Machine Learning Aided Discovery of a New NIF Design

DSI/ UC Data Science Workshop

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The Team

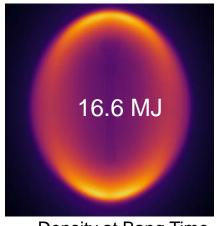
- Brian Spears
- John Field
- Scott Brandon
 - UQPipeline Team
- Ryan Nora
- Steve Langer
- Joe Koning
 - HYDRA Team

- Dave Munro
- Jim Gaffney
- Michael Kruse
- Michael Buchoff
- Jim Hammer
- Paul Springer
- ICF HDC Team
 - D. Ho & L. Berzak Hopkins

- Luc Peterson
- Kelli Humbird (TAMU)

We have discovered a new kind of robust Inertial Confinement Fusion implosion

- Suggested by an AI system (Random Forest) trained on the largest ICF simulation dataset ever created
 - Trinity Open Science Phase I (LANL)
- Optimal implosion is an ovoid, not sphere, challenging known physics
- Presence confirmed by new simulations not in the original dataset – digging into "why"
- We are building tech to enable these kinds of discoveries



Density at Bang Time

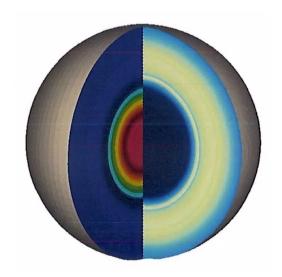
J. L. Peterson, et al., Physics of Plasmas, **24**(3):032702 (2017)

Machine learning on a large ensemble of simulations has pointed to a new class of robust implosions

Fall 2015: Can we make NIF Designs more resilient?



We want this

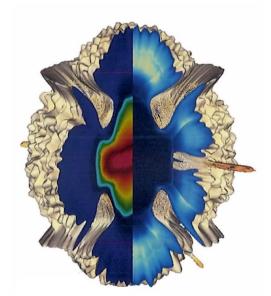


D. Clark

Fall 2015: Can we make NIF Designs more resilient?



But can get this



Can we withstand these kinds of imperfections?

D. Clark





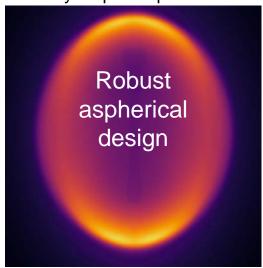
Machine Learning said yes! But the results were unexpected

Machine learning helped uncover an unexpected, robust NIF ICF capsule design

- Enabled by large-scale HPC ensemble simulation
- Post-facto learning on processed results
- Computer architecture matters
- Machine learning brings you back to the physics

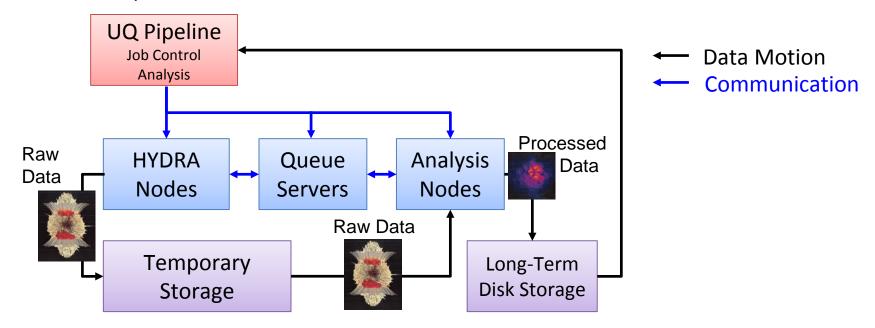


Density map of imploded shell

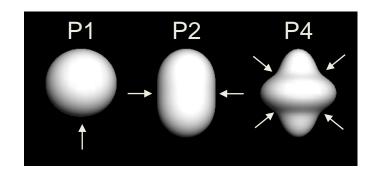


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 Turned Trinity into a server farm with in-transit analysis

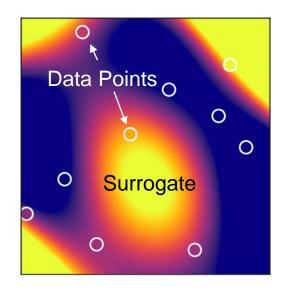


- Turned Trinity into a server farm with in-transit analysis
- Ran a bunch of simulations of NIF implosions (30x more than any previous study)



- 9 ways to mess up a NIF implosion (parameters)
- Successfully completed 60k simulations
- 39 Million CPU Hours
- 5 PB Raw Data, 100 TB Processed & Zipped

