Cognitive Simulation models for inertial confinement fusion

LPA Workshop

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LLNL-PRES- 830976

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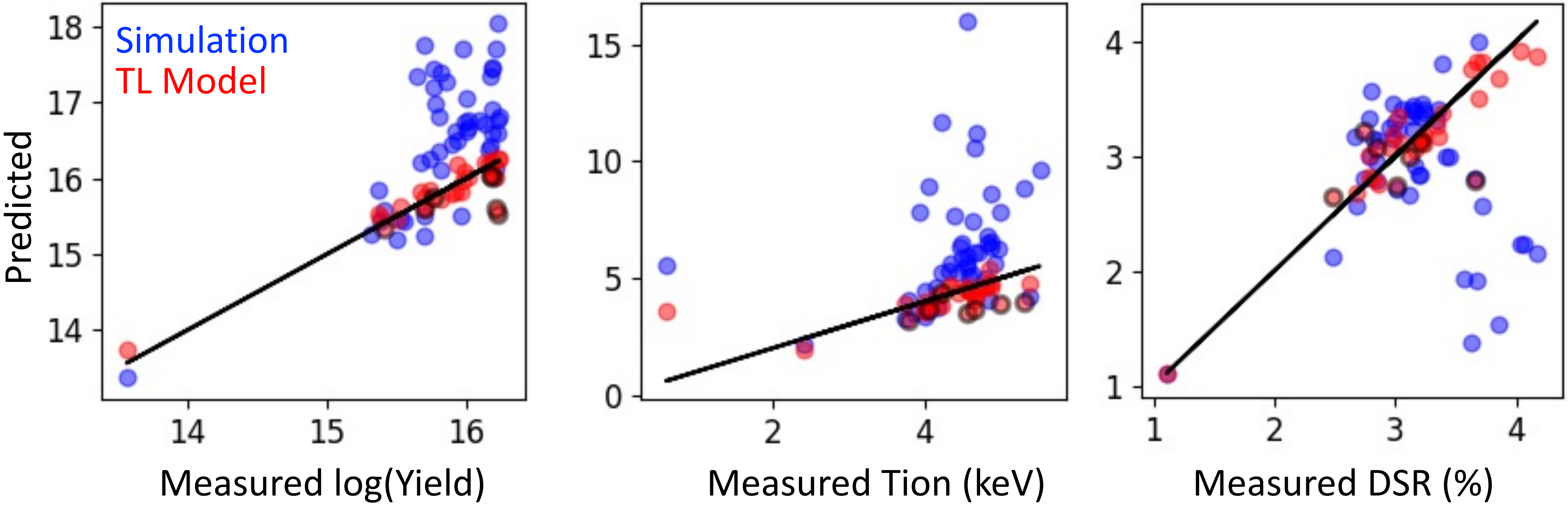
Inertial confinement fusion simulations are not consistently predictive of ICF experiments



How can we reduce the discrepancy using the simulation and experiment knowledge we have on hand?

We are advancing transfer learning as a method for combining simulation and experiments into a common, predictive model

- We've developed two approaches to transfer learning for ICF
  - Direct drive ICF – "Input to output" TL
  - Indirect drive ICF – TL with autoencoders

- These data-informed models are a new tool for design optimization, exploration, and improving understanding of model discrepancies

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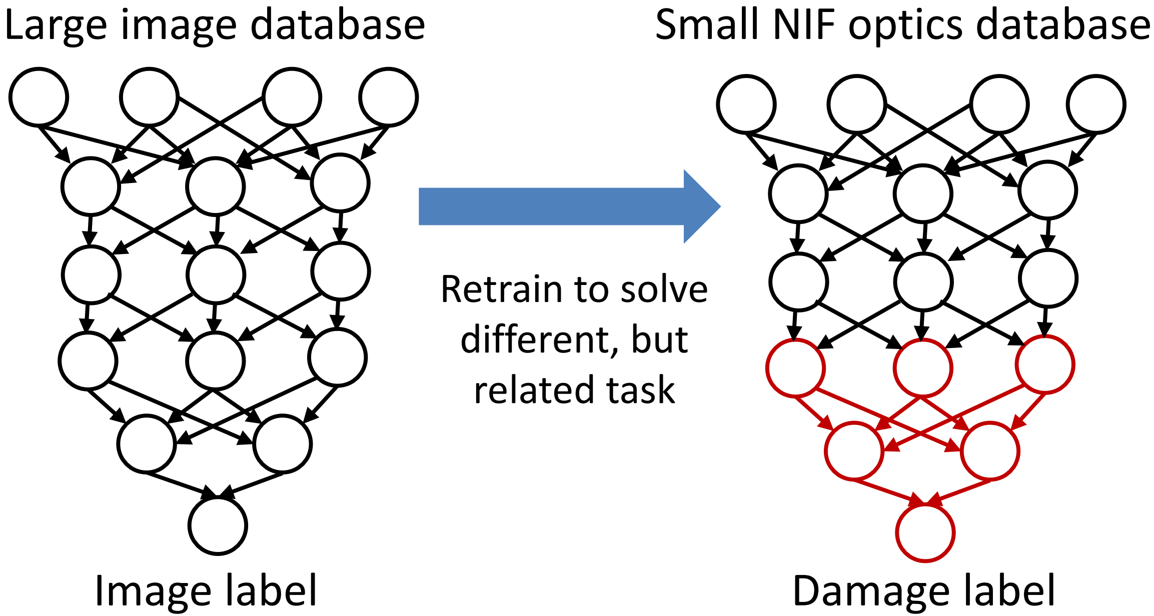
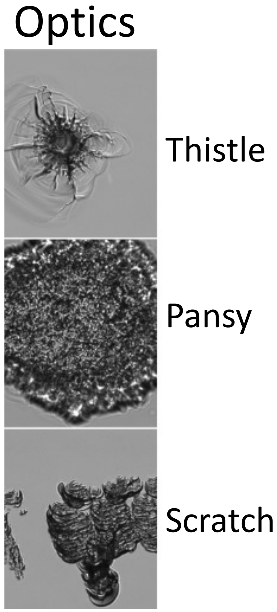
“Transfer learning” is when a network trained to solve one task is retrained to solve a different task with limited data



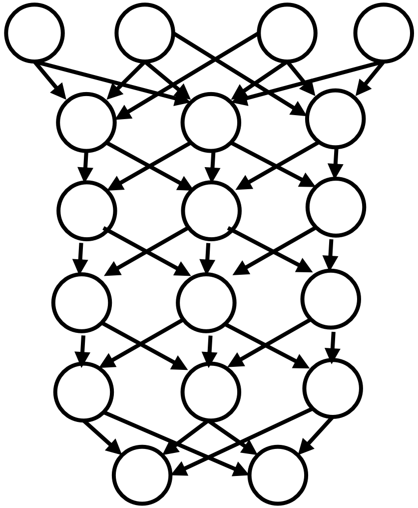


Can transfer learning be used to “transfer” between simulations and experiments?

Transfer learning provides a map from inputs to outputs using large simulation ensembles and sparse experimental data

Train NN on large database of inexpensive simulations

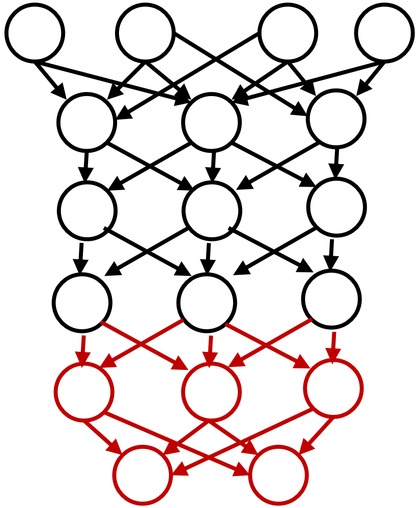
Simulation Inputs



Simulation Outputs

Freeze all but the last layers of the network, retrain on sparse, expensive data

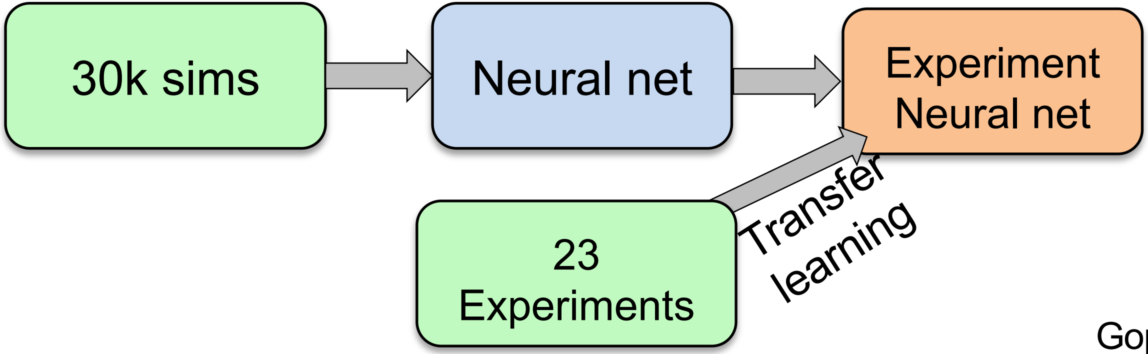
Experiment Inputs



Experiment Outputs

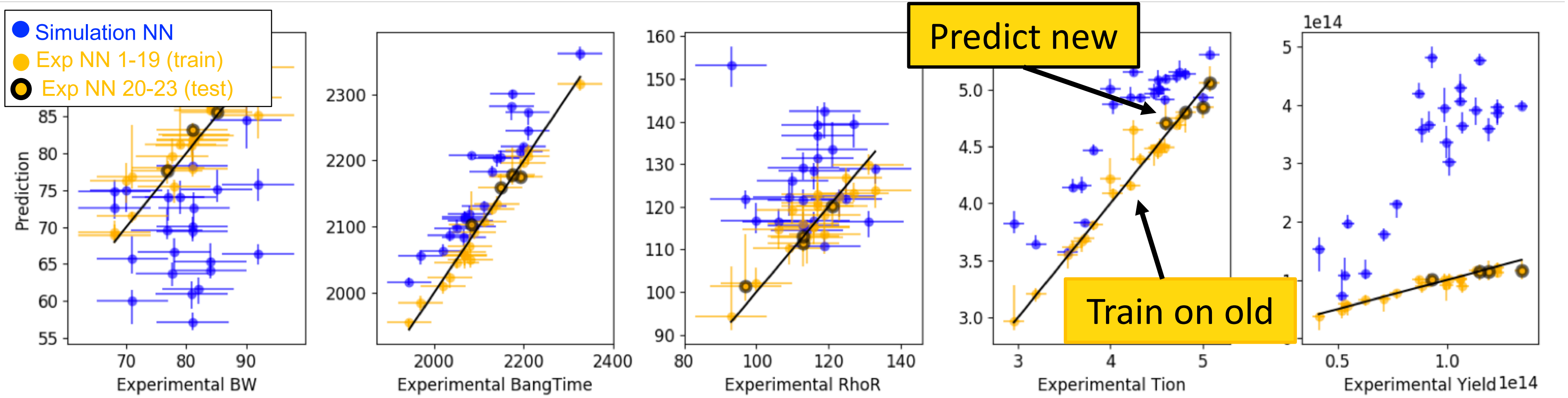
Can TL predict future Omega ICF experiments with higher accuracy than simulations?

