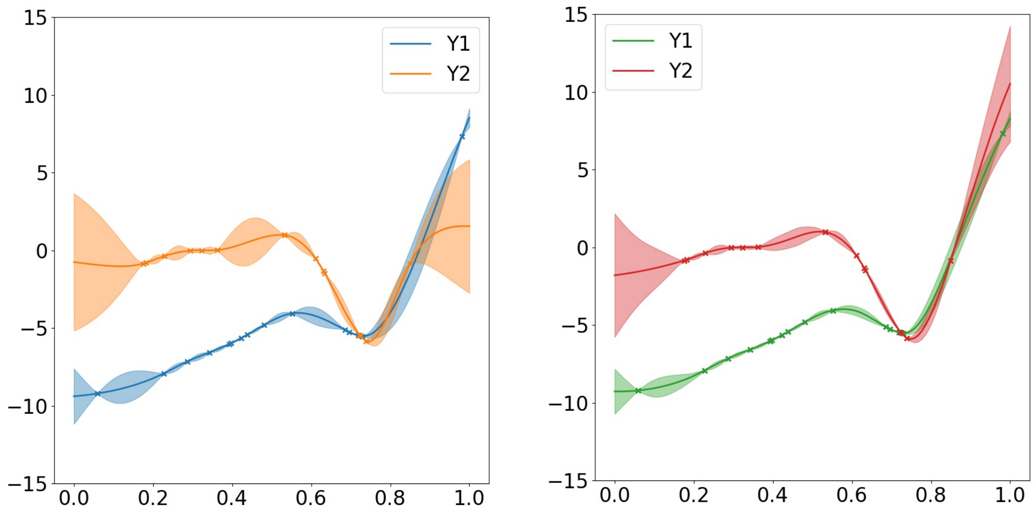


DNNs are a powerful and flexible tool to to learn general non-linear mappings, but getting well quantified uncertainties is a challenge

While powerful, this approach has drawbacks

- obscures the underlying physics
- Can be difficult to enforce known physical constraints

Co-predicted Gaussian processes (GP)

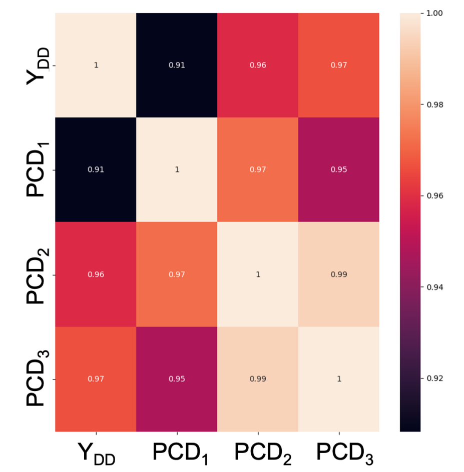


Individual GPs

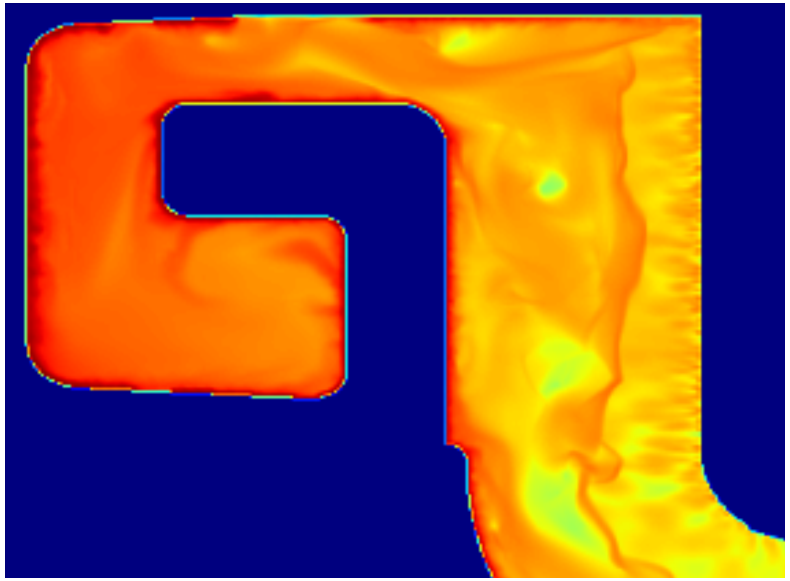
Co-predicted GPs

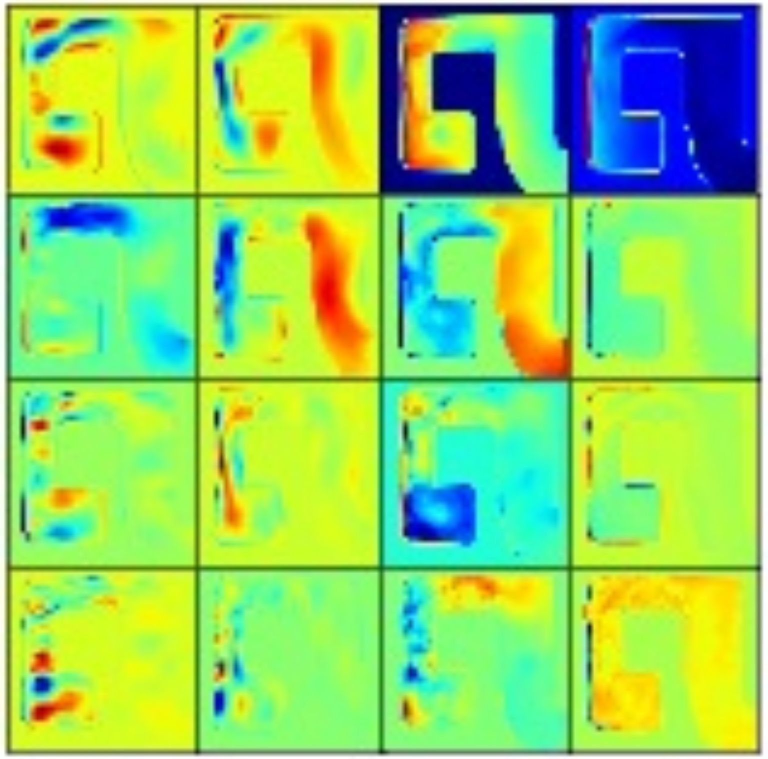
Co-prediction provides a way to leverage and preserve correlations between multiple outputs w/ uncertainties

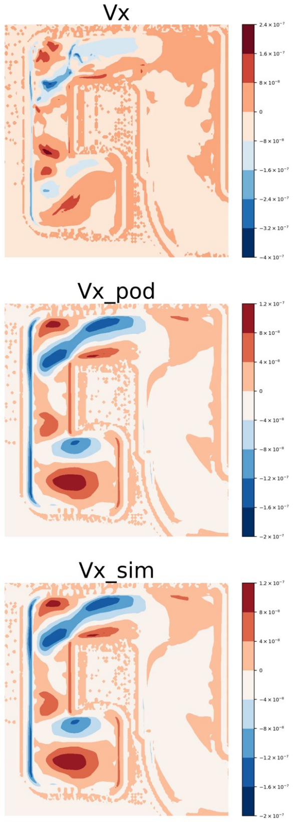
- Kathryn Maupin (1463) and Anh Tran (1441)



We are exploring ways to surrogate dynamical systems in a way that is generalizable and physics preserving







Resistive MHD models are the workhorse for designing and interpreting experiments on Z.

Dynamical model surrogates could provide a powerful tool for efficiently exploring designs and sensitivities

