Cognitive Simulations for Inertial Confinement Fusion

Computational Methods Roundtable

American Nuclear Society Annual Meeting
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LLNL-PRES-823142

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Lawrence Livermore National Laboratory

A little bit about my journey from A&M Nuclear Engineer -> LLNL ICF design physicist

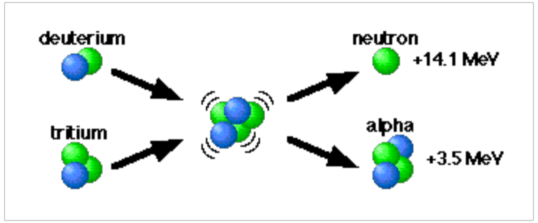
I spent many years at Texas A&M
- BS Physics, BS Nuclear Engineering, TAMU, Dec 2013
- MS Nuclear Engineering, TAMU, May 2016 (adjoint methods for rad diffusion)

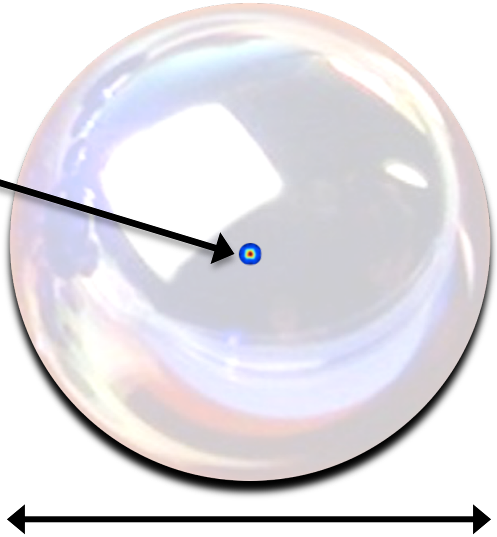
- Summer intern @ LLNL in 2016 – Machine learning for ICF
- Moved to LLNL for Livermore Graduate Scholars Program, 2017-2019
- Completed PhD in May 2019
  - "Machine learning guided discovery and design for ICF"
- Joined LLNL as a Design Physicist in May 2019
  - Currently work in inertial confinement fusion, weapons physics, post-detonation nuclear forensics, and even modeling the spread of COVID-19

LLNL is home to the National Ignition Facility (NIF) -- a 2MJ laser used for Inertial Confinement Fusion research

Inertial Confinement Fusion (ICF) compresses deuterium-tritium (DT) fuel to high density, temperature, and pressure

- Conditions for ignition:
  - Reduce volume by 30,000x
  - Pressures of hundreds of Gbar
  - Temperatures of 10^6 K
  - Density of 1000x liquid DT density
  - Ignite chain fusion reaction
  - Get more energy yield out than absorbed by the capsule



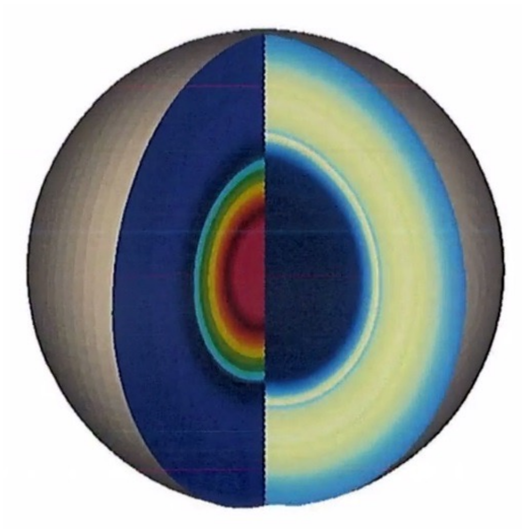


~2 mm diameter

Image: L. Berzak Hopkins

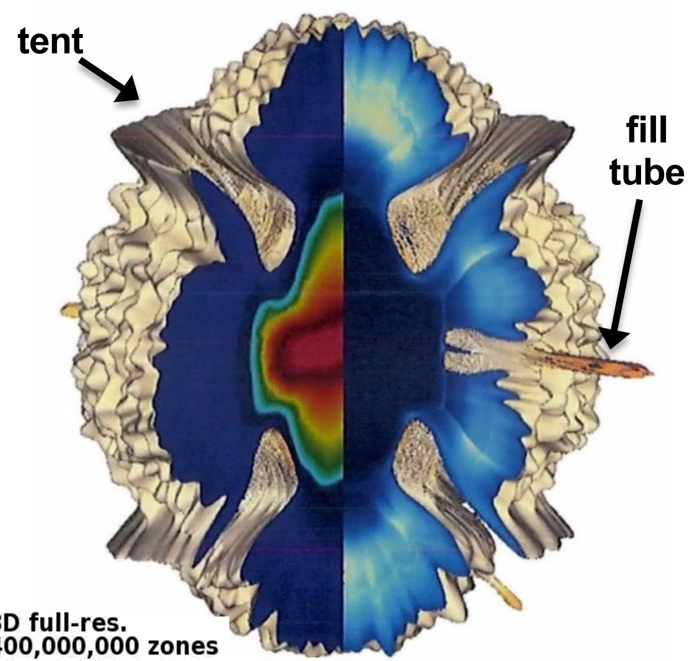
Achieving a round, symmetric implosion is a critical challenge for ICF

Expectation



1D
500 zones
1 CPU
5 minutes runtime

Reality



3D full-res.
400,000,000 zones
6144 CPUs
1 month runtime

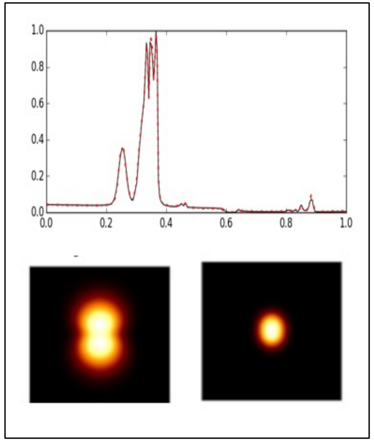
Machine learning is improving how we simulate, design, and understand ICF implosions