- The data* includes:
  - 30k 1D LILAC simulations
  - Spans a 9D input space with varying laser pulse & capsule dimensions
  - 23 experiments
    - Experimental measurements of yield, bang time, Tion, rhoR, burnwidth



*Data provided by Varchas Gopalaswamy & Riccardo Betti

Transfer learned neural networks are *more predictive* of future Omega experiments than simulations



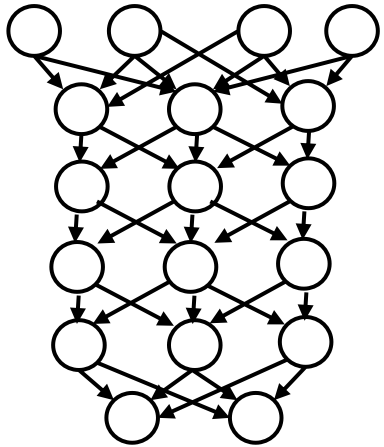
Experimentally informed Neural Network can predict future Omega experiments

*Error bars produced by training ensembles of neural nets

"Transfer Learning to Model Inertial Confinement Fusion Experiments"
Humbird et al, IEEE Plasma Science (2020)

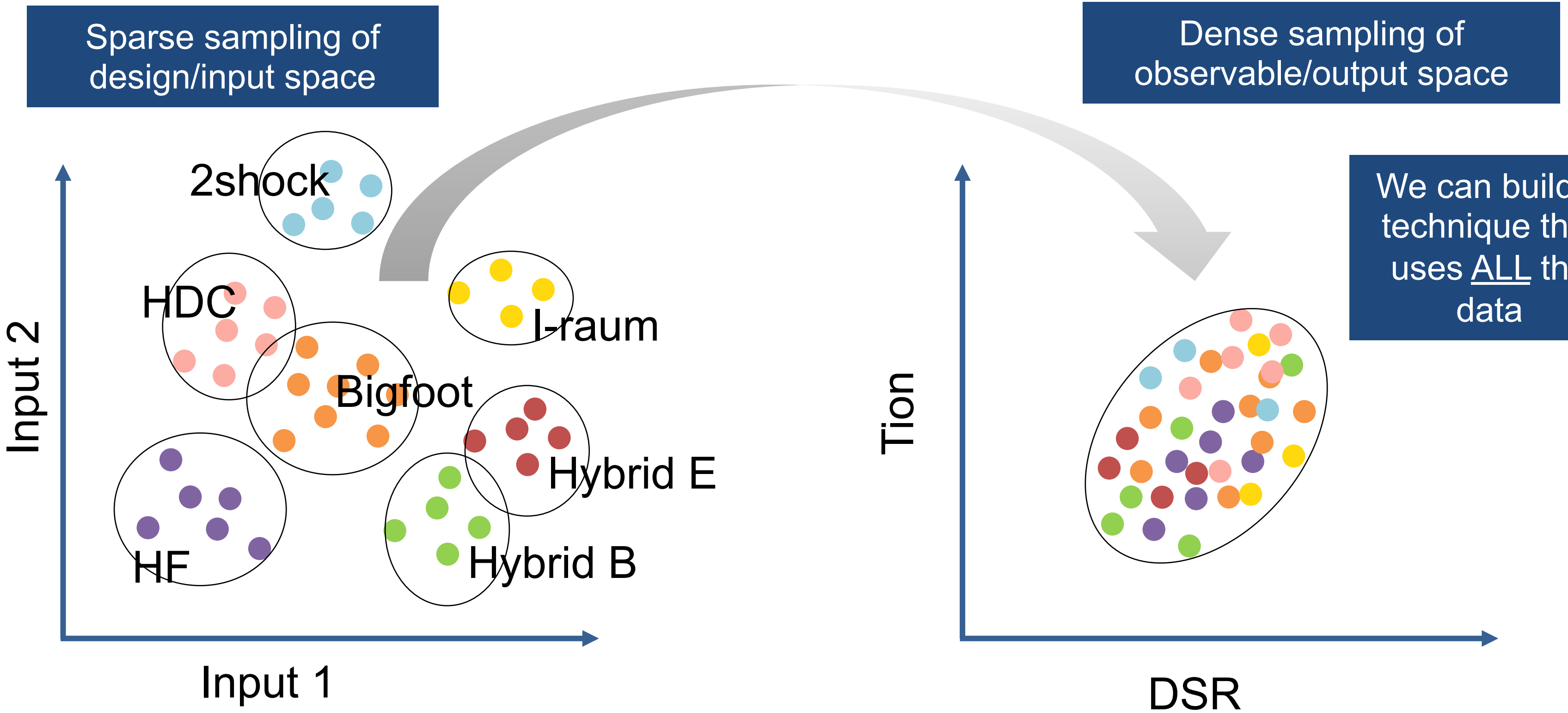
Applying "input to output" transfer learning methods to indirect drive ICF is challenging

- For Omega, capsule simulations are analogous to the experiment; for NIF it's hohlraums
- The NIF experimental design space is *broad* and *sparsely populated*
- Hohlraum simulations are very expensive



Novel transfer learning techniques are needed to create predictive models of indirect drive experiments

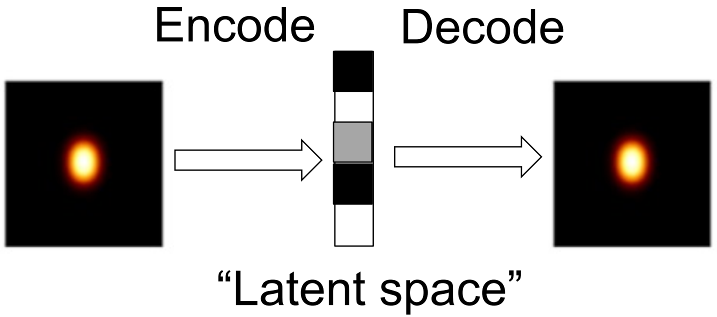
The input space for NIF is sparsely populated, but the observable *output space* for DT shots are often similar



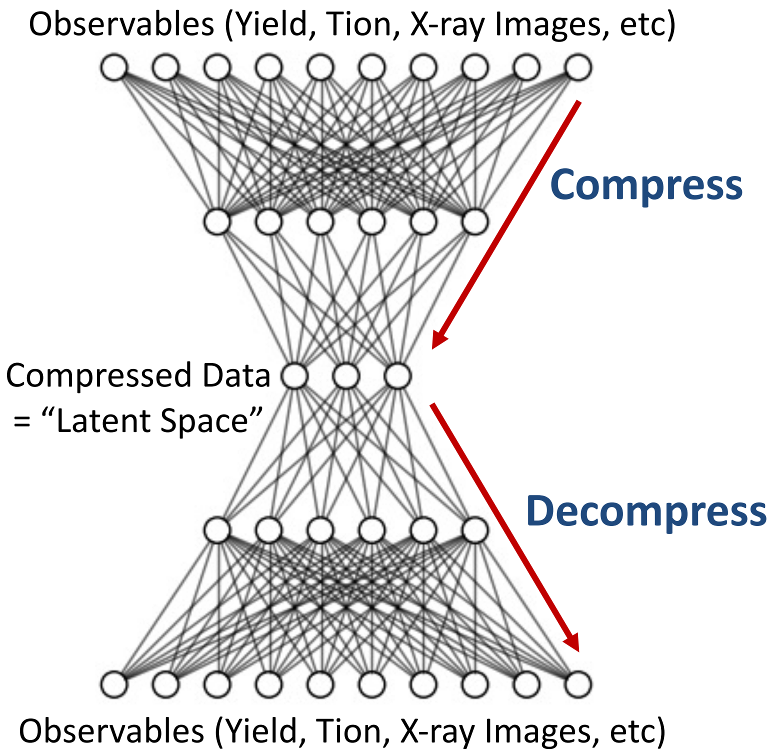
We can build a technique that uses ALL the data

We are exploring a different approach to transfer learning based on the output space of NIF experiments

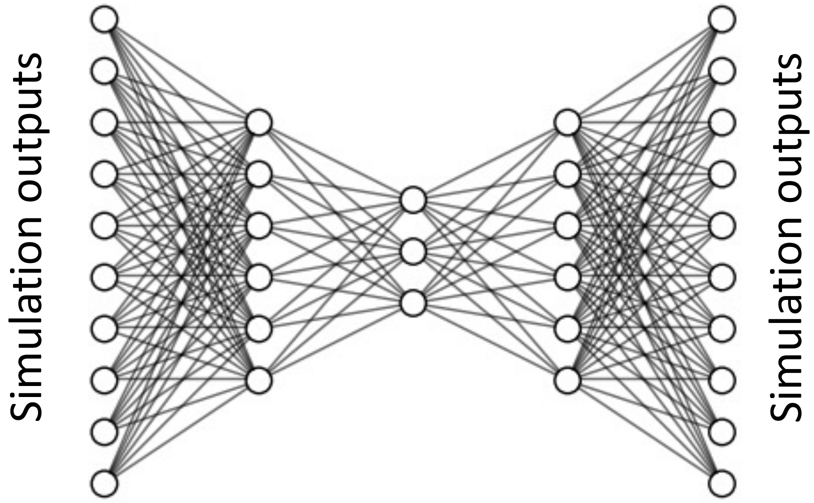
- Autoencoders are a type of neural network traditionally used for data compression



- Latent space formed by learning correlations and redundancies in the input data

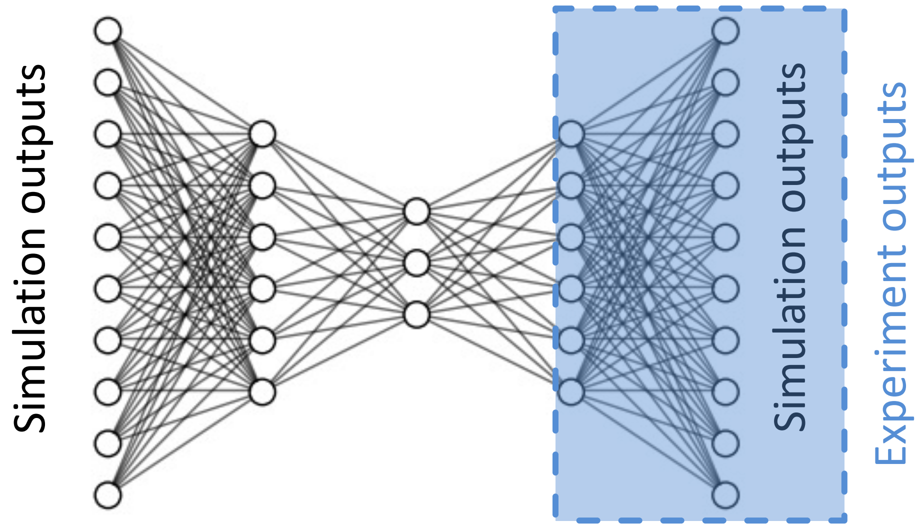


Can we transfer learn an autoencoder to map from *simulation outputs* to *experimental outputs*?