SINDY – Proper orthogonal decomposition coupled to library-based model discovery

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MICHIGAN STATE UNIVERSITY

Gina Vasey

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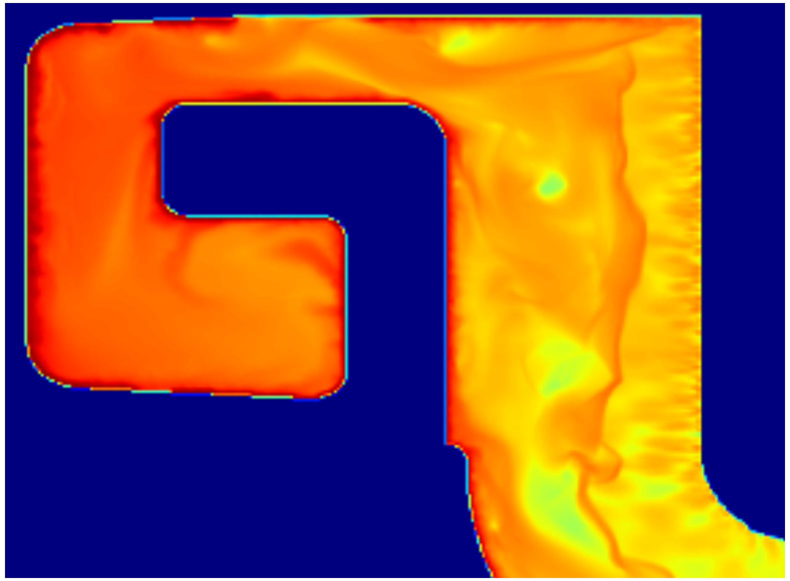
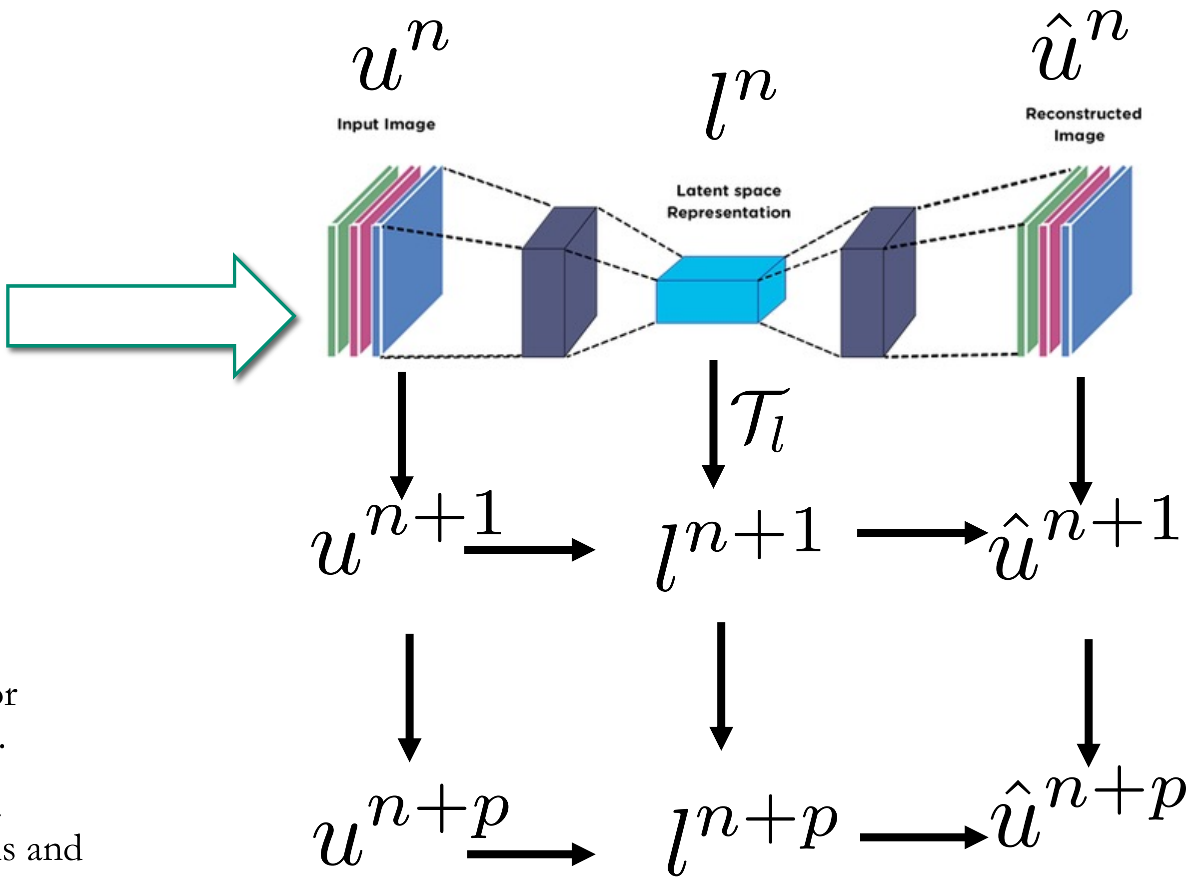
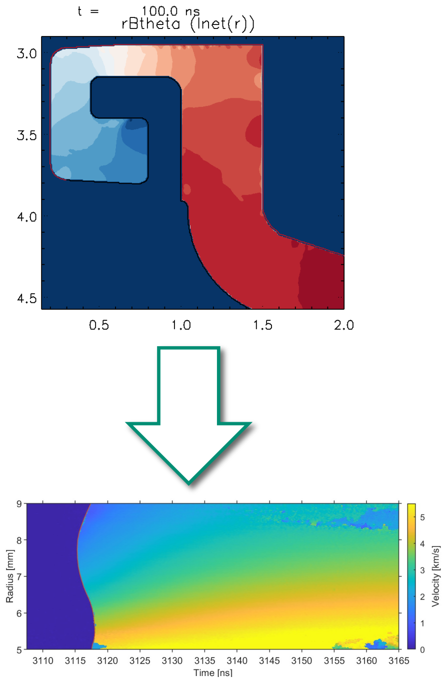




Autoencoder-based compression, ResNet to learn dynamics in latent space



Synthetic observable

Resistive MHD models are the workhorse for designing and interpreting experiments on Z.

Dynamical model surrogates could provide a powerful tool for efficiently exploring designs and sensitivities

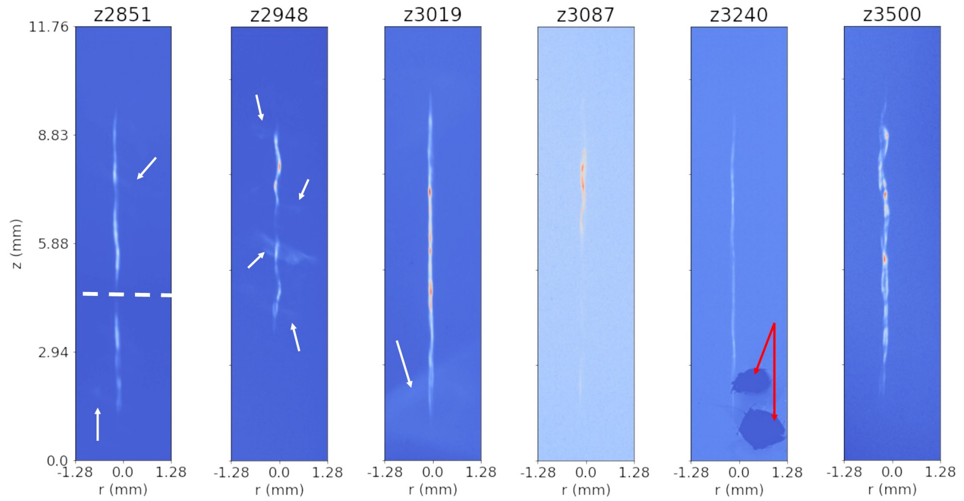
R.G. Patel (1441)

These methods pose challenges when applying to systems with strong transients and advection

Challenge

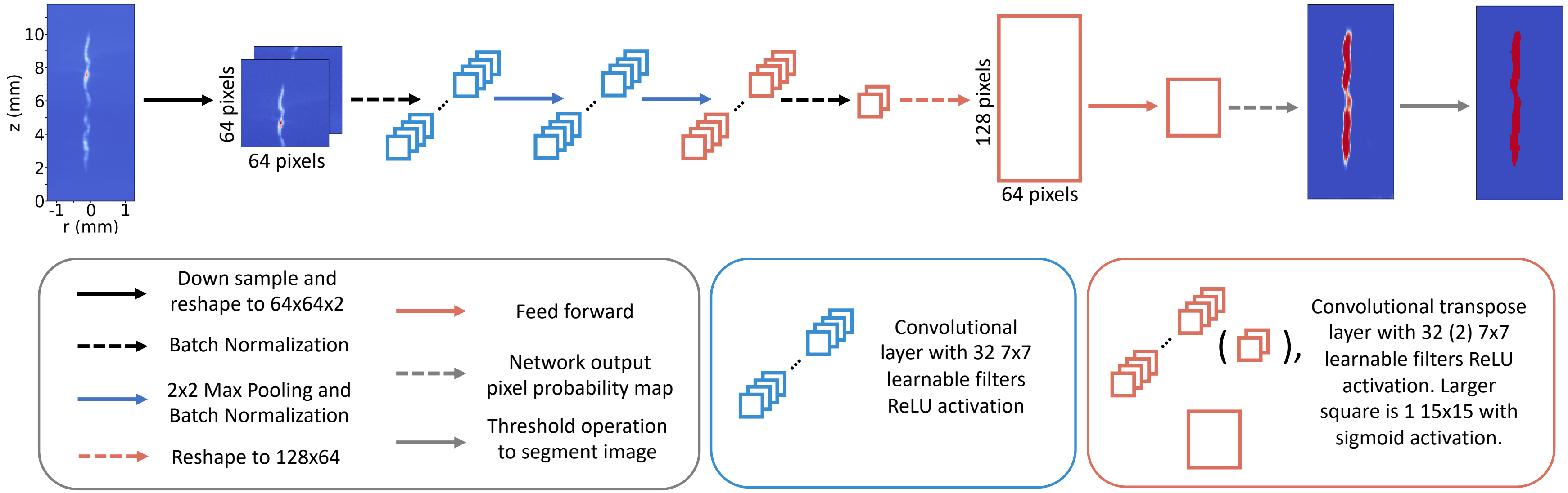
- We produce copious amounts of data on a single experiment. Processing and interpreting raw data is labor intensive and can introduce bias and uncertainty
- Machine learning provides us with a path towards automating and streamlining this process while providing uncertainties for common tasks like background subtraction

Image segmentation is a critical task when attempting to quantify features in experimental images



Experimental images exhibit rich data features, complex backgrounds, and intermittent defects

An autoencoder was developed using synthetic training data to automate segmentation of the data from background