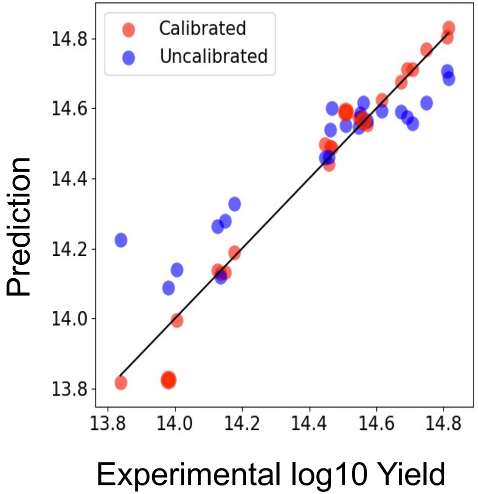
ML workflows for database generation

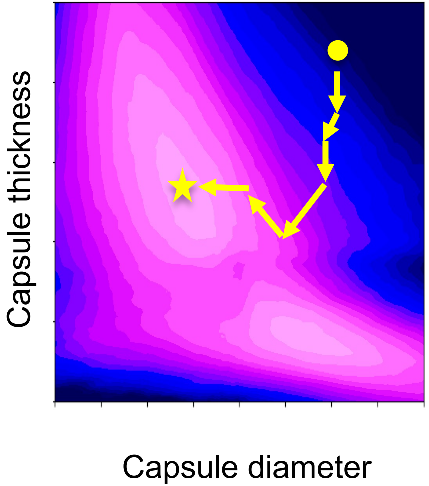
ML code acceleration & heterogeneous computing

Models that merge simulations and experiments

Rapid experimental design optimization

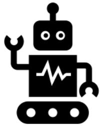






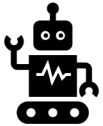
Guiding questions

- **What is machine learning?**



Guiding questions

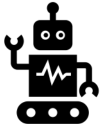
- **What is machine learning?**



- **Why is this important for ICF?**

Guiding questions

- **What is machine learning?**



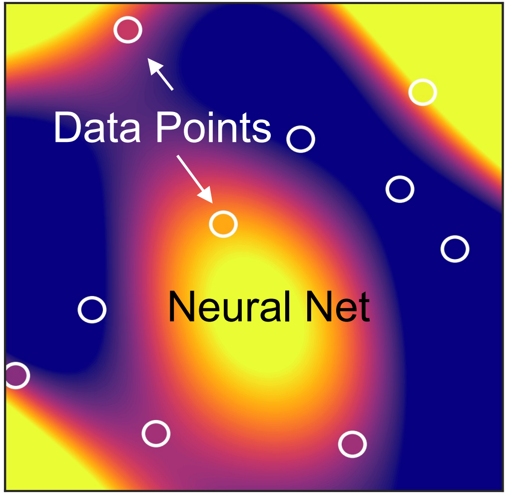
- **Why is this important for ICF?**

- **Alexa, what's my next shot?**

- What is machine learning?

A machine learning algorithm improves its *performance* at a given *task* based on *experience*

- Task: predict a numerical value given numerical input $y^* = f(\mathbf{x})$
- Experience: data; examples; observations $\{(y_1, \mathbf{x}_1), (y_2, \mathbf{x}_2), \ldots, (y_n, \mathbf{x}_n)\}$
- Performance: nearness of a prediction to the true value $$\text{MSE} = \sum_{i=0}^{n} (y_i - f(\mathbf{x}_i))^2$$
- Learning: improving performance with exposure to additional experience



We use ML models as fast approximations to expensive simulations

Isn’t that just curve fitting?

Isn’t that just curve fitting?

Y Hacker News new | comments | ask | show | jobs | submit

▲ nerdponx on July 17, 2017 | parent | favorite | on: The Limitations of Deep Learning

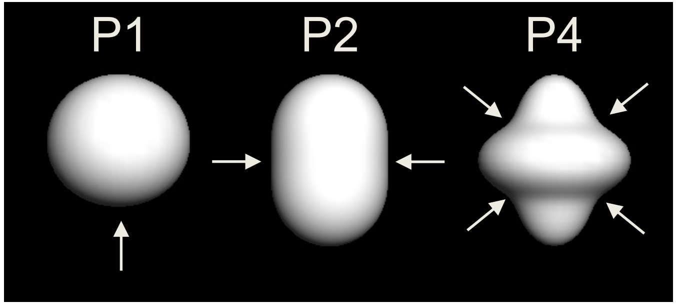
Well said. It's just curve fitting.

- Why is it important for ICF?

- Why is it important for ICF?
  - Rapid design exploration
  - Acceleration of ICF simulations
  - Efficient data generation

In 2016 we generated the Trinity Open Science I Database - the largest database of ICF simulations ever created (at the time...)