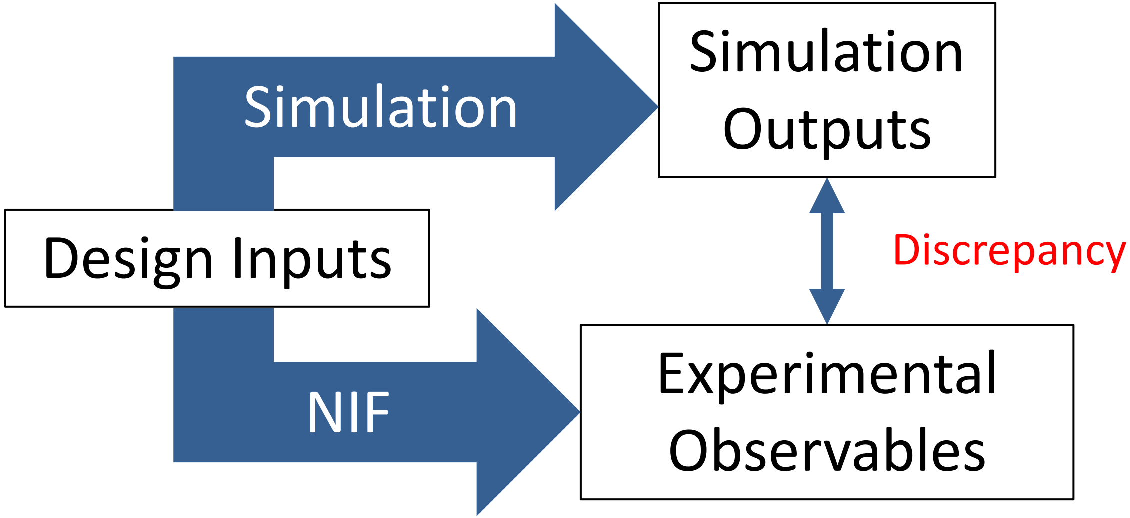
Step 1: Train an autoencoder to learn relationships between outputs from a large simulation database

Can we transfer learn an autoencoder to map from *simulation outputs* to *experimental outputs*?



Step 2: Use predicted simulation outputs and corresponding experimental outputs to transfer learn the autoencoder

A transfer learned model provides a new tool that improves our design loop



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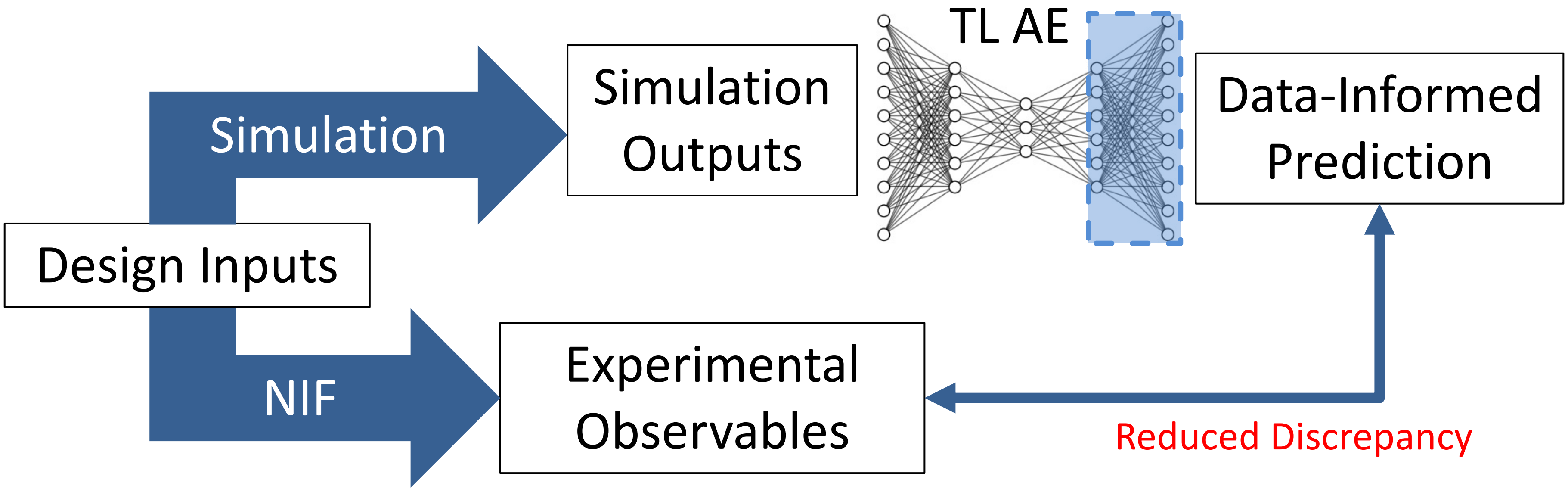

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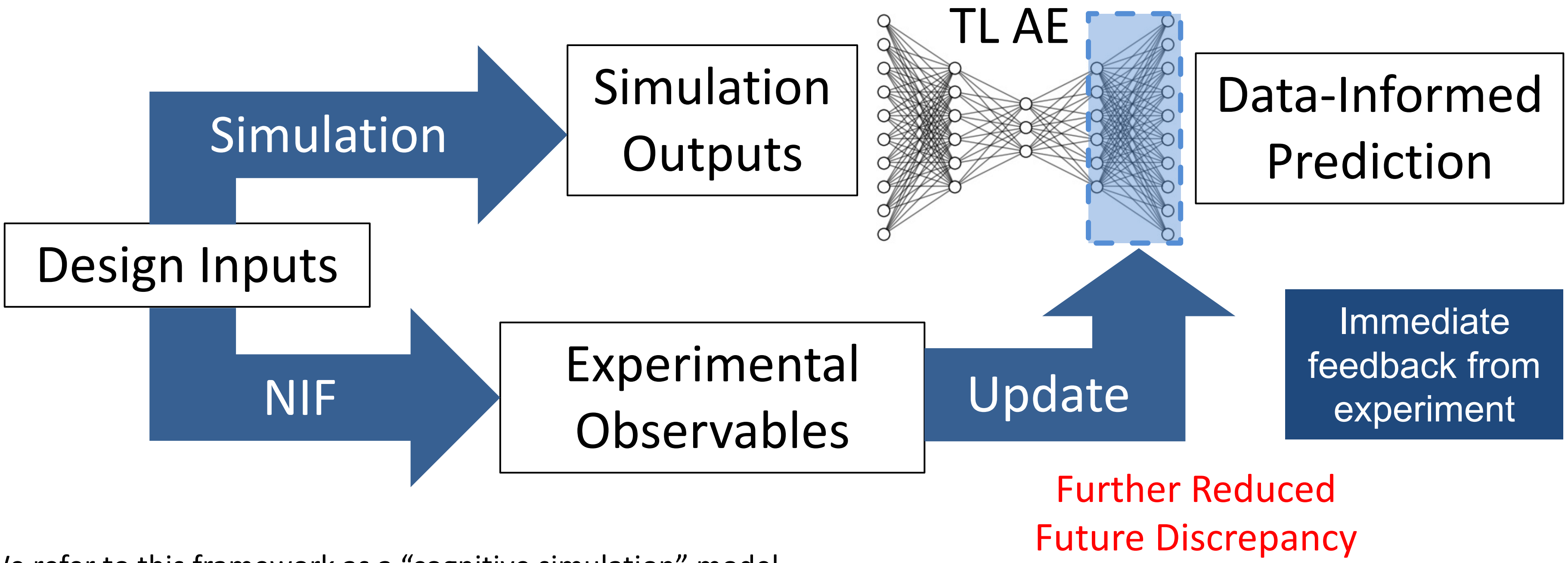
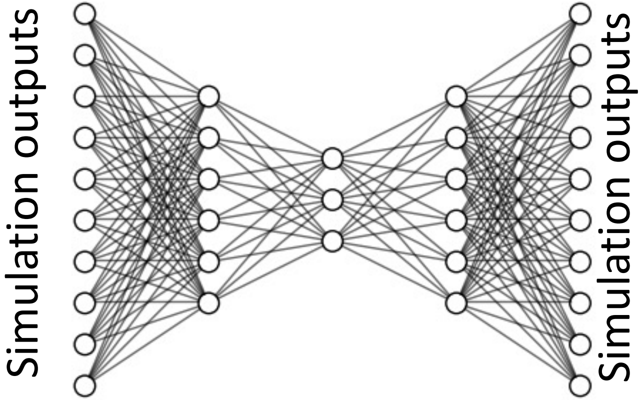


*We refer to this framework as a "cognitive simulation" model

Humbird, KD, et al. "Cognitive simulation models for inertial confinement fusion: Combining simulation and experimental data." *Physics of Plasmas* 28.4 (2021)

NIF DT shots from a variety of campaigns are included in the CogSim model

- Train the autoencoder on existing databases of ~160k capsule simulations



Uses ALL the data: 2shock, I-raum, HDC, Bigfoot, Hybrid campaigns

*Hydra Python Deck, courtesy of Jay Salmonson

NIF DT shots from a variety of campaigns are included in the CogSim model

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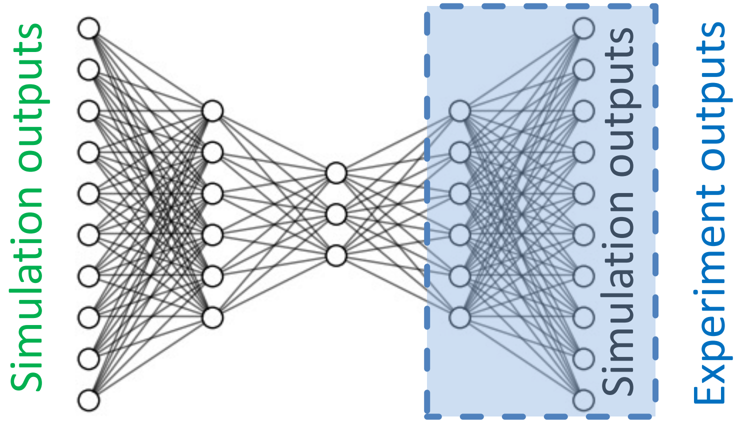
- Create a set of (Simulation Predictions, Experimental Measurements) for a set of ~50 previous NIF DT shots



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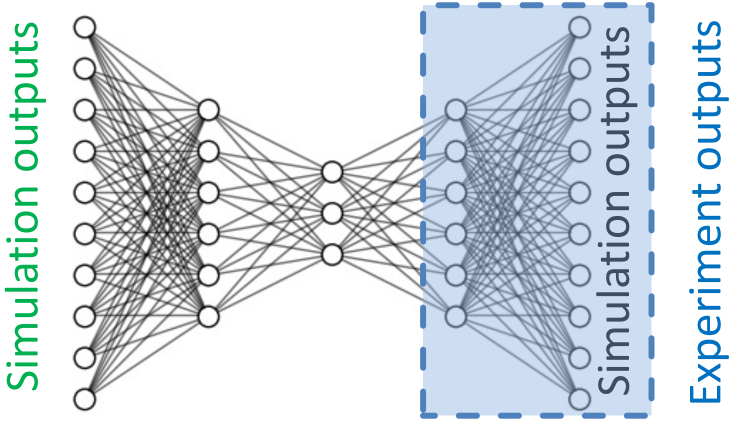
- Create a set of (Simulation Predictions, Experimental Measurements) for a set of ~50 previous NIF DT shots