Down sample and reshape to 64x64x2

Batch Normalization

2x2 Max Pooling and Batch Normalization

Reshape to 128x64

Feed forward

Network output pixel probability map

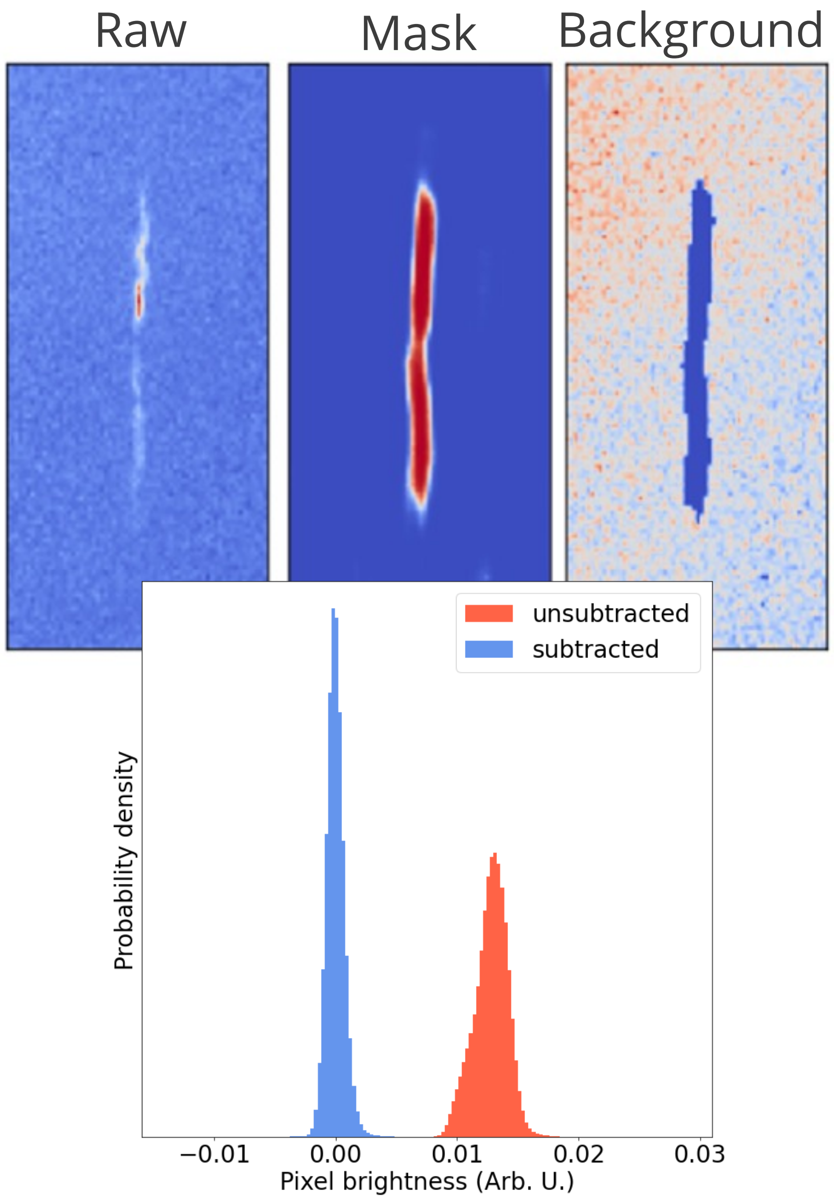
Threshold operation to segment image

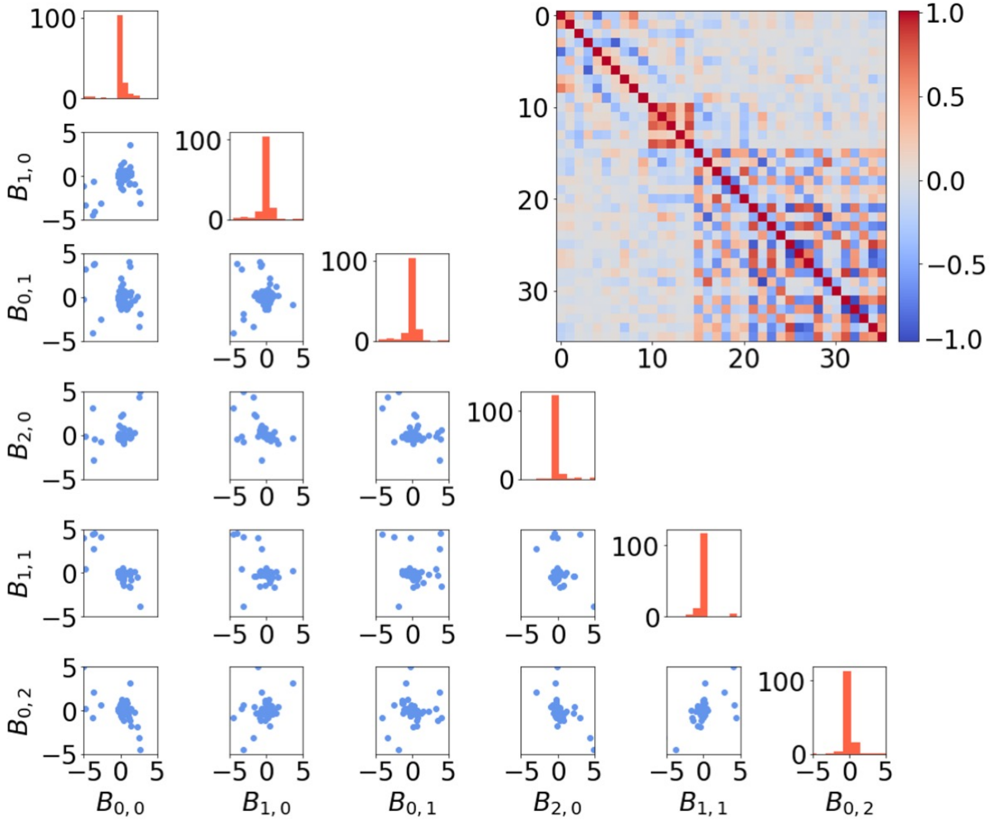
Convolutional layer with 32 7x7 learnable filters ReLU activation

Convolutional transpose layer with 32 (2) 7x7 learnable filters ReLU activation. Larger square is 1 15x15 with sigmoid activation.

W.E. Lewis et al., under review

This capability allows us to mine our existing data to quantify backgrounds, noise statistics, and defects





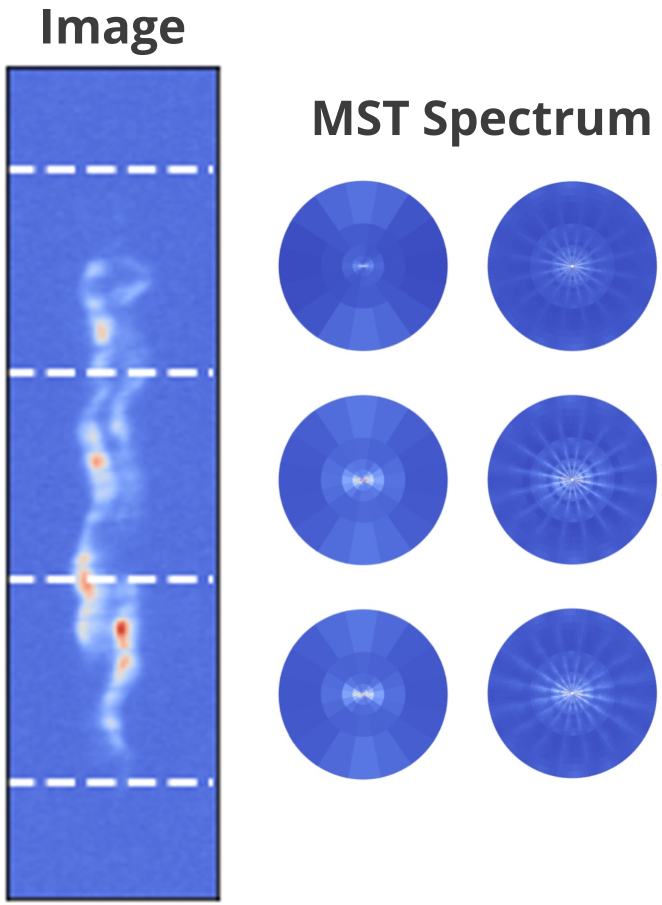
Accurately quantifying our noise and background allows us to