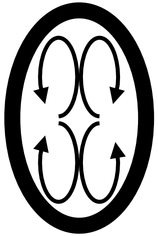
- 3-shock HDC Ignition Design
  - HYDRA 2D Capsule (D. Ho)
- Varied 9 parameters
  - Time-varying drive asymmetry
    - Legendre Modes P1, P2, P4
  - Time-varying drive amplitude
  - Capsule gas fill density
- Successfully completed over **60k simulations**, 39 Million CPU Hours (Trinity @ LANL),
  5 PB Raw Data

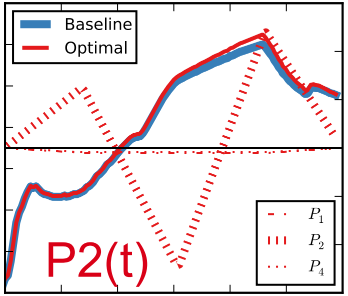


Goal: build surrogate model and search 9D design space for a high performing implosion

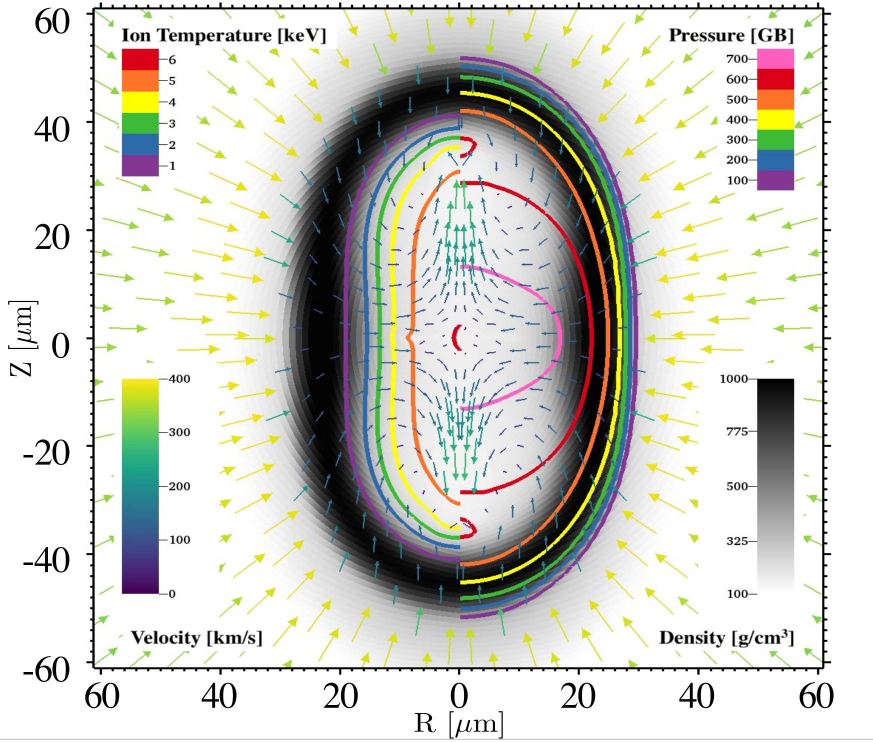
ML applied to this database led us to discover *new physics* in ICF implosions ("ovoid" implosions)

Time varying P2 generates large scale zonal flows





Burn-Off Configuration at Peak Energy Production

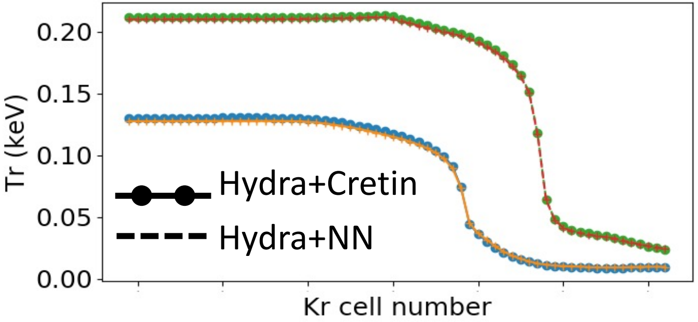


"Zonal flow generation in inertial confinement fusion implosions", Peterson, Humbird, et al. Physics of Plasmas 24, 032702 (2017).

Images: L. Peterson

ML opacity calculations lead to 10X+ speed ups for ICF simulations

We trained an accurate neural net to emulate the atomic physics code Cretin



Deep learning for NLTE spectral opacities

Cite as: Phys. Plasmas **27**, 052707 (2020); https://doi.org/10.1063/5.0006784
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G. Kluth, K. D. Humbird, B. K. Spears, J. L. Peterson, H. A. Scott, M. V. Patel, J. Koning, M. Marinak, L. Divol, and C. V. Young

COLLECTIONS

EP This paper was selected as an Editor's Pick

(Download Image)

Lawrence Livermore National Laboratory and Silicon Valley-based Cerebras Systems have installed the company's CS-1 artificial intelligence (AI) computer into Lassen, making LLNL the first institution to integrate the cutting-edge AI platform with a large-scale supercomputer. The integration creates a radically new type of computing solution, enabling researchers to investigate novel, AI-driven approaches to predictive modeling and "cognitive simulation." Photo by Katrina Trujillo/LLNL.

LLNL pairs world's largest computer chip from Cerebras with Lassen to advance machine learning, AI research

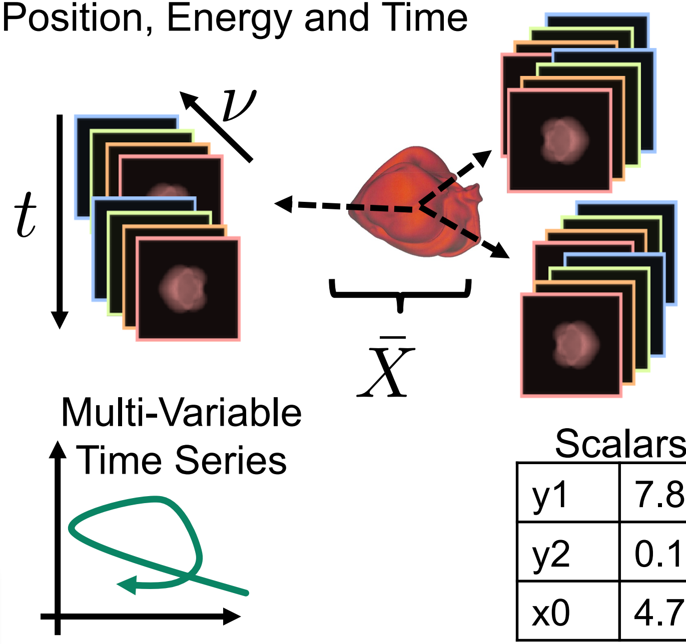
ML-accelerated High Performance Computing workflows enable rapid data generation