- Start TL with one experiment, update the model after each shot in chronological order



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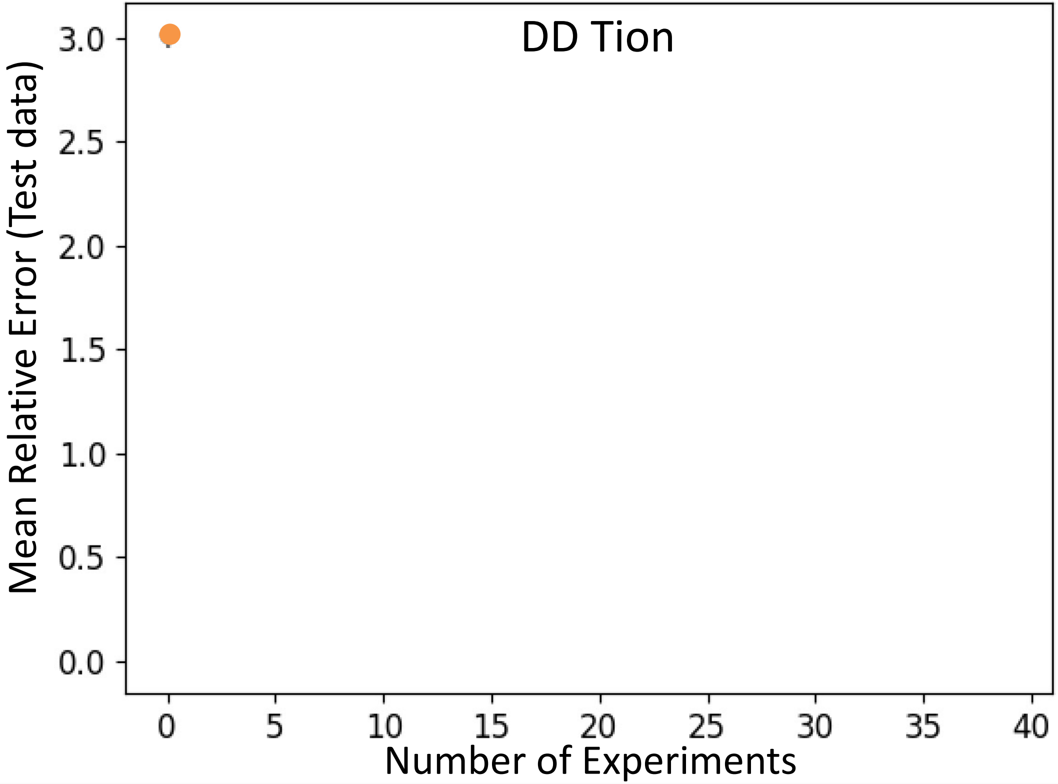
As we acquire data the mapping from predictions -> experimental measurements becomes more accurate

- *Test* predictive capability by predicting the 7 recent holdout shots in the database (HyE, 2shock, Iraum)



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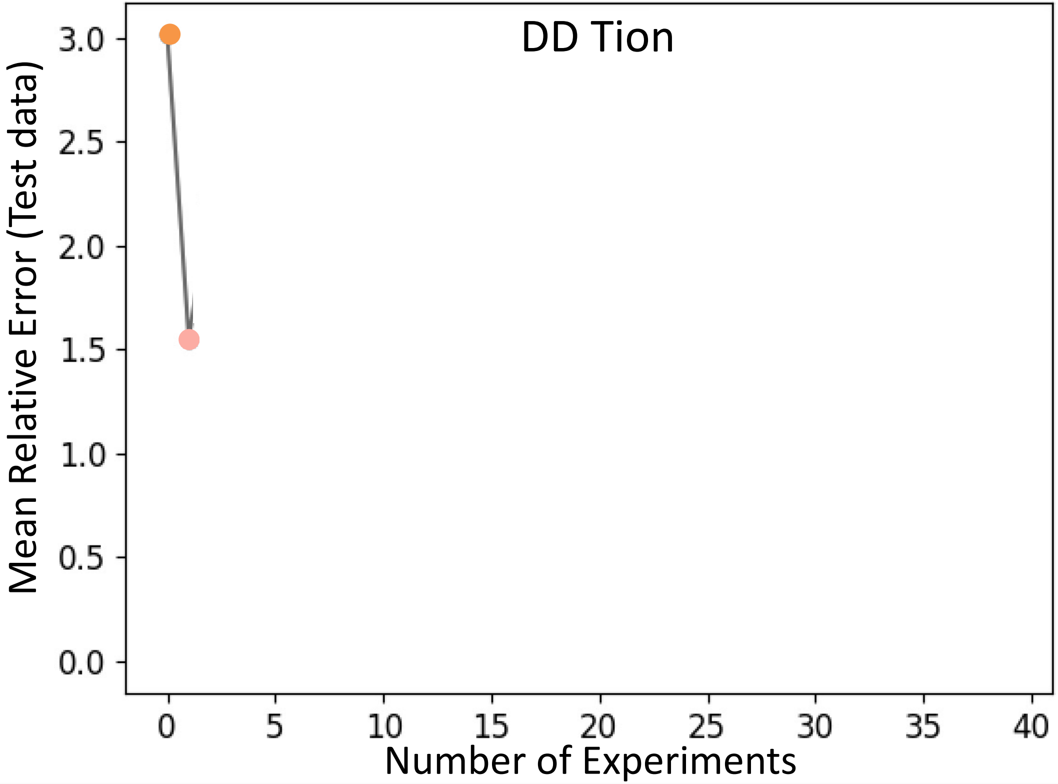

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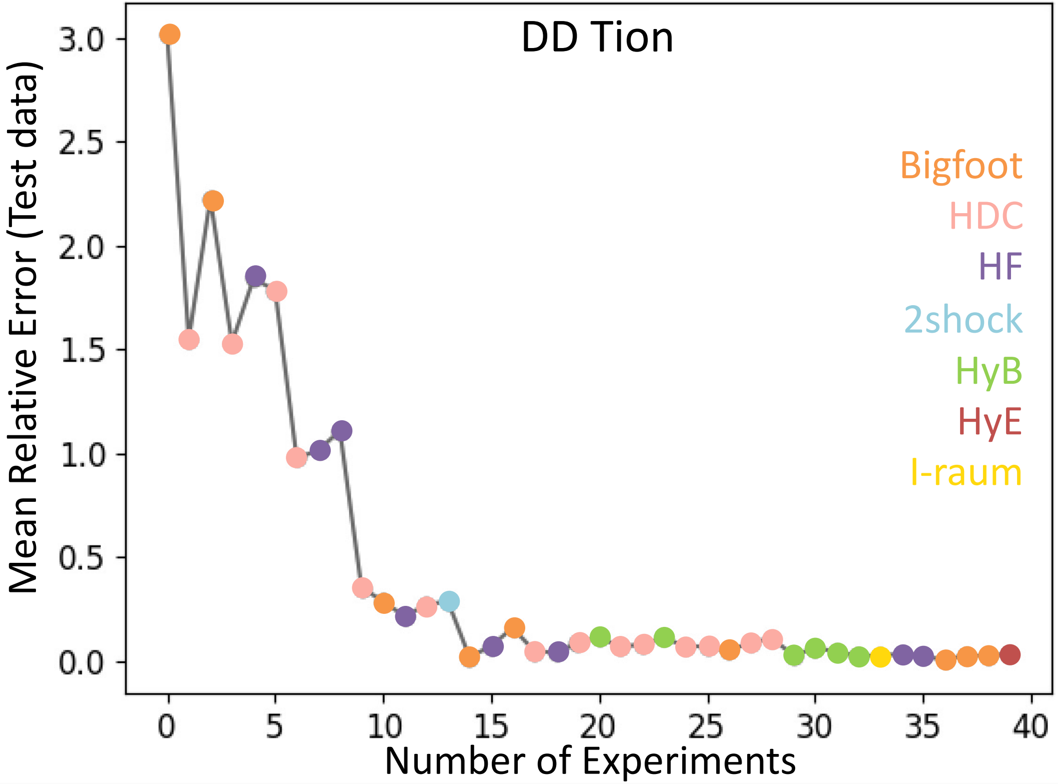
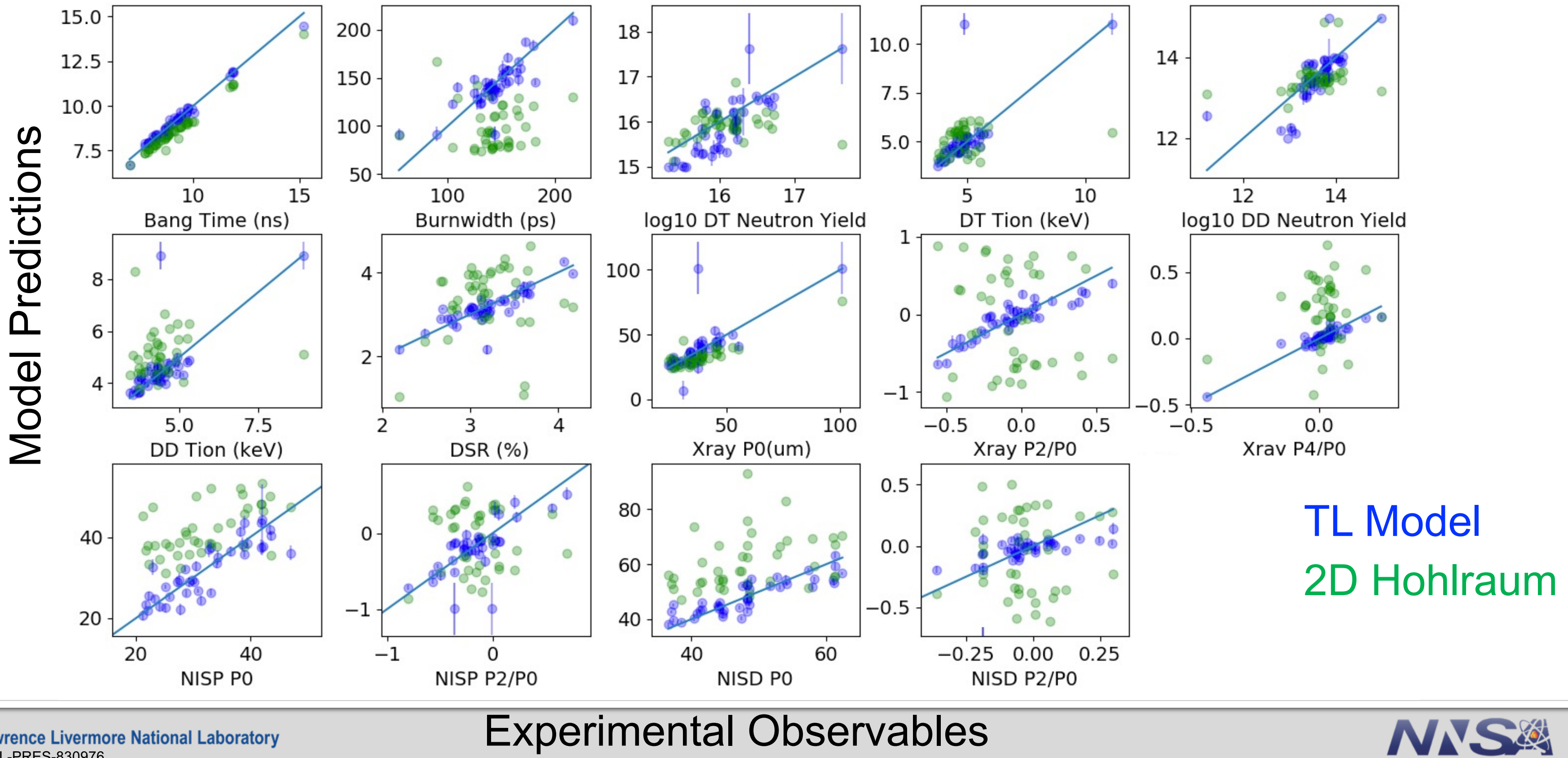
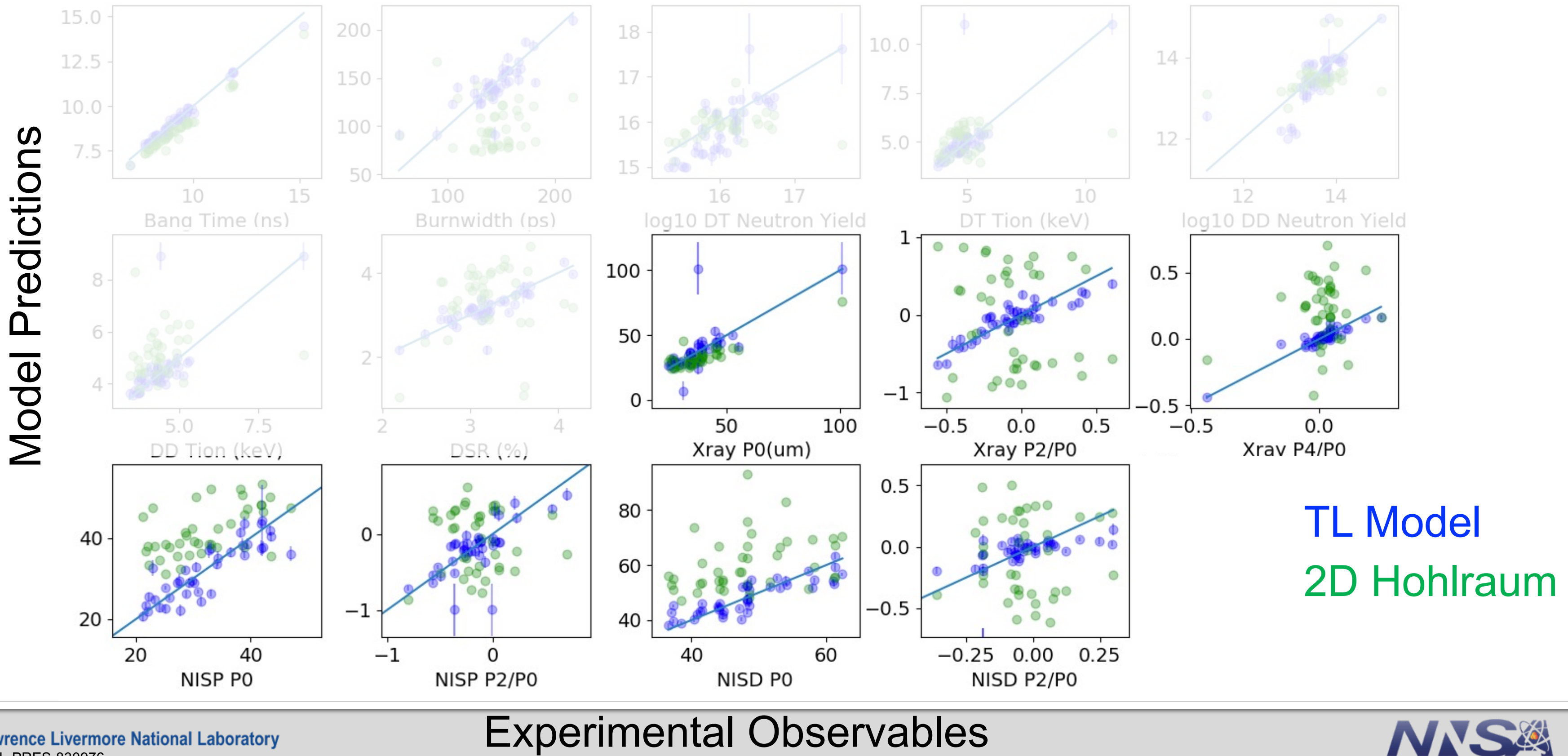