- Turned Trinity into a server farm with in-transit analysis
- Ran a bunch of simulations of NIF implosions (30x more than any previous study)
- **Trained a ML model to fill in the gaps



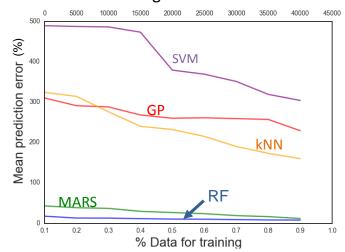




Random Forest surrogates, of all those tested, are the most accurate models for this dataset

- Tested multiple machine learning algorithms
 - Gaussian process, multivariate adaptive regression splines, nearest neighbor regression, support vector machines, random forests
- Dimensionality, volume of data, complexity of response surface (cliffs, peaks) make accurate interpolation challenging
- Random forest regressor most accurately models this ICF data

Mean error for yield models as a function of training data set size



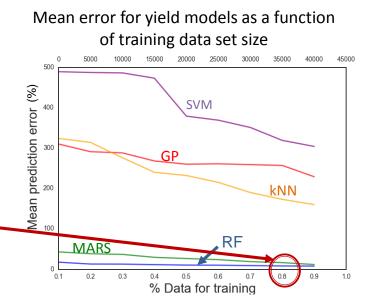
Slide: K. Humbird



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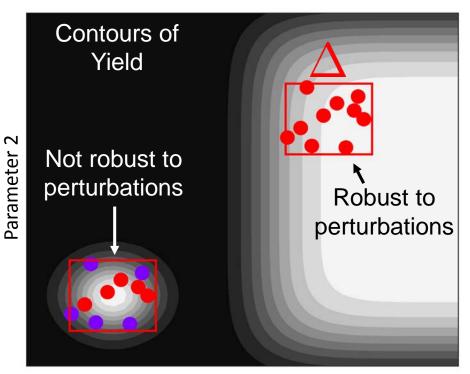
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Random forest yield model has 8% mean error when trained on 80% of the data



Slide: K. Humbird

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- **Trained a ML model to fill in the gaps
- **Optimized the ML model for "robustness"

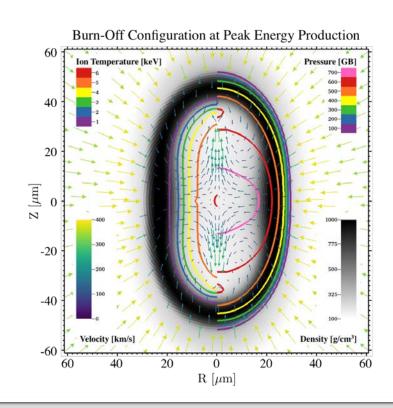


Parameter 1





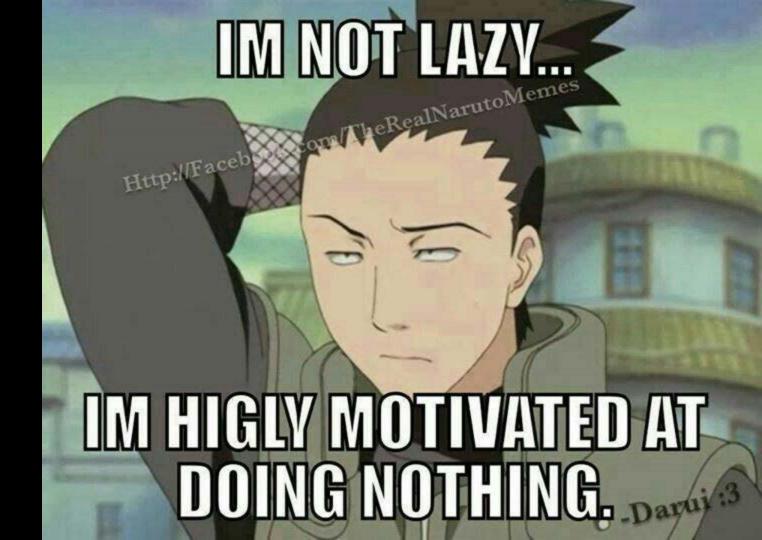
- Turned Trinity into a server farm with in-transit analysis
- Ran a bunch of simulations of NIF implosions (30x more than any previous study)
- **Trained a ML model to fill in the gaps
- 4. **Optimized the ML model for "robustness"
- 5. Ran new simulations at the predicted sweet spot & <u>dug into the physics</u>