Merlin + Sierra "JAG" database

- 100 Million 3D thin-shell ICF Simulations
- Multi-modal physics-based data
- 4.8 Billion Hyperspectral Multi-View Images
- Timeseries
- Scalars

Merlin
github.com/LLNL/merlin

Hyperspectral Images:
Position, Energy and Time



Scalars

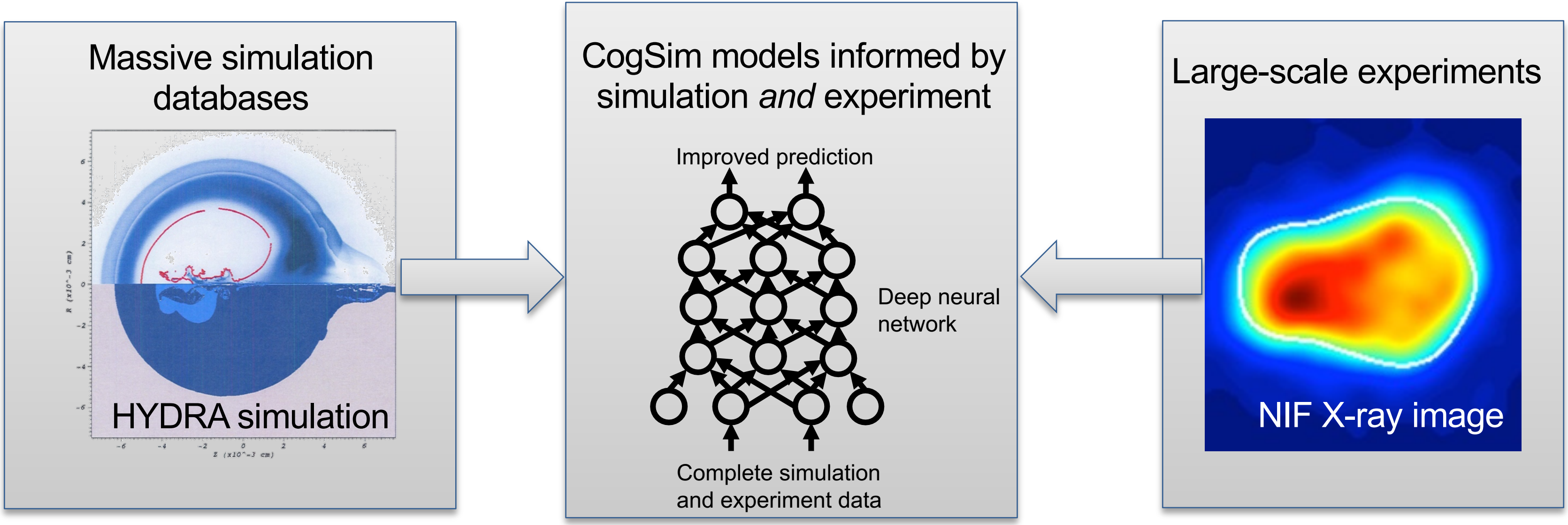
y1	7.8
y2	0.1
x0	4.7

data-science.llnl.gov/open-data-initiative

We've shared this dataset to strain models and training methodologies

- Alexa, what’s my next shot?

Accelerated simulations + novel machine learning methods are enabling us to make the best use of simulation and experimental data



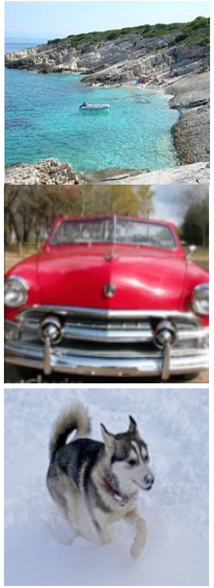
“Cognitive Simulations” are informed by simulation and experiment, and get more accurate as new data is acquired

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

Ocean

Car

Dog



Large image database

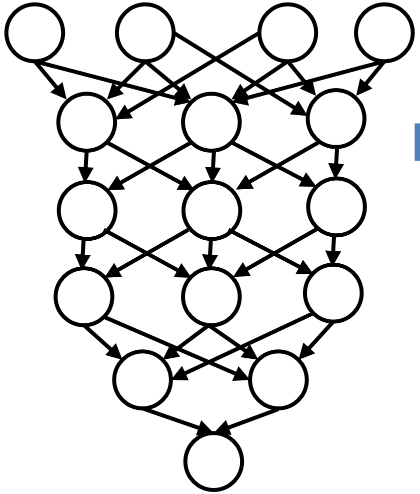
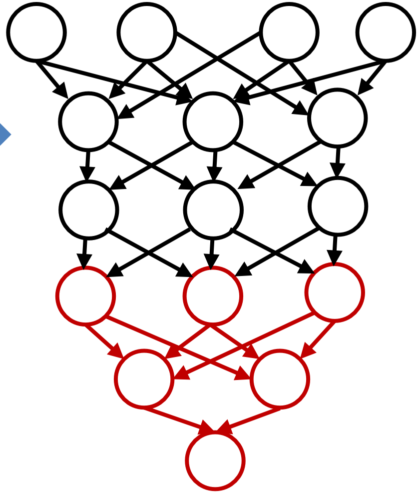


Image label

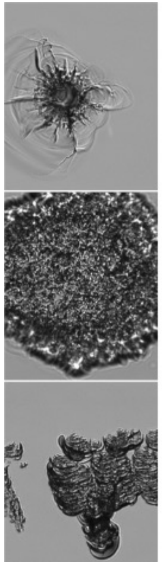
Retrain to solve different, but related task