The CogSim model is more accurate than simulations for a wide variety of NIF experiments



The CogSim model can correct the significant mismatch in shape between the simulations and experiments



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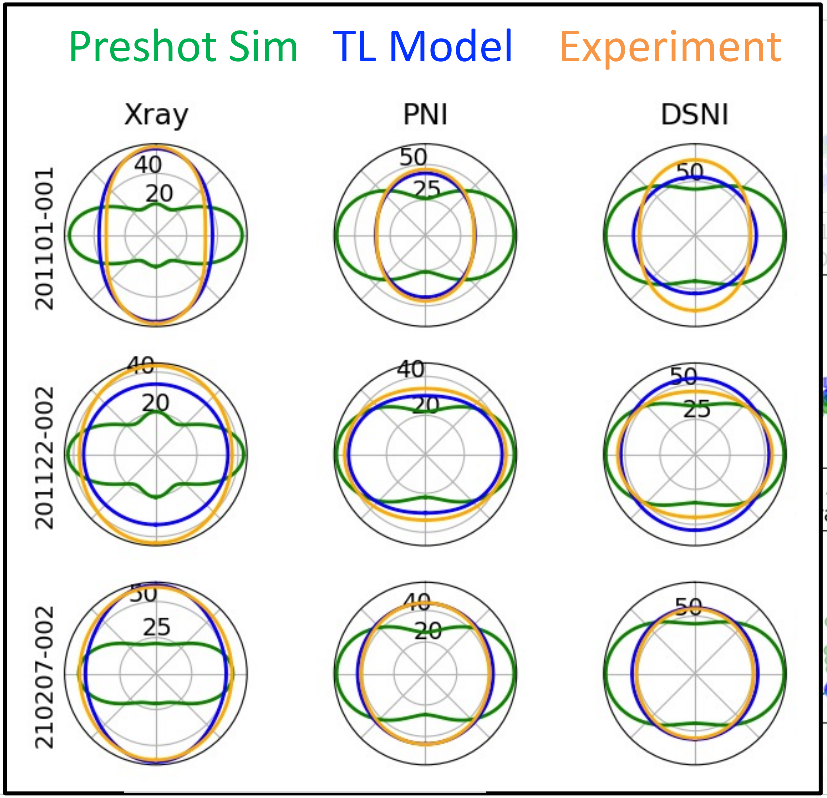
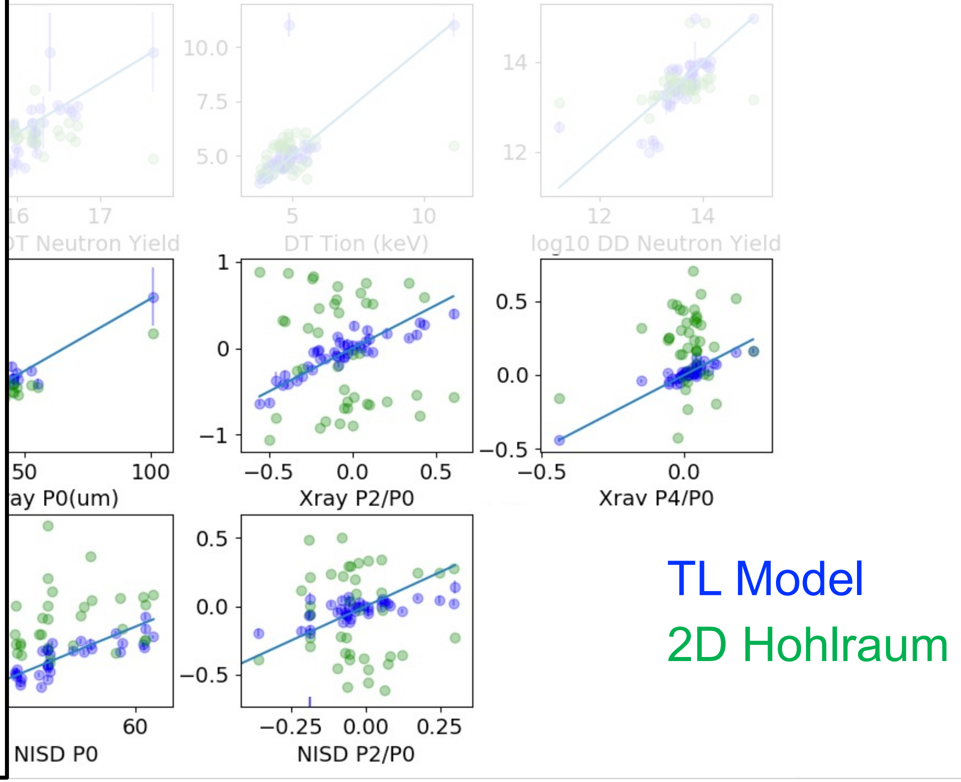




Experimental Observables

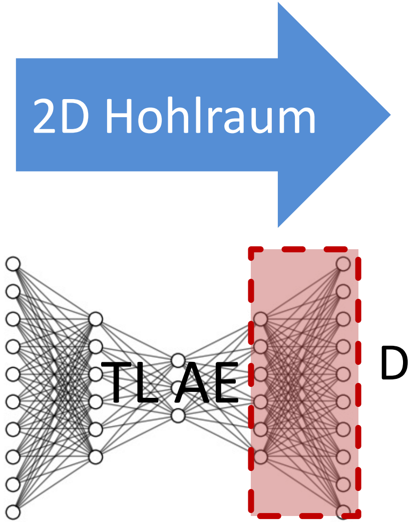
We are advancing transfer learning as a method for combining simulation and experiments into a common, predictive model

- We've developed two approaches to transfer learning for ICF
  - Direct drive ICF and the "traditional" TL approach
  - Indirect drive ICF – TL with autoencoders

- These data-informed models are a new tool for design optimization, exploration, and improving understanding of model discrepancies

Data-informed maps of the ICF design space could guide us toward high performing designs efficiently

Parameter
Scan
(peak power,
pulse length)



Simulation
"Map"

Data-informed
"Map"

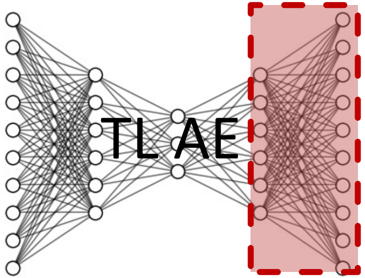
Data-informed maps of the ICF design space could guide us toward high performing designs efficiently