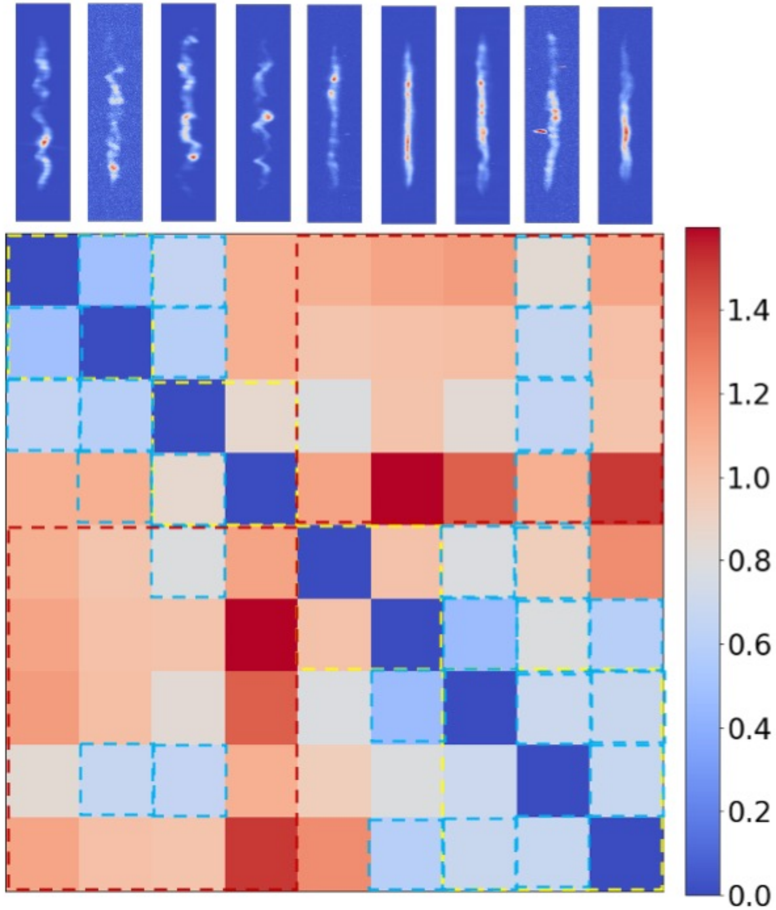
- make more realistic synthetic data models
- Incorporate realistic models in inference to capture uncertainties
- Quantify diagnostic and data requirements

W.E. Lewis et al., under review

The reduced image database is being used to develop *model-free* metrics to quantify relationships between experiments

Fixed weight convolutional networks provide a route to image comparison.



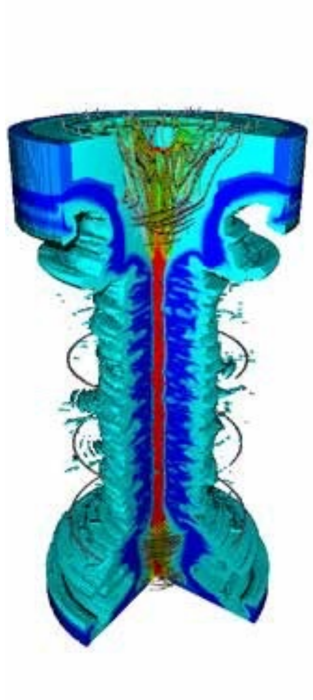


- The MST[1,2] is used as a basis to form a metric with which to compare images
- Texture subtraction in MST-space provides insensitivity to noise
- Resolution and registration sensitivities are quantified
- Effectively separates images with different morphologies

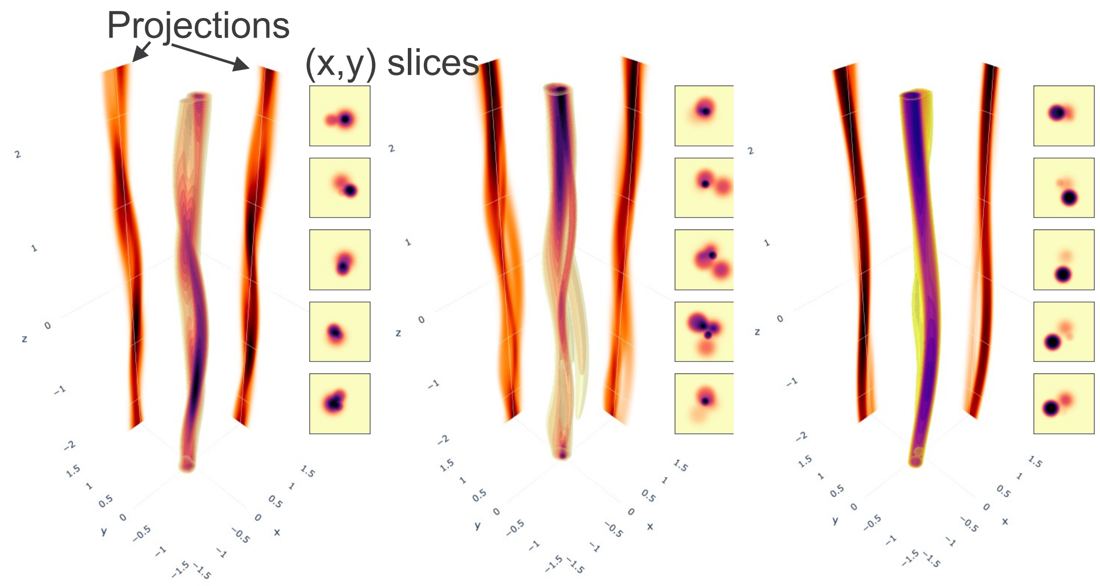
[1] J. Bruna and S. Mallat IEEE Trans. Pat. Analysis and Mach. Intelligence **35**, 1872 (2013).
[2] M. Glinsky *et al.* Phys. Plasmas **27**, 112703 (2020).

W.E. Lewis et al., in preparation

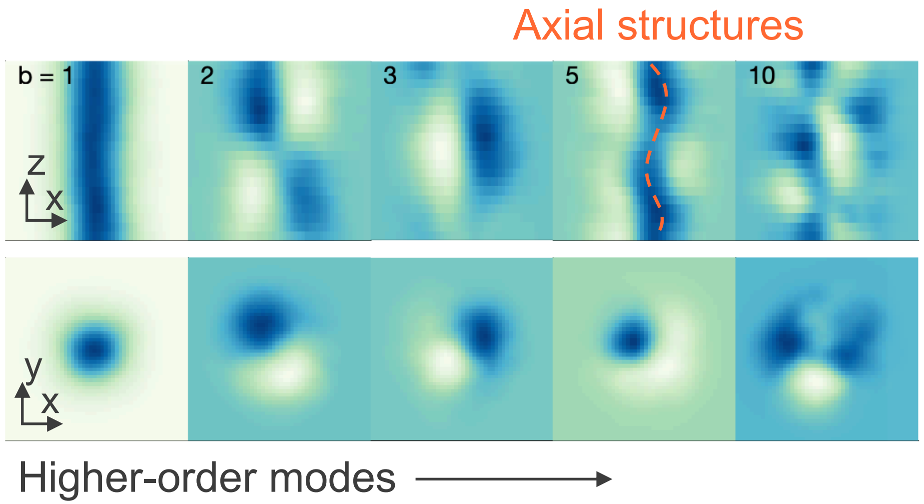
Measuring fuel volumes in 3D is important for MagLIF, but challenging due to limited diagnostic views and rich structure



3D training volumes (MagLIF-like, helical blobs)

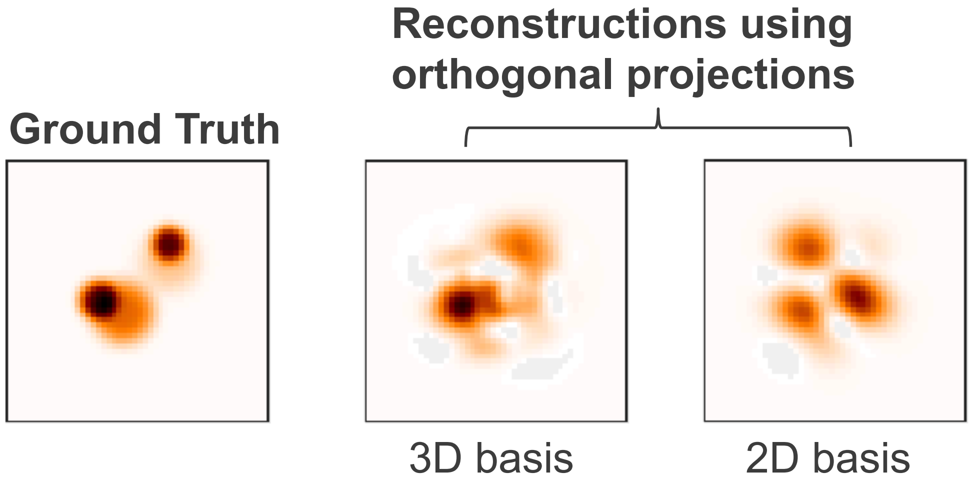


Slices of 3D basis functions from SVD



- Compute fundamental modes from large set of 3D training volumes and use for full 3D reconstruction

Reconstructions from just 2 views using learned 3D basis functions reproduce key morphological features