Small NIF optics database



Damage label

Optics



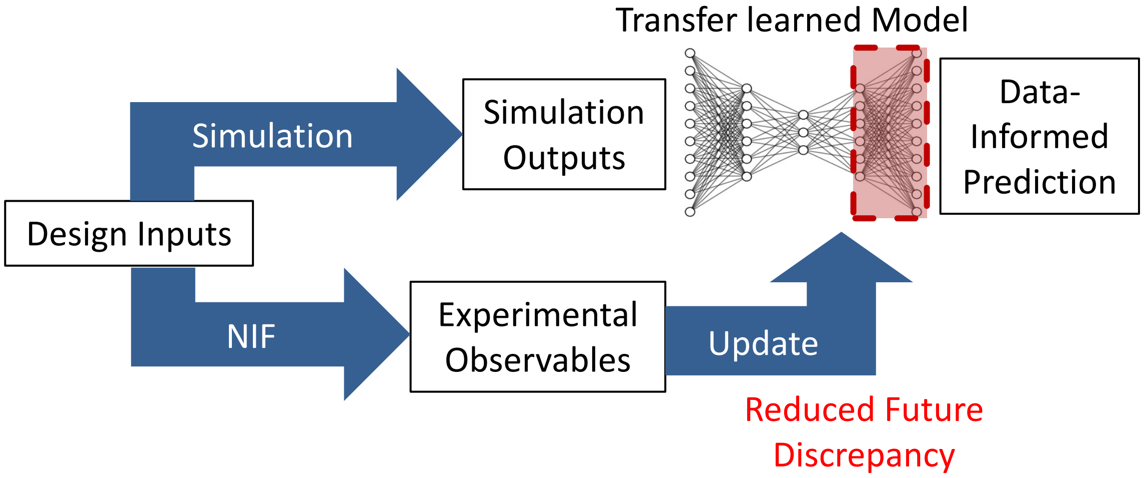
Thistle

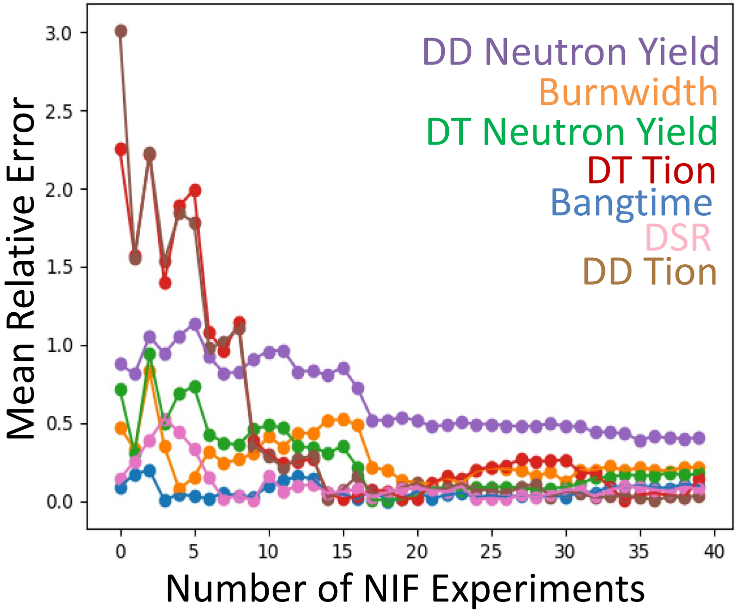
Pansy

Scratch

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

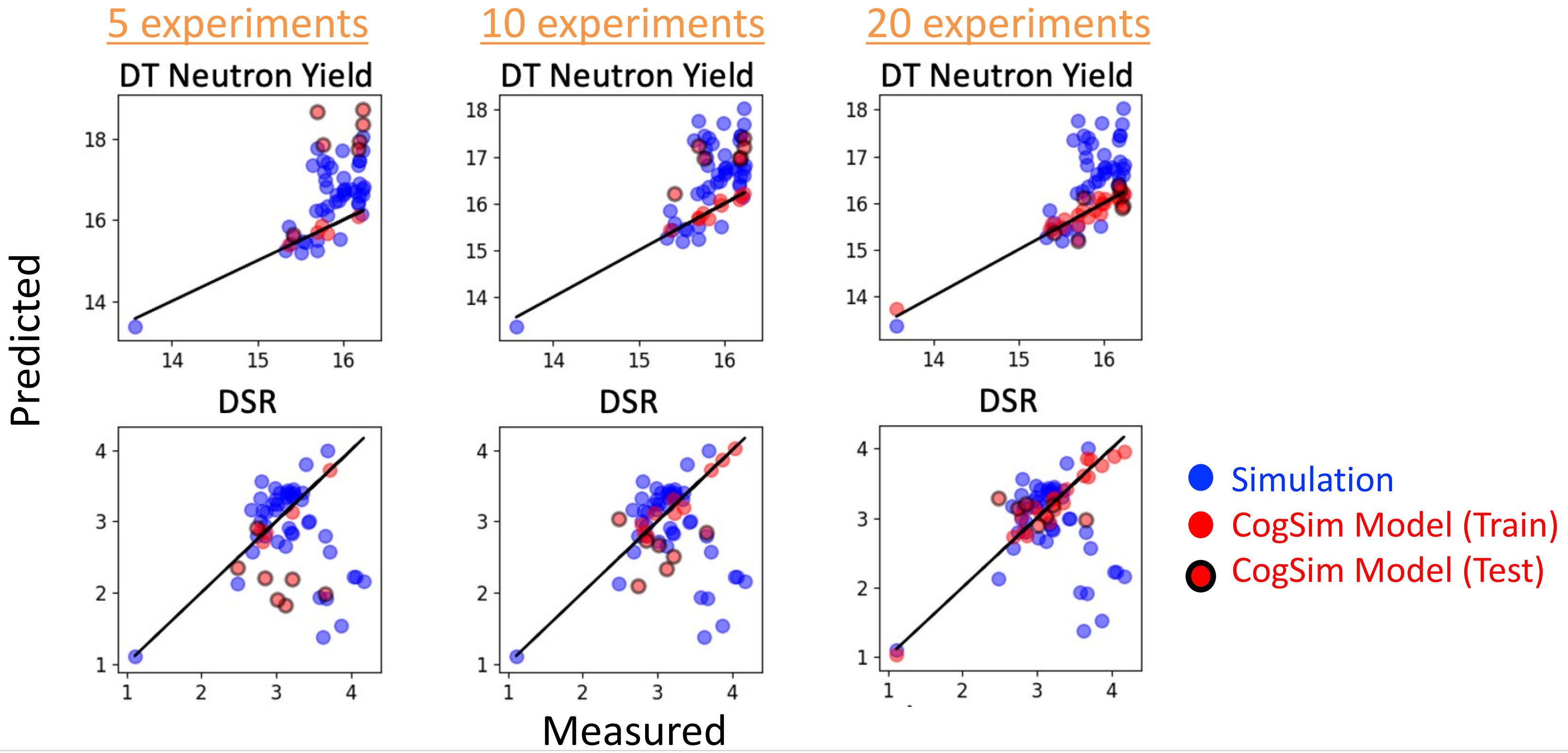
We've adapted this technique to make "cognitive simulation" models of NIF experiments