2D Hohlraum

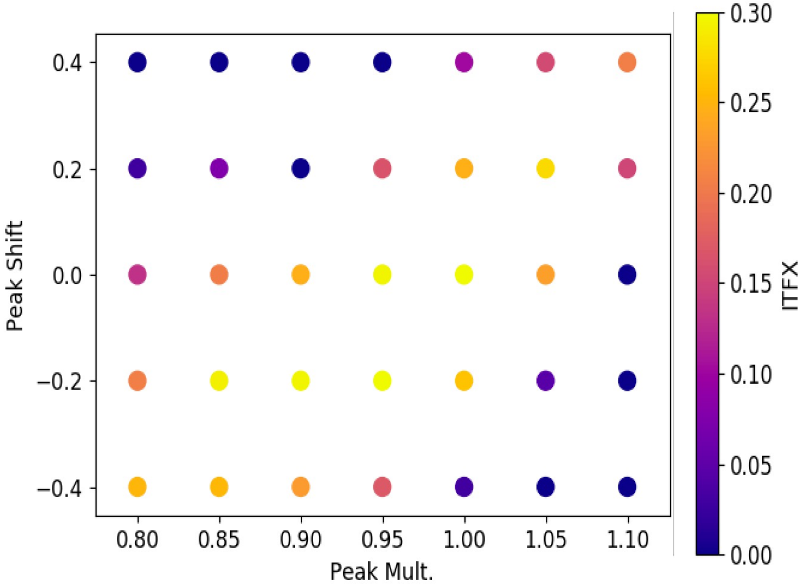
Simulation “Map”

Parameter Scan

(peak power, pulse length)

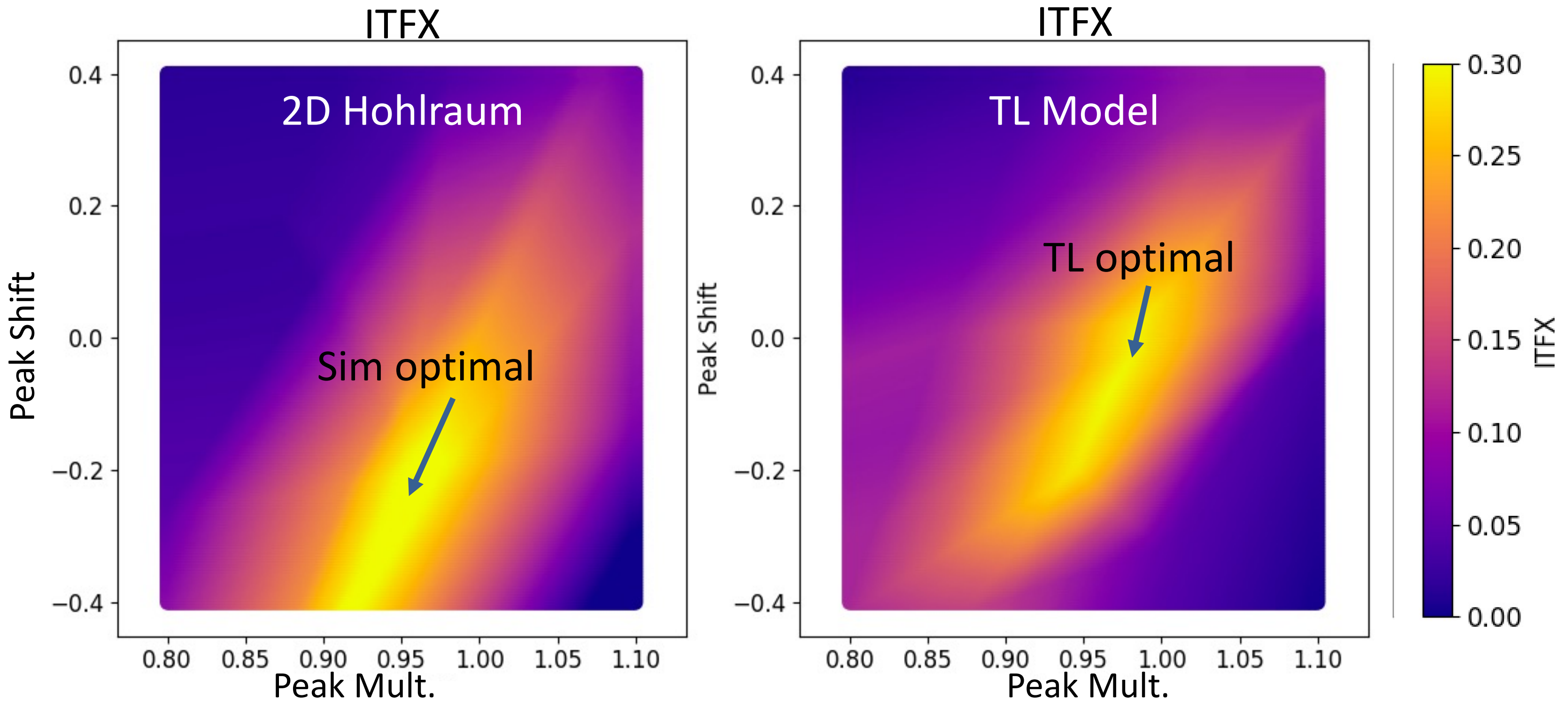


Data-informed “Map”



- Run hohlraum simulations to map out 2D parameter space
- Search Sim only, Sim+Data maps for “best design”

Data-informed map predicts the "best design" is in a different location than the simulation map



ITFX = 1/0.25(Y/1.2e16)*(DSR/0.07)^2.3

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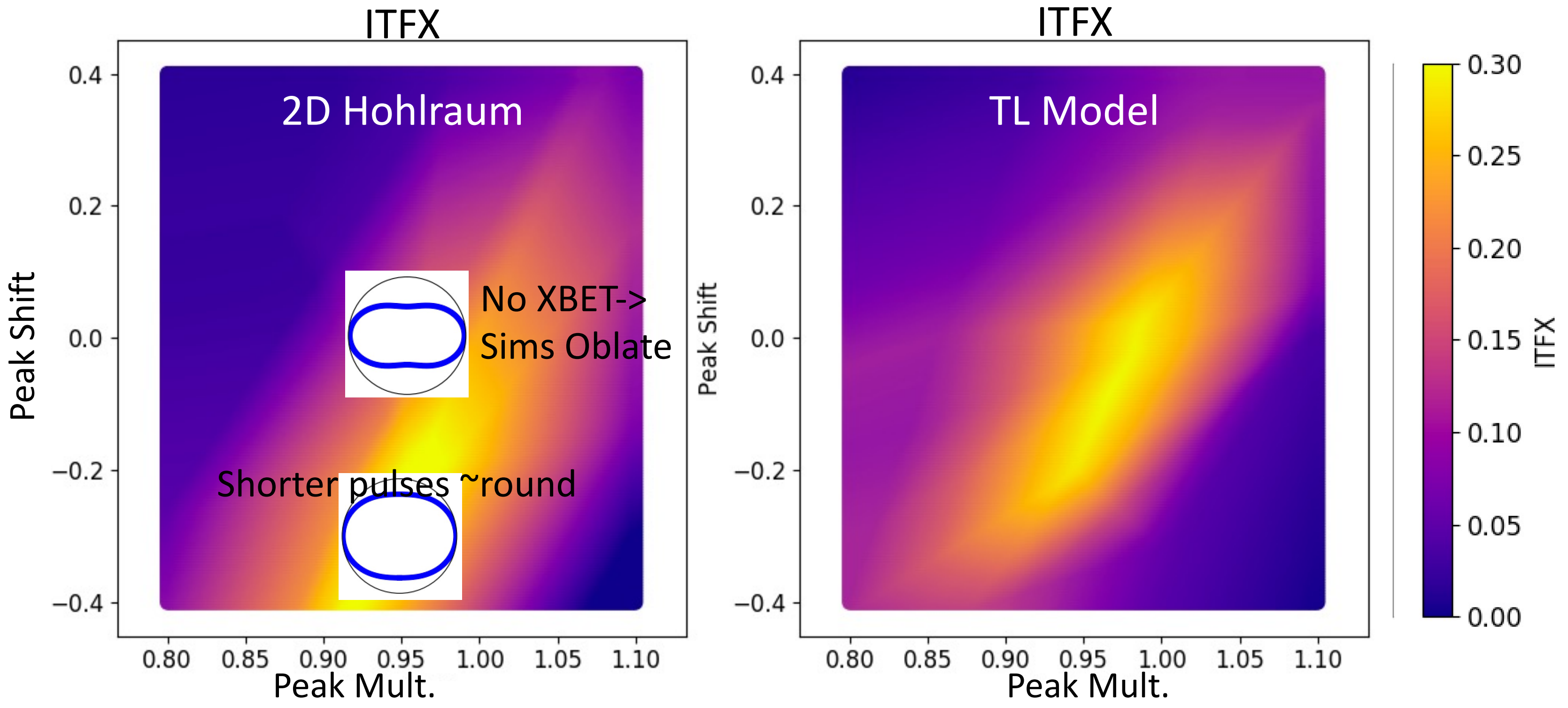

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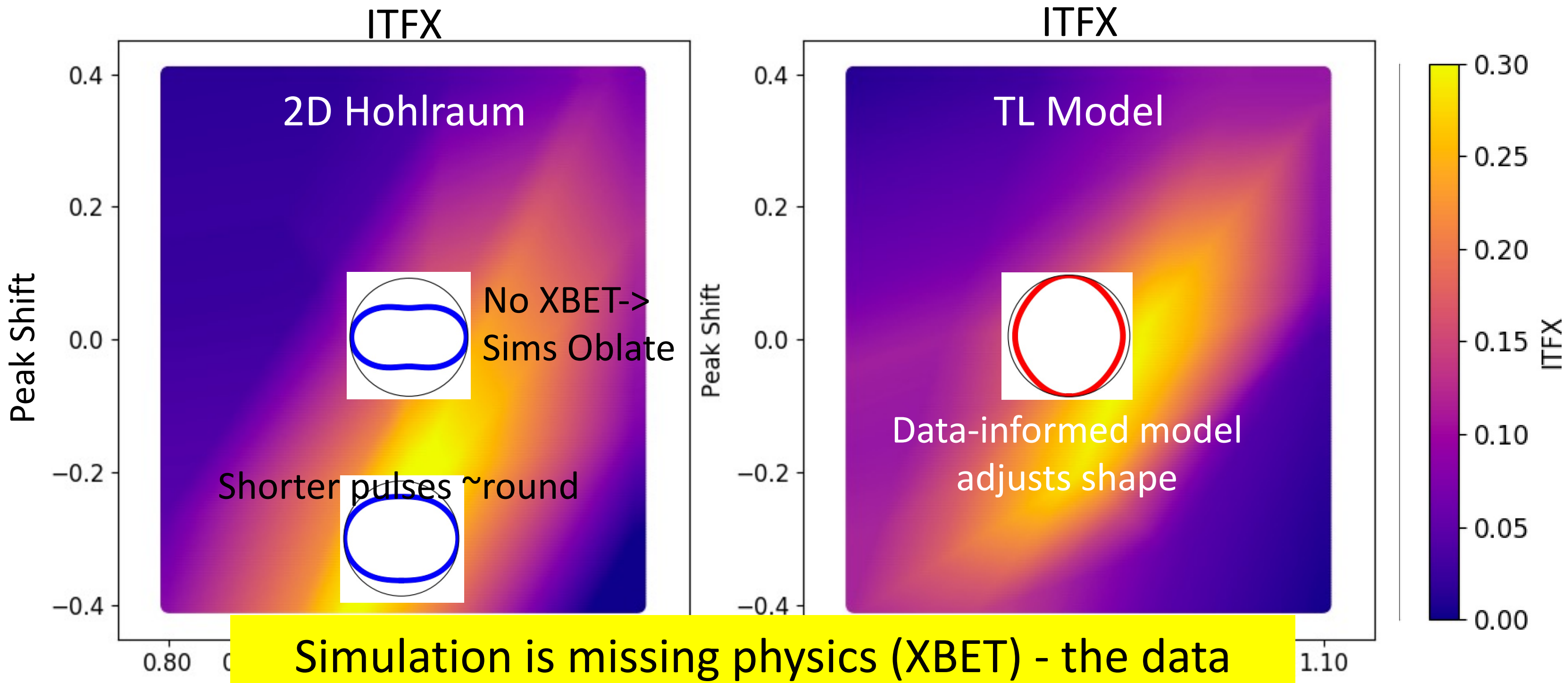
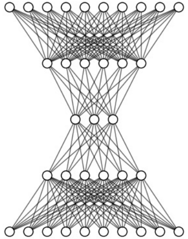