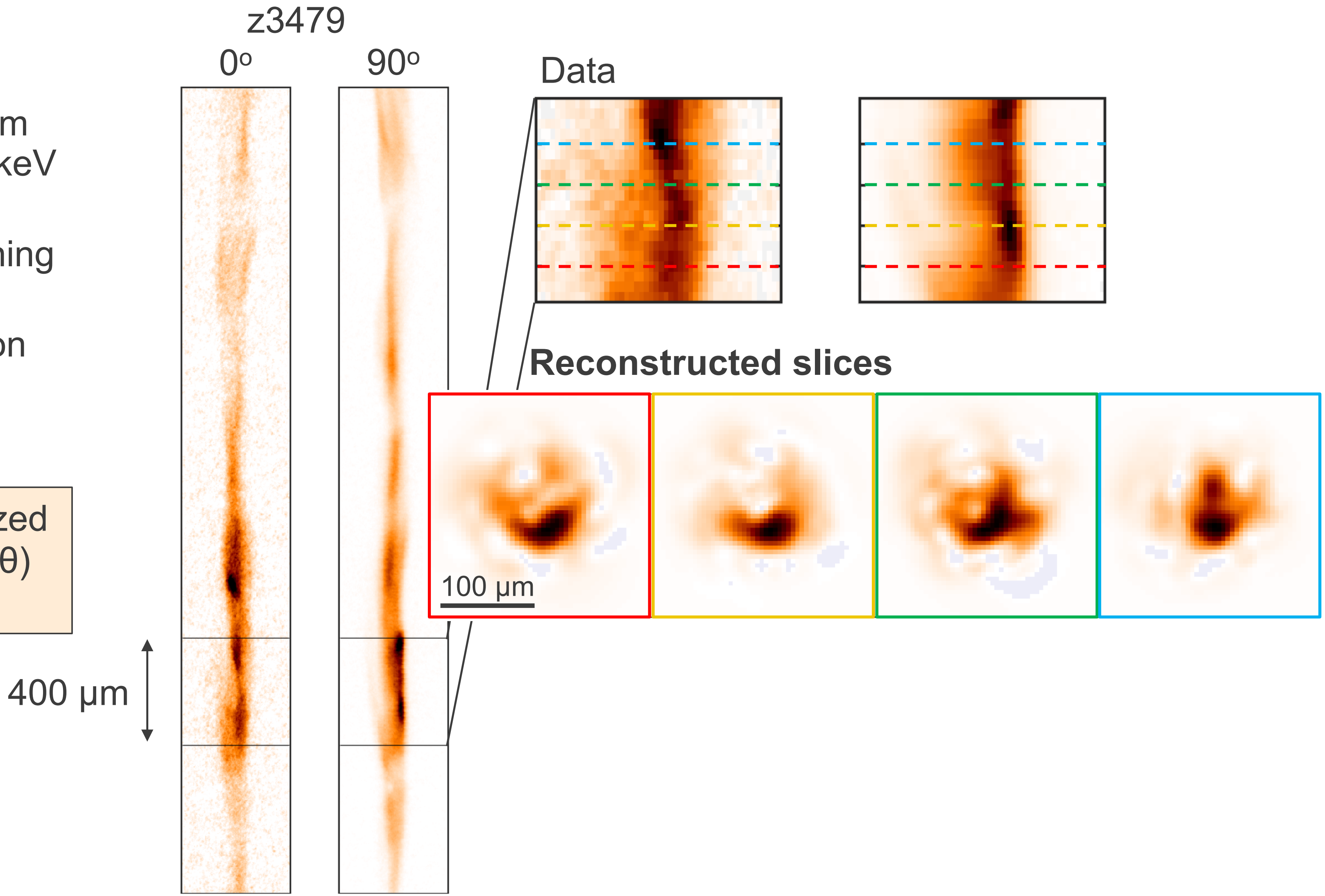
SVD = Singular Value Decomposition

Work by J.R. Fein

Initial 3D reconstructions of a MagLIF stagnation column show asymmetric hot spots

- Reconstruct volume patch from orthogonal projections at 7.2 keV using learned 3D SVD basis
- Extend to full volume by stitching overlapping patches together
- Projections from reconstruction match data to within <15%

*Projections are intensity-normalized assuming slowly varying liner ρR(θ) and center-of-mass aligned

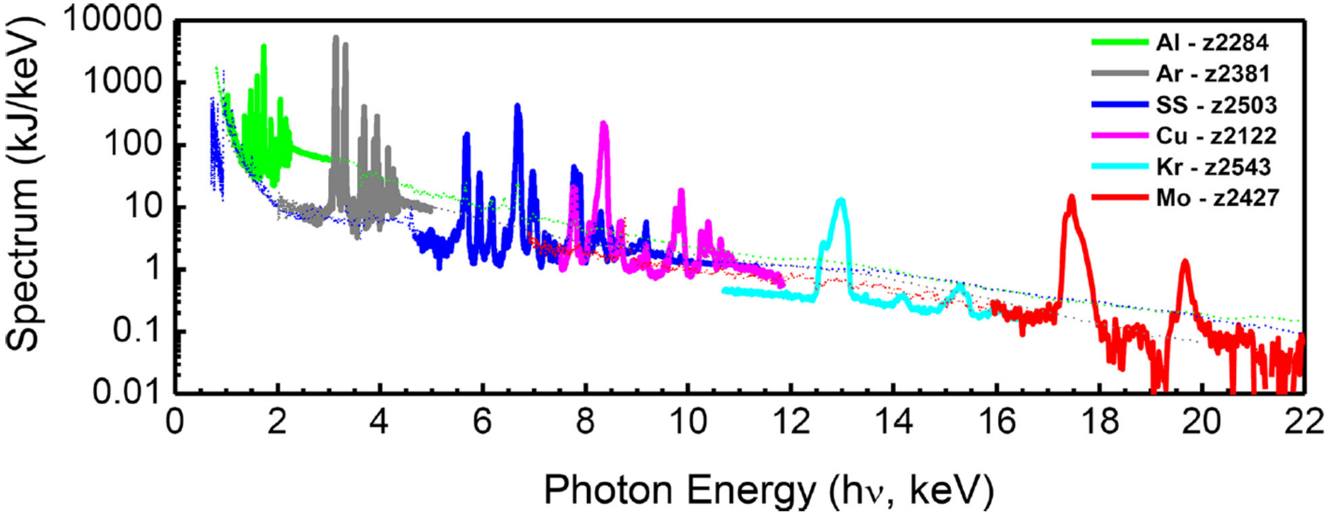


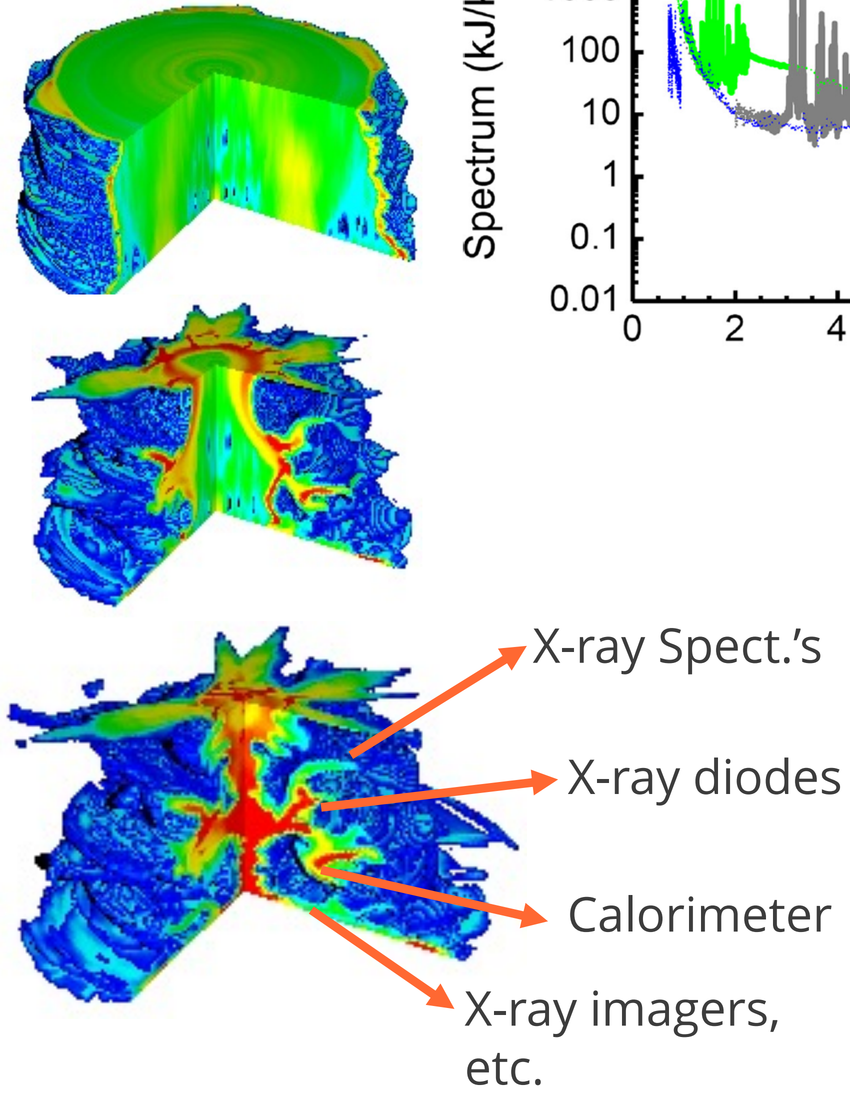
Work by J.R. Fein

Challenge

- Diagnostics and experiments are largely intuition driven
- How do we ensure that we are configuring our instruments and experiments in such a way that we can maximize the information we gain?

Accurately quantifying x-ray source outputs on Z is a critical step in survivability research





How should we configure our instruments to minimize uncertainty in the inferred x-ray output and spectrum?