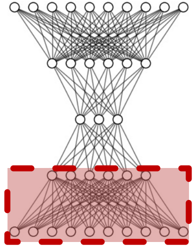
CogSim models are updated after each experiment, becoming increasingly accurate over time

CogSim models get better as we add more experimental data



We're developing the tools to run machine learning-guided experimental campaigns

Sim. inputs → Run simulation → Evaluate CogSim Model



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

Run optimal experiment → Update TL Model

Maps get better

Better maps drive design

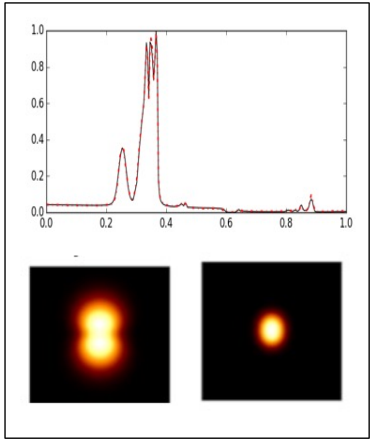
Machine learning is improving how we simulate, design, and understand ICF implosions

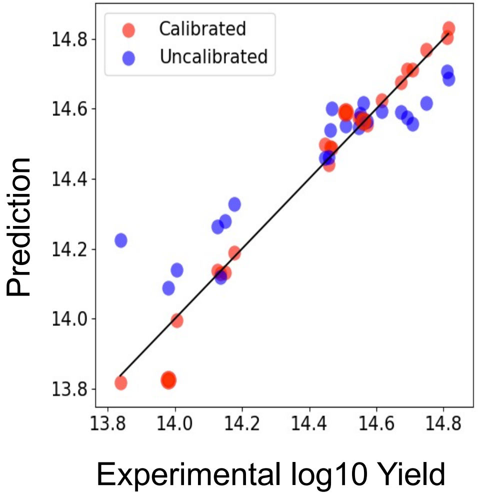
ML workflows for database generation

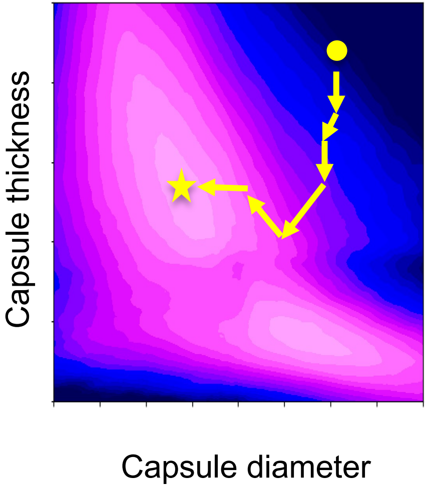
ML code acceleration & heterogeneous computing

Models that merge simulations and experiments

Rapid experimental design optimization







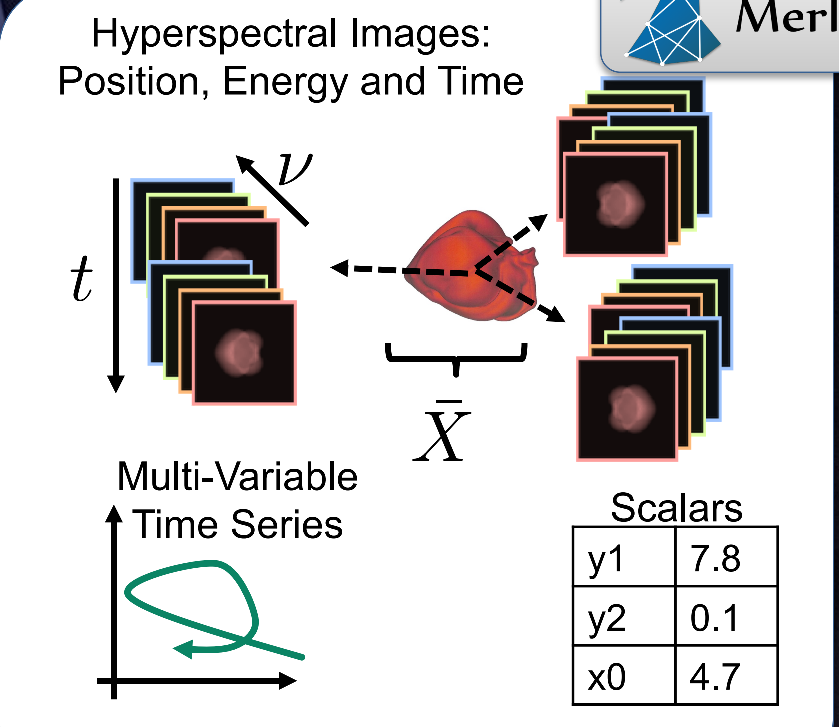
I'm proud to be a part of a great team of researchers