Simulation is missing physics (XBET) - the data informed model corrects for this missing physics

Transfer learning could play a central role in an ML-driven experimental campaign

Sim. inputs → Run simulation → Simulation outputs



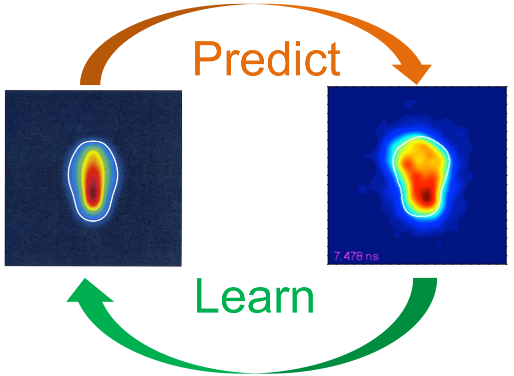
Expected exp. outputs → Use optimization algorithm select new inputs → Sim. inputs

Simulation outputs → Run optimal experiment → Update AE → Expected exp. outputs

Maps get better
Better maps drive design

Transfer learning creates "CogSim" models that are predictive of ICF experiments

- Transfer learning combines large simulation databases with sparse experimental data to create predictive models
- Models are readily updated as we acquire more experimental data
- The models offer a new design tool
  - Track discrepancies across designs to inform model improvement needs
  - Use empirically realistic tools to design future implosion platforms



Transfer Learning merges simulation + experiment to produce a model that is predictive of ICF experiments

Acknowledgments

- Brian Spears
- Luc Peterson
- Jay Salmonson
- Bogdan Kustowski
- Chris Young
- Annie Kritcher
- Jim Gaffney
- Michael Kruse
- Ryan Nora
- Debbie Callahan
- Omar Hurricane
- The Hybrid-E and I-Raum teams

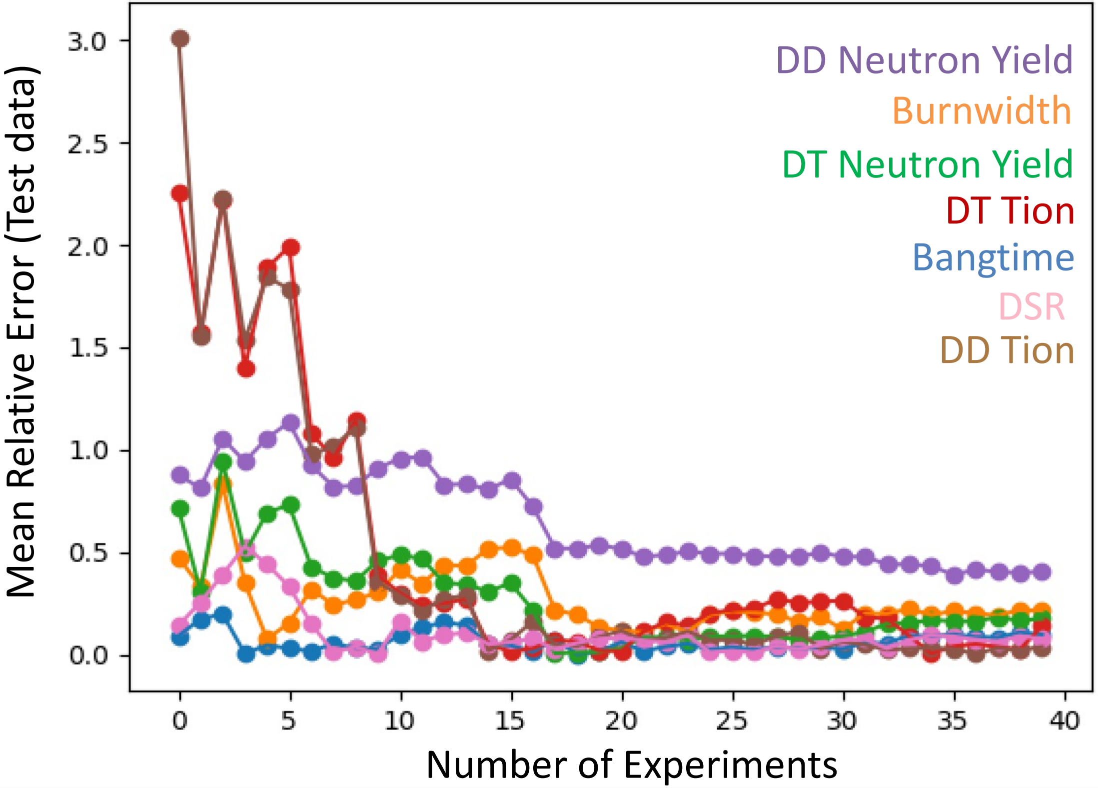
“Where can physicists find their place in the much broader community of machine learning?”

- We bring difficult and new problems to the field that differ significantly from more mainstream ML applications (advertising, search, object detection, language processing, etc)
  - Sparse data, multimodal data, models that need to respect physical constraints, high consequence decision making

- Scientific ML is an emerging field – we’re pushing ML tools into regimes for which they weren’t necessarily developed, and asking scientists to be patient during the development of these tools
  - Physicists need to learn the limits of ML and understand many solutions will not be “off the shelf” ML tools.
  - Conversely, the ML collaborators need to take time to understand the application to decide what ML strategy is most appropriate to answer the questions at hand.

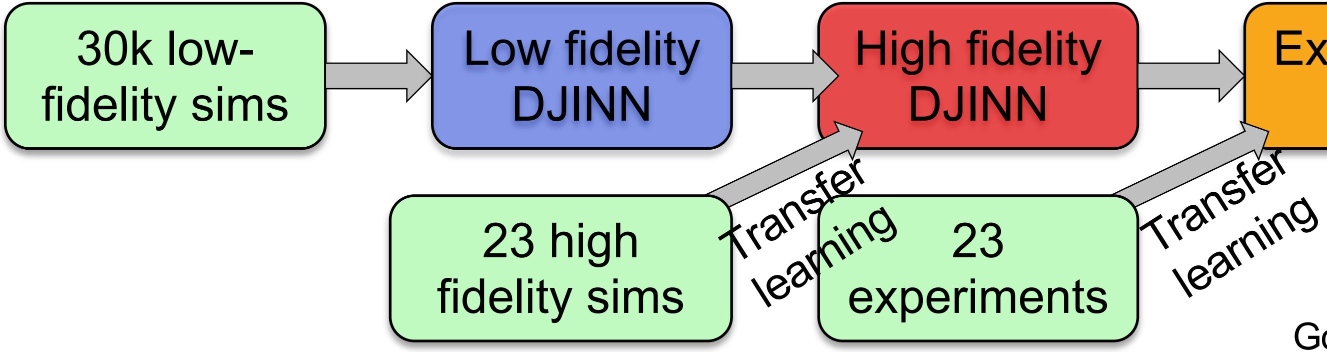
As we acquire data the mapping from predictions -> experimental measurements becomes more accurate

- Perform transfer learning iteratively, adding one experiment at a time in chronological order
- *Test* predictive capability by predicting the 7 most recent shots in the database



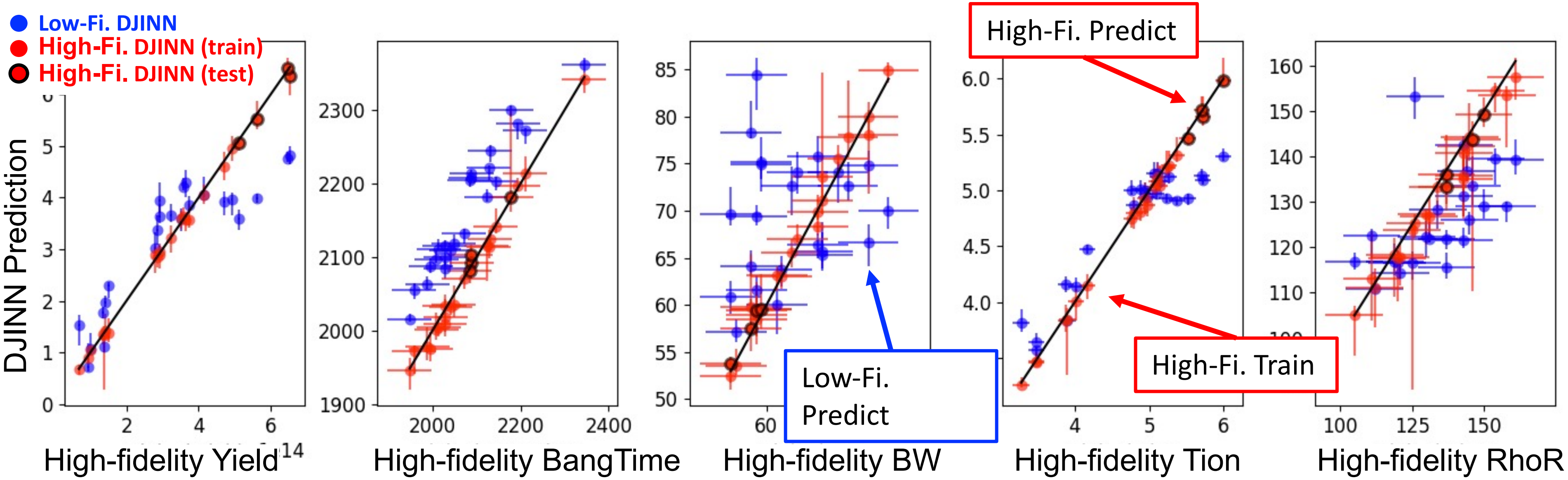
Can DJINN+TL predict future Omega experiments with higher accuracy than simulations?