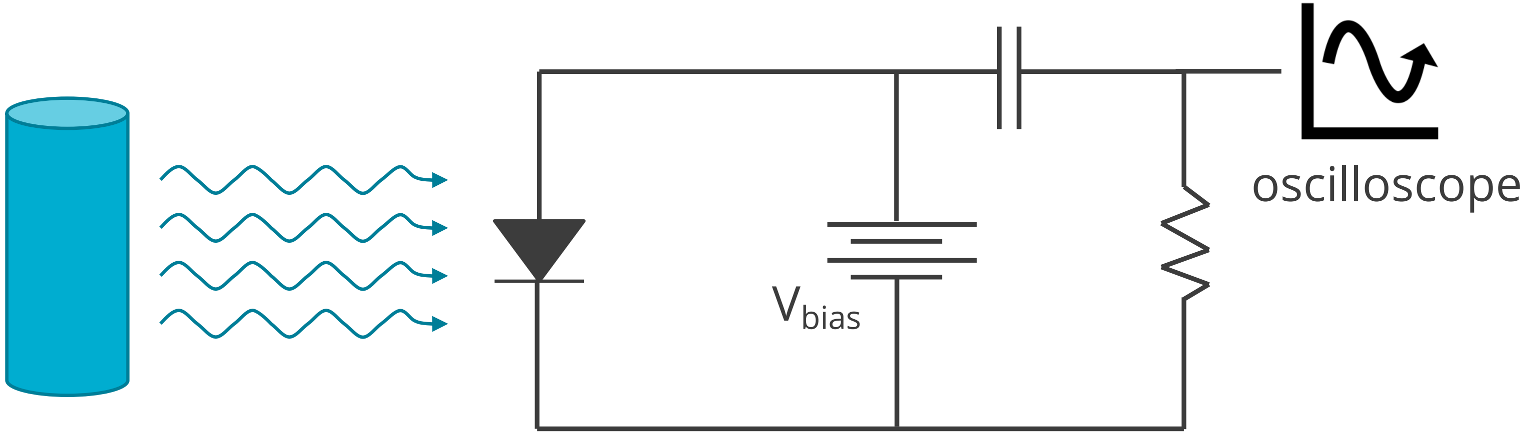
Which instruments should we use?

What calibrations should we invest in to provide the highest impact on our measurements?

We constructed a simplified problem to develop a method for optimizing filtered x-ray power detectors

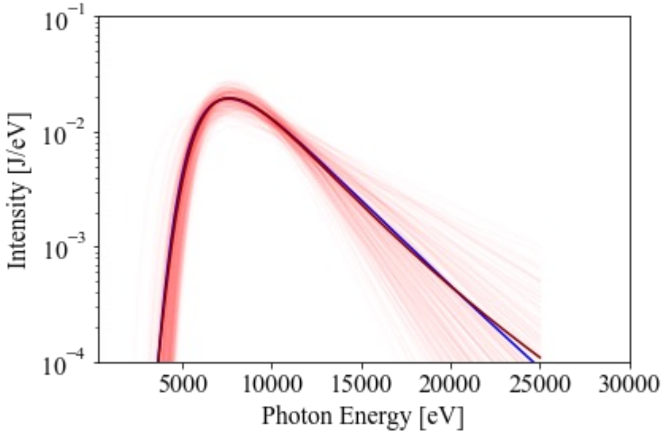
PCDs are a workhorse diagnostic on Z, but their highly integrating nature makes it difficult to extract source information

Using a database of 1D MagLIF simulations we were able to optimize the detector and filter configurations to minimize uncertainty in source temperature, areal density, and total output

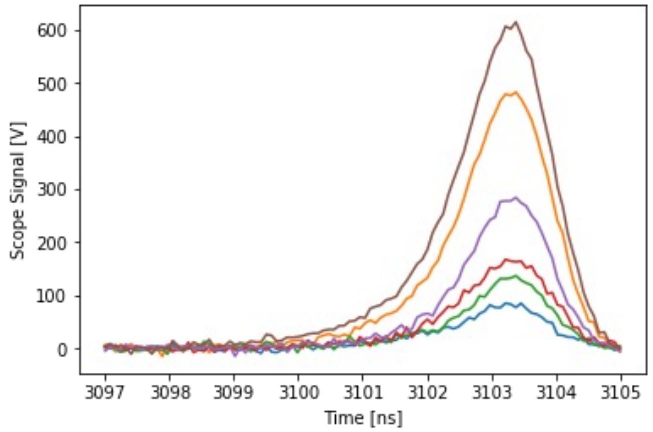


Need to add a penalty to the optimization

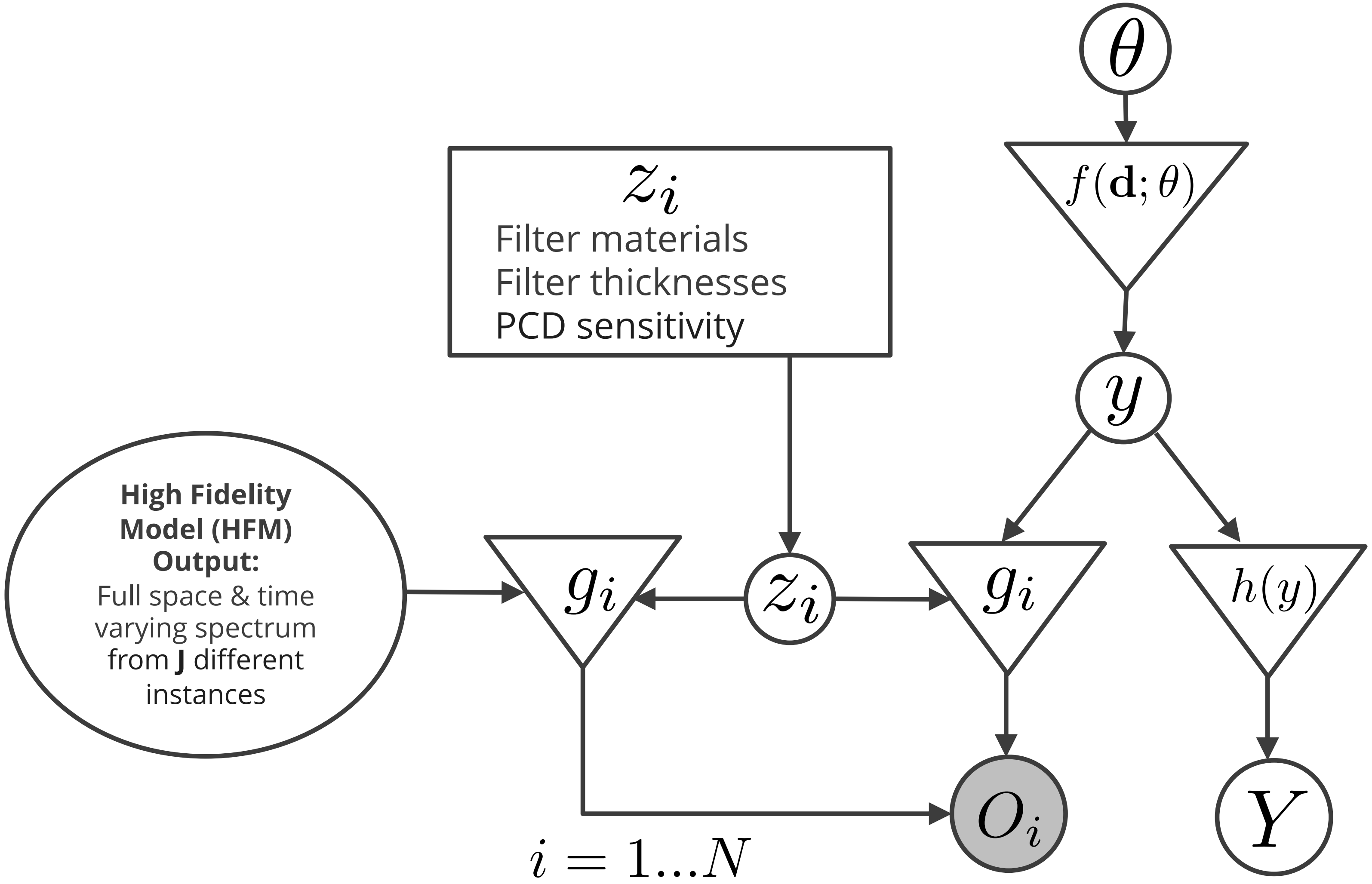
Source Spectrum



Filtered Power Signals



In order to optimize the instrument configuration we must evaluate the quality of the inference at each proposal