- Brian Spears
- Luc Peterson
- Bogdan Kustowski
- Chris Young
- Jay Salmonson
- Jim Gaffney
- Michael Kruse
- Ryan Nora
- Debbie Callahan
- Omar Hurricane

Lawrence Livermore National Laboratory

Merlin* + Sierra: An unprecedented physics based dataset

- 100 Million 3D thin-shell ICF Simulations
- Oversampled 5D Space
- Multi-modal physics-based data
- 4.8 Billion Hyperspectral Multi-View Images
- Timeseries
- Scalars



data-science.llnl.gov/open-data-initiative

Merlin

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ML is enhancing our simulation and experimental capabilities at all levels of the design process

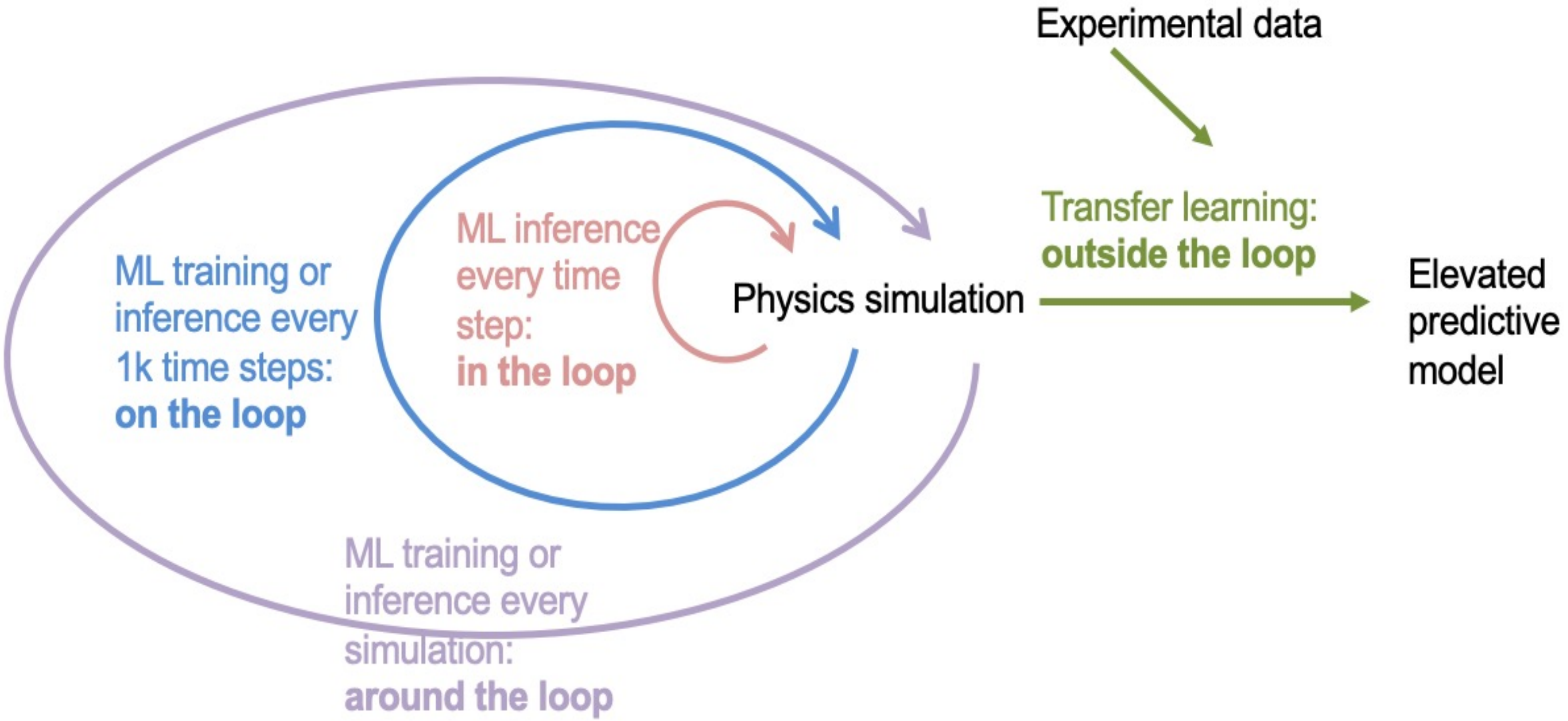
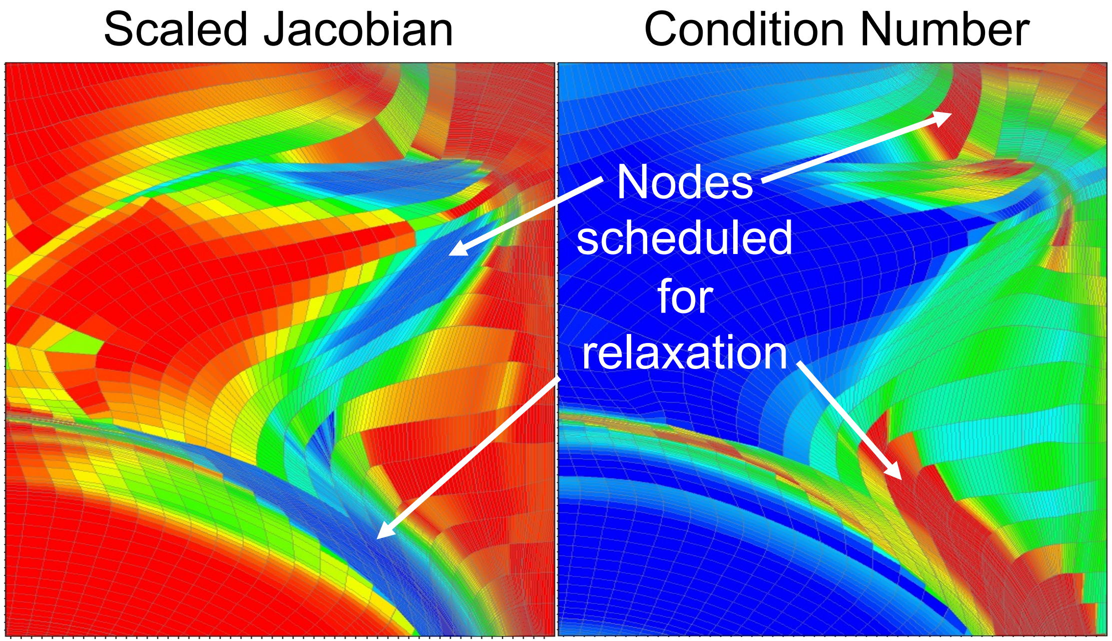
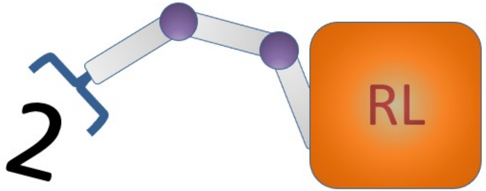