- Use the same data as before
  - 30k low fidelity 1D LILAC simulations
    - Spans a 9D input space with varying laser pulse & capsule dimensions
  - 23 experiments
    - 1D High-fidelity simulations
    - Experimental measurements of yield, bang time, Tion, rhoR, burnwidth

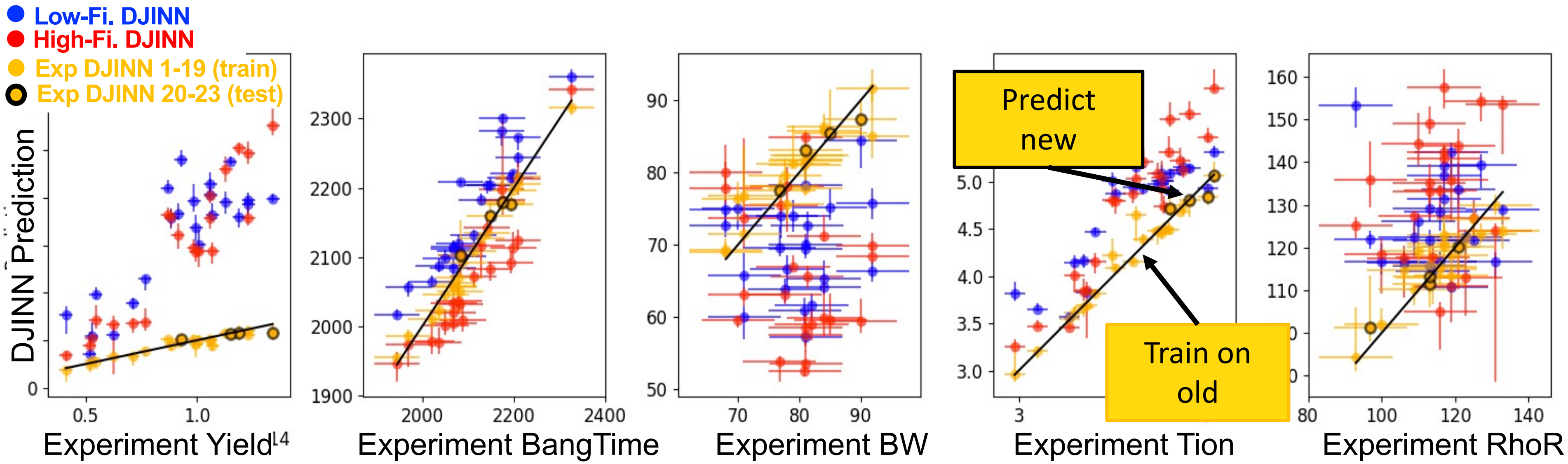


*Data provided by Varchas Gopalaswamy & Riccardo Betti

DJINN+TL: predict high-fidelity simulations with low computational cost



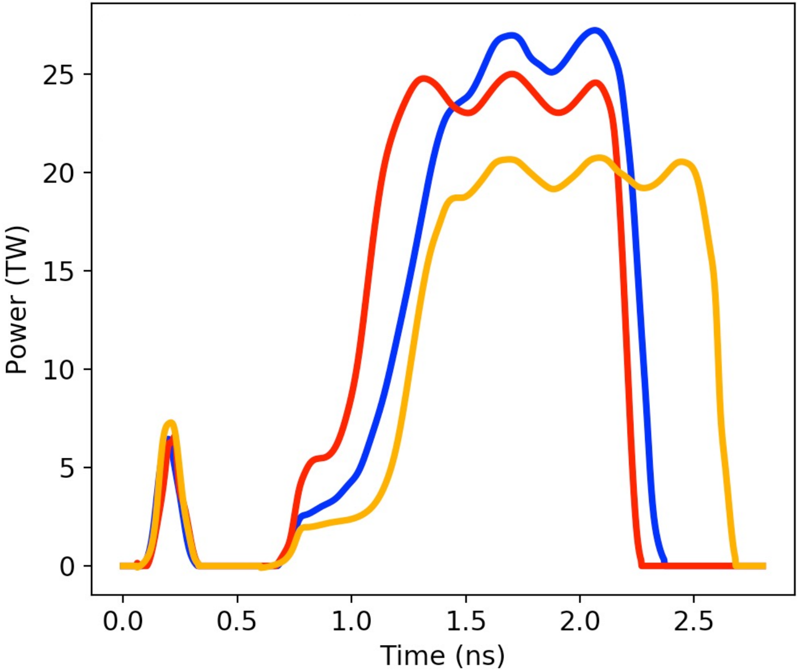
DJINN+TL: *more predictive* of future Omega experiments than simulations



Experiment DJINN models can predict future Omega experiments

Each model suggests a different optimal* implosion

DJINN: Optimal Laser Pulses



Optimal Capsules

*Maximum Yield·$(\rho R)^2$

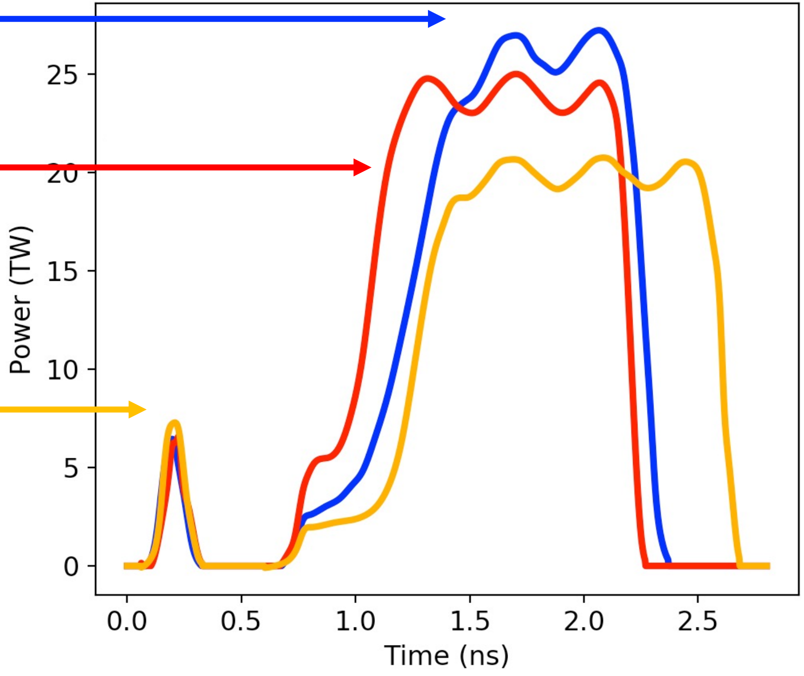
Each model suggests a different optimal* implosion

Max 1D Yield

Fix LPI but maintain velocity

Control hydro. instabilities at higher ρR

DJINN: Optimal Laser Pulses



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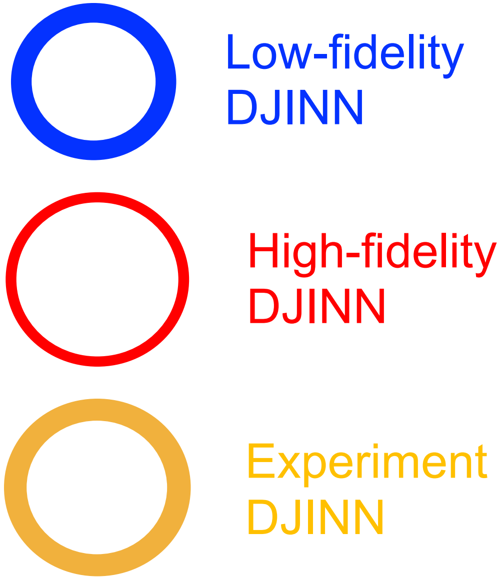
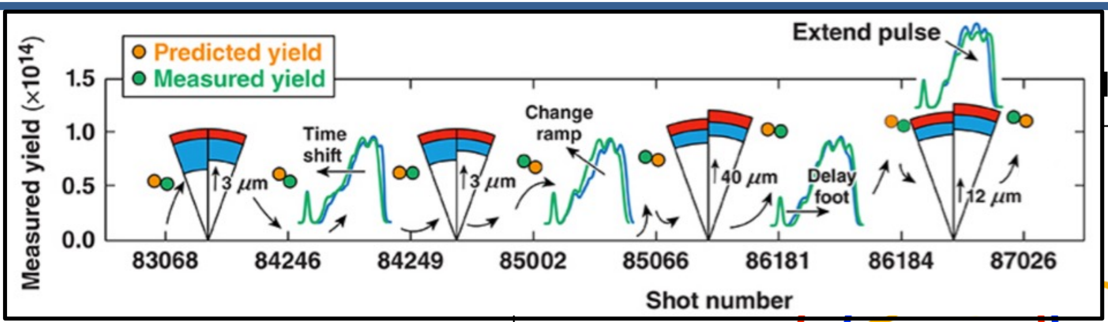


*Maximum Yield·$(\rho R)^2$

DJINN optima are consistent with physics-guided iterations



*Betti et al, 2018

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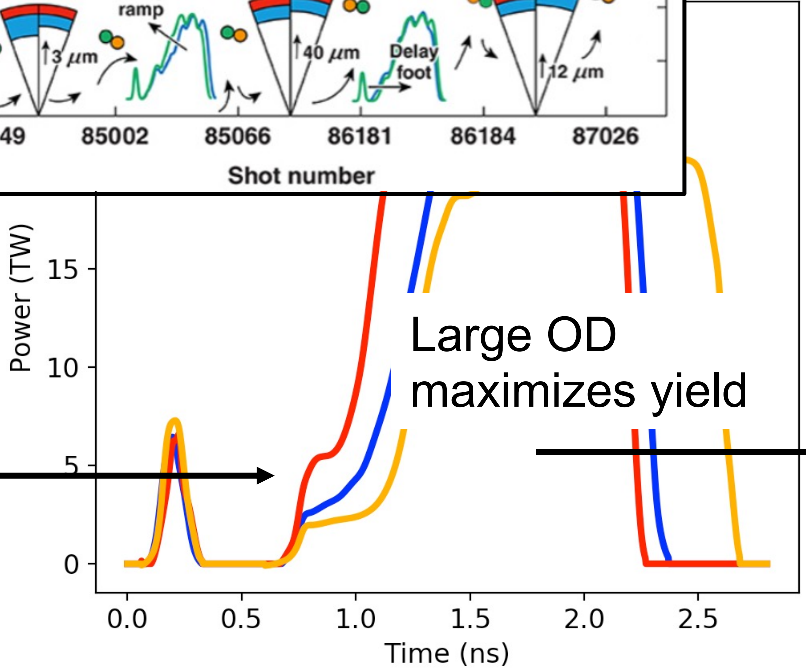
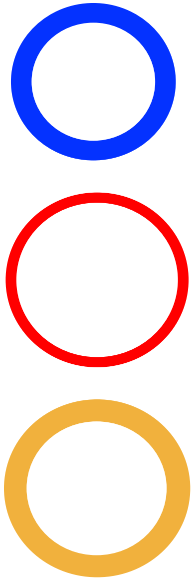


Large OD maximizes yield

Adjusting picket and foot improves ρR

Optimal Capsules



Low-fidelity DJINN

High-fidelity DJINN

Experiment DJINN

*Maximum Yield·$(\rho R)^2$