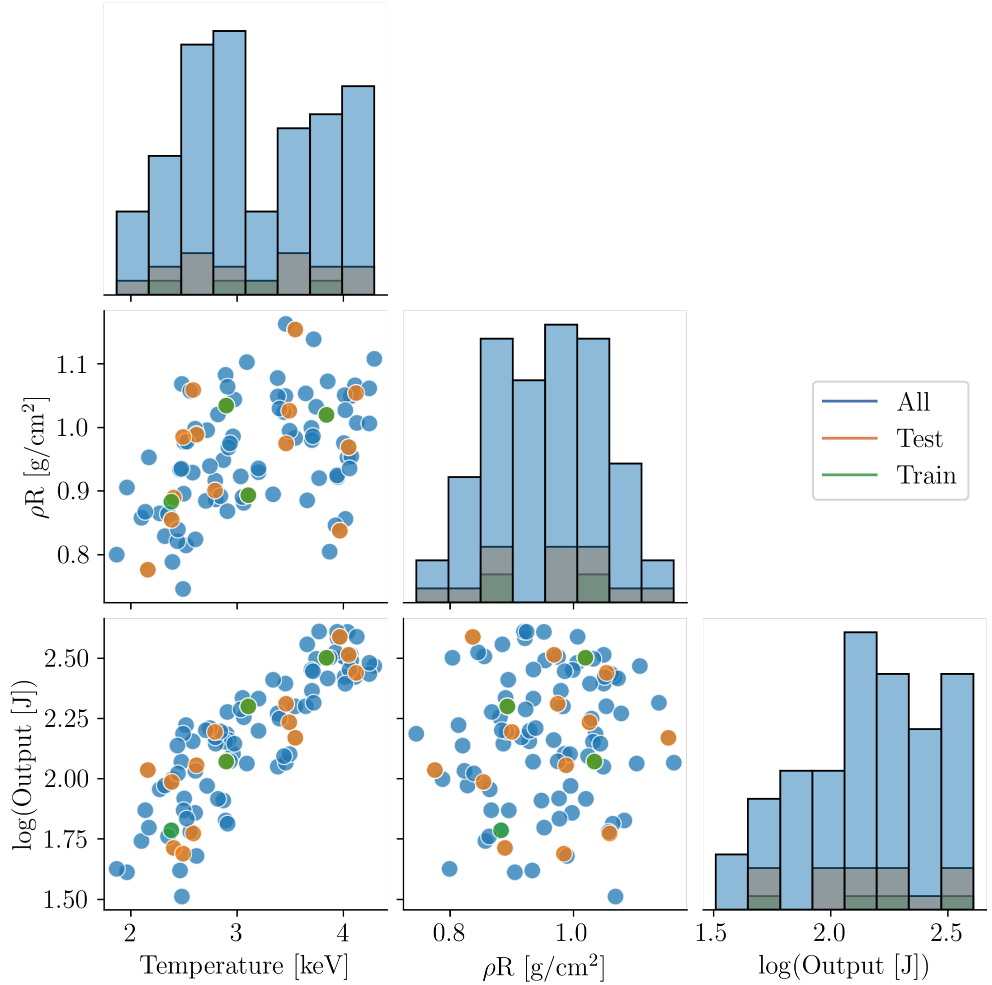
Procedure

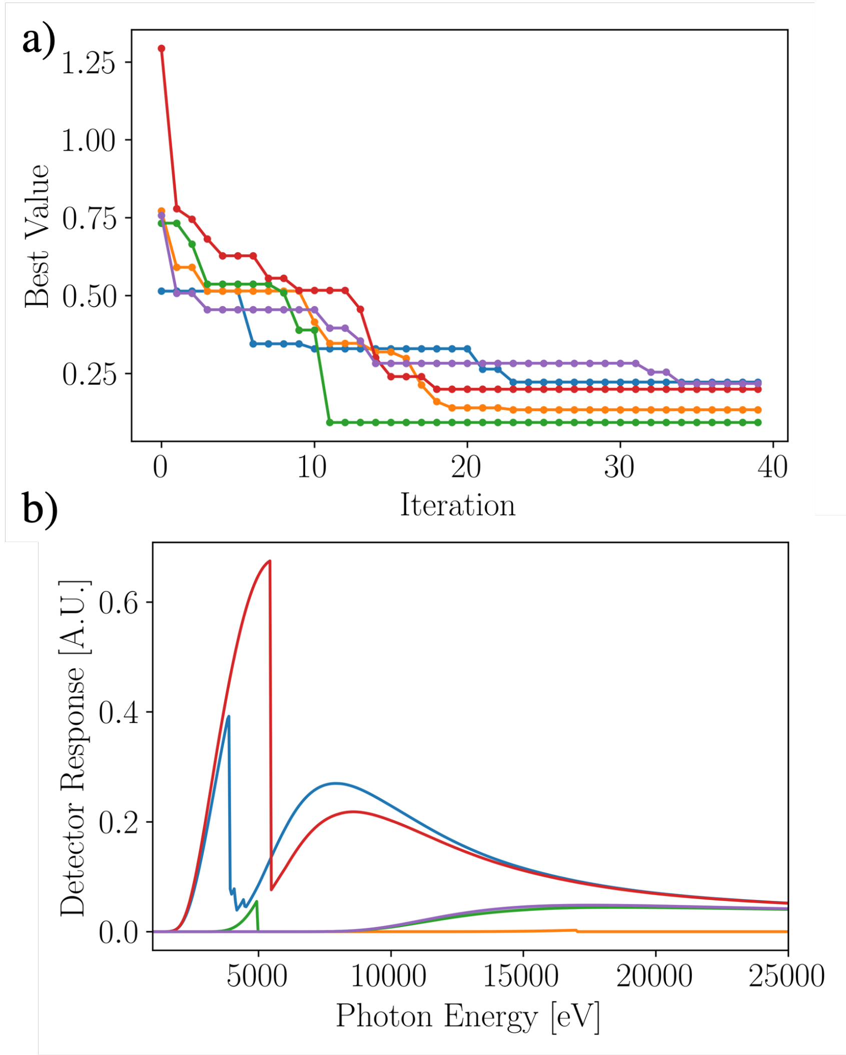
1. Choose z_i (filter material and thickness for each element)
2. Create O_i from HFM output for each element with chosen configuration
3. sample posterior with chosen configuration and new O_i
4. Compute MSE from posterior samples
5. Fit GP and compute EI to select new point
6. Go back to (1) with new choice, iterate until stopping criterion is reached

$$\mathcal{M} = \log(MSE + \lambda L) \quad Z_{\mathrm{opt}} = \underset{z_i}{\mathrm{argmin}} \sum_{j=1}^{J} \mathcal{M}_j$$

P.F. Knapp et al., under review

We leverage an ensemble of high fidelity calculations to train and validate our optimization procedure





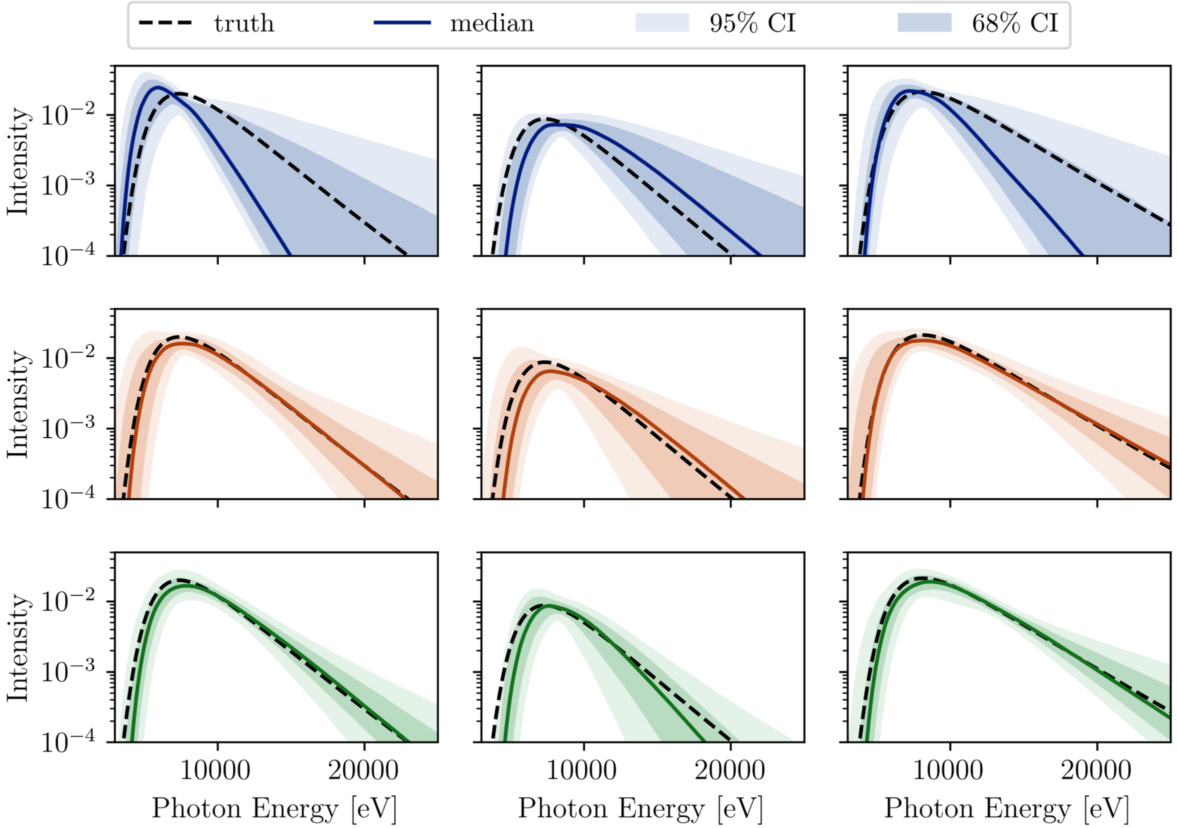
Bayesian optimization is used, allowing mixed continuous & categorical variable