Figure: Brian Spears

Reinforcement learning is automating mesh management in ICF codes



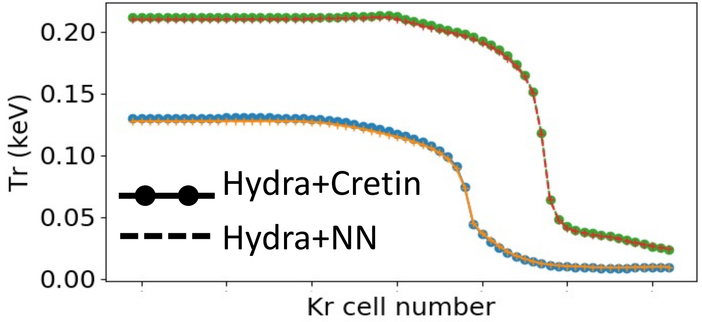


C. Yang, J. Salmonson, C. Young

In the loop

ML opacity calculations show potential for 10X+ speed ups for integrated ICF hohlraum simulations

We trained an accurate neural net to emulate the atomic physics code Cretin



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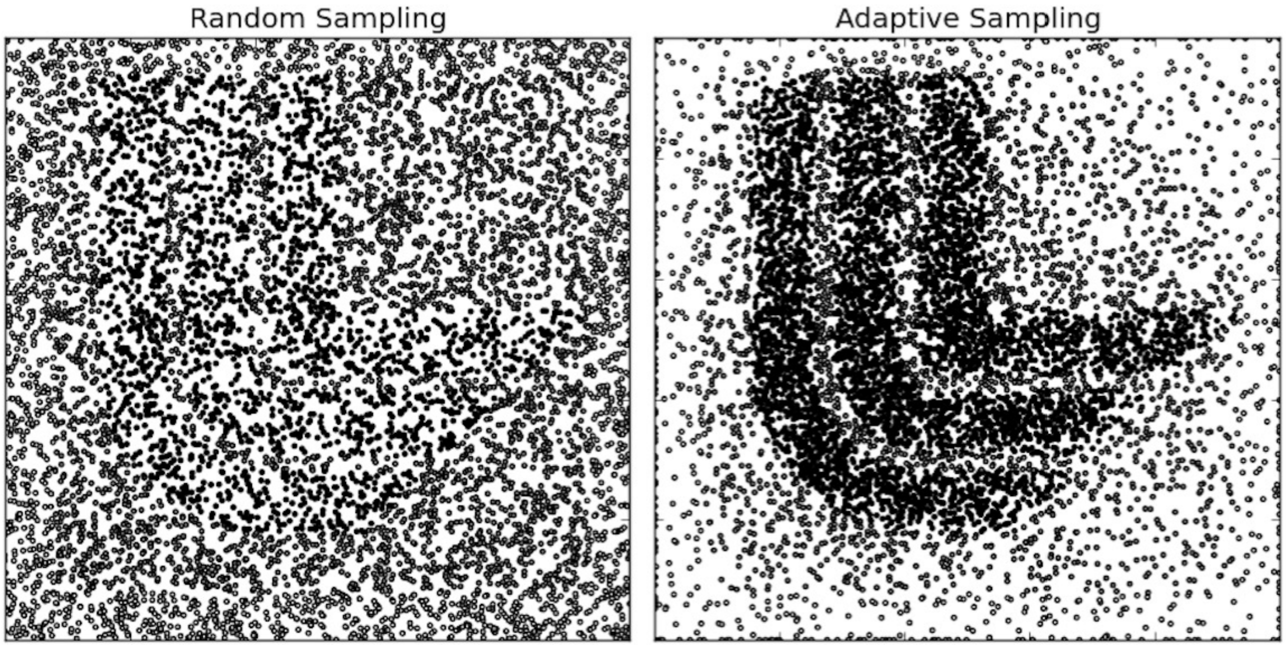
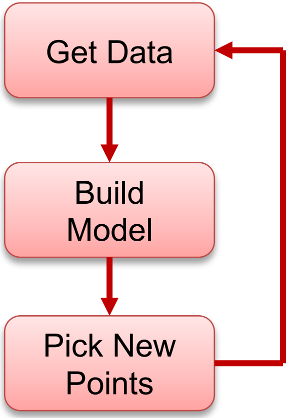
LLNL pairs world's largest computer chip from Cerebras with Lassen to advance machine learning, AI research

ML-driven sampling strategies enable us to run simulations that maximize information gain





Impala Active Learning Algorithm
Peterson CODA 2018

Instead of relying on existing datasets to train our models we can actively seek out good new data