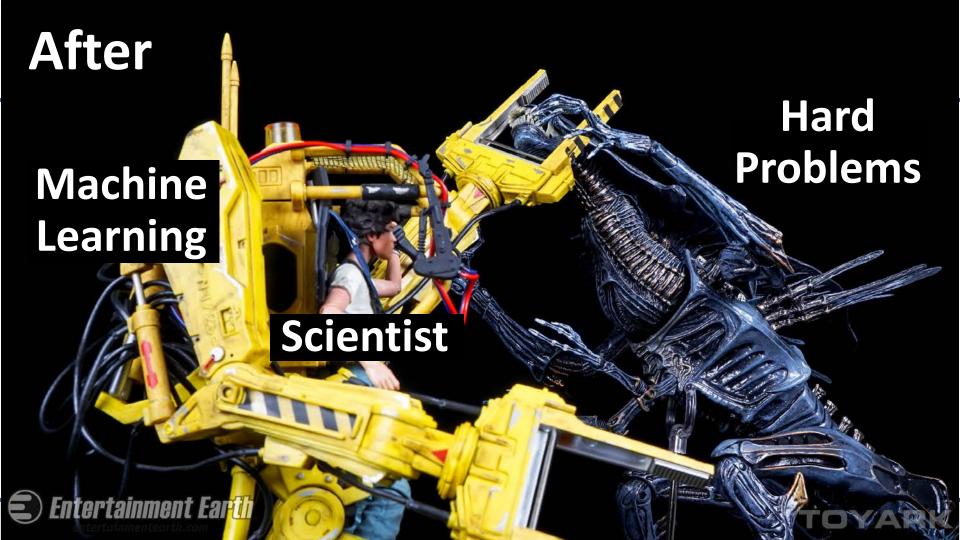


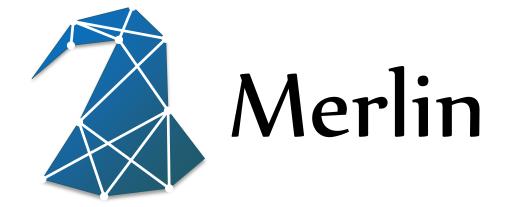


The Trinity Ovoid changed my view on how machine learning could help my do my job [HPC-enabled science].

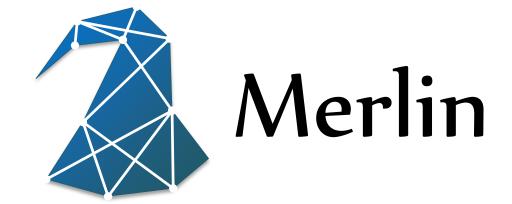
Before



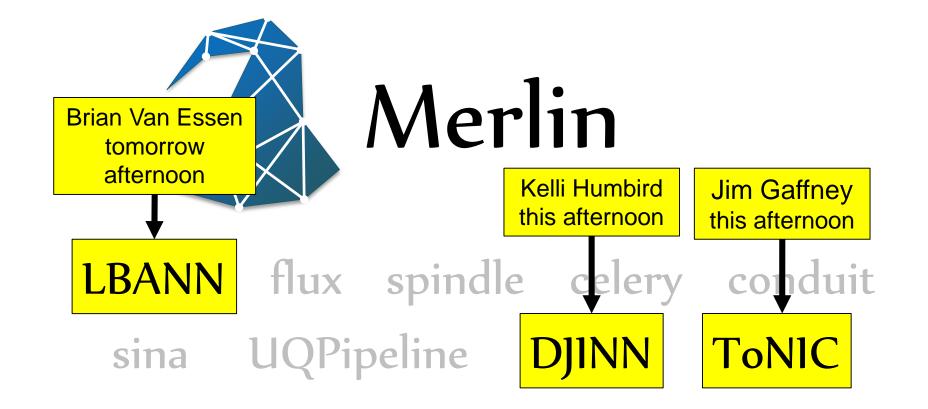




Machine Learning for HPC Workflows



LBANN flux spindle celery conduit sina UQPipeline DJINN ToNIC



We're aiming to make a "splash" for early Sierra access

- Generate 1 billion semi-analytic ICF implosion simulations
 - Oversample a high-dimensional space
 - Train a deep learning model on a physics problem
 - Develop new physics insight
- Shareable data for the machine learning community
 - Beyond MNIST and ImageNET
 - Several billion images, plus scalars, time histories
- Challenging and meaningful problems unique to the Laboratory



1 Billion Sims!

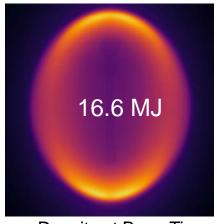




An exciting opportunity to establish Lab leadership in cognitive computing and data science

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Thank You!



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