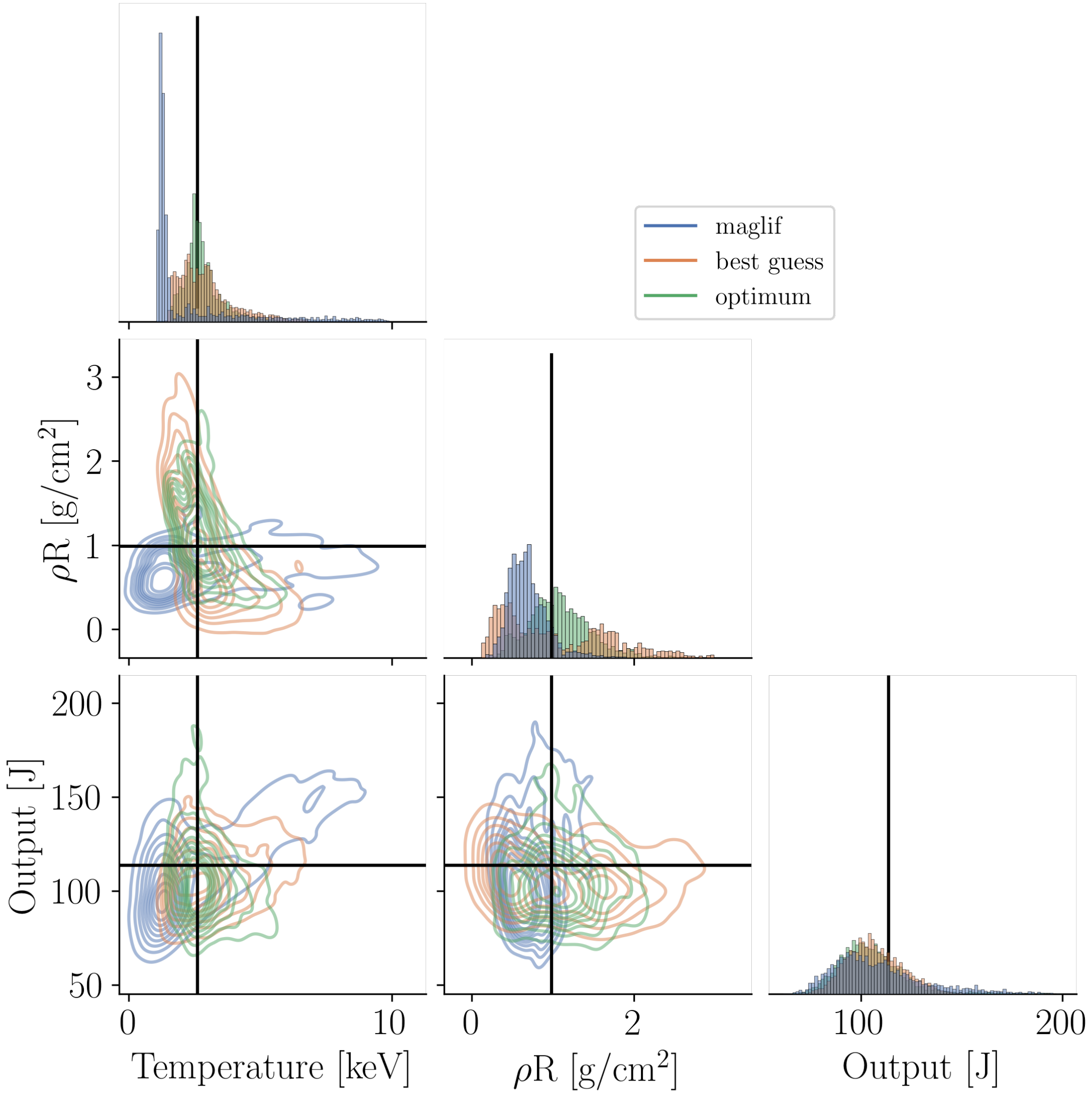
Due computational cost, only 4 training and 16 validation points were selected from the ensemble

Support points were used to ensure the samples represent the distribution

P.F. Knapp et al., under review

Our optimized configuration outperformed two reference cases in both fitting the output spectrum and other reduced quantities





P.F. Knapp et al., under review

With our collaborators at GA Tech we are developing efficient methods to optimize experiments

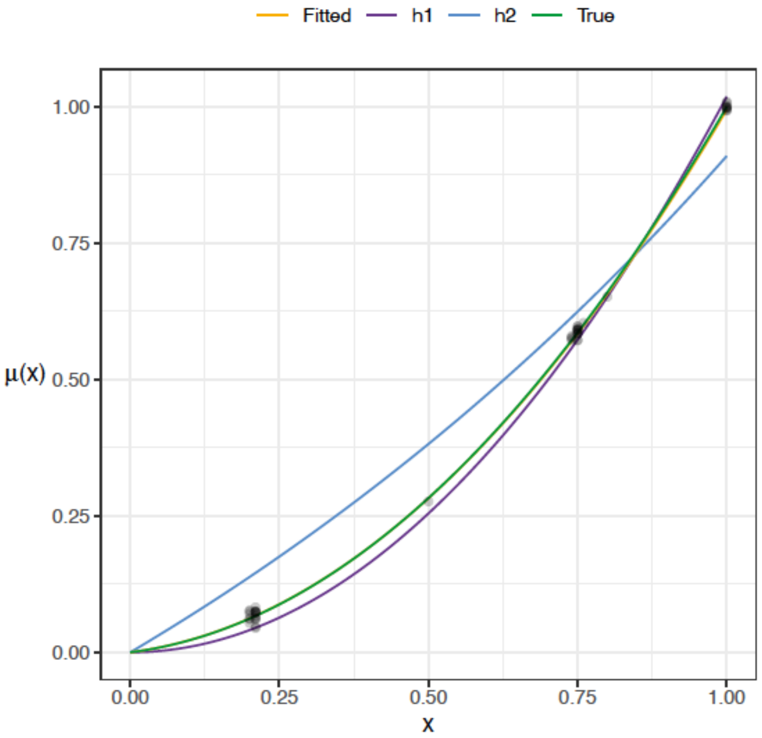
The ability to field experiments that effectively distinguish between competing hypotheses is at the core of the scientific method

$$\mu(x) = \lambda h_1(x;\theta_1) + (1-\lambda)h_2(x;\theta_2)$$

Find x that minimizes uncertainty on λ, subject to priors on θ

$$\mathcal{I}(\beta,\theta_1,\theta_2,\mathbf{X}) = \frac{1}{\sigma^2}\sum_{i=1}^{n} g_i g_i^T$$

Use the information matrix to find x



Georgia Tech

V.R. Joseph

C.F.J Wu

A fully Bayesian approach to experiment design

Testing shows the method is efficient and effective, outperforming methods in the literature

Need to generalize to many parameters, varying λ, nested models, and implement in a pipeline with simulation & diagnostic models

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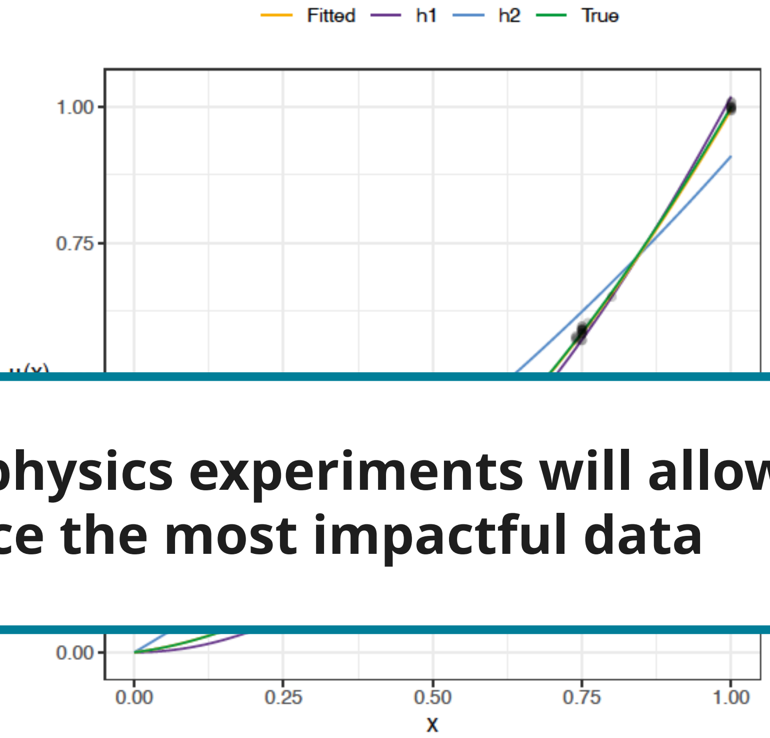
Applying this tool to the design of multi-physics experiments will allow us to guide our experiments to produce the most impactful data

Use the information matrix to find x



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Summary

We are developing and applying modern data science tools to dramatically reshape the way we conduct expensive, high impact experiments

- Applied a Bayesian data assimilation tool to make inferences from disparate experimental data
- Utilized deep learned surrogate models to accelerate greedy optimization and sampling algorithms while retaining physical fidelity
- Developed methods to process and quantify images and reconstruct 3D volumes from sparse views
- Developing dynamical surrogate models that respect underlying physics
- The future is the application of these tools in concert to optimize the use of scarce experimental and personnel resources, maximizing our ability to gain new and impactful information

Next Steps and Gaps

Our vision is an enormous technical challenge, but the payoff is tremendous

- The application of this to ICF and HED science is new and we are rapidly making progress, but there is much more work ahead
  - Good inferences require good data – we need robust methods to reduce our data with confidence
- Bayesian inference is expensive
  - Surrogate models provide a means to do this efficiently, but obtaining data and training the models is challenging
- Surrogate models that preserve physics and provide us access to the underlying processes are critical for applications like experiment design
  - Existing methods have limitations when applied to ICF and HED systems
- Robust and efficient methods to sample and optimize experiments for maximal impact