Boiler Modeling for Flexible Operations

[Chris Guenther and Mehrdad Shahnam (NETL)]
[Yong Liu, Tarak Nandi, Jennie Stoffa (Leidos)]
]

NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DEPARTMENT OF ENERGY

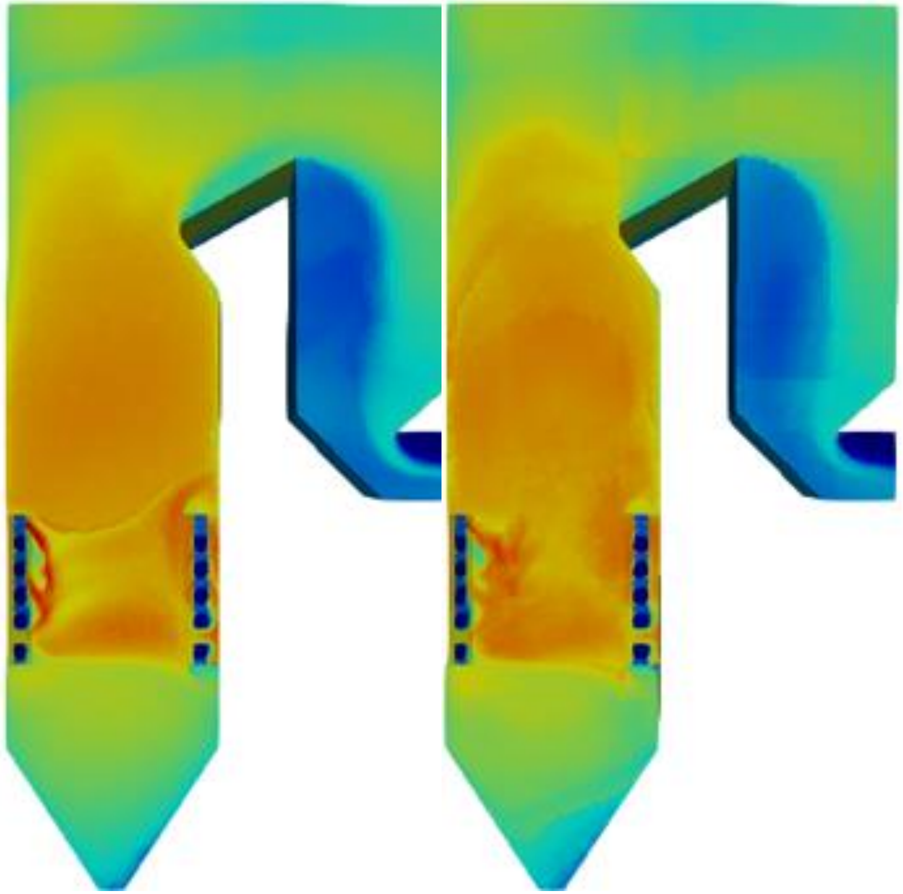
Motivation

Why Do We Need These Tools?

These tools can quickly assess new energy plant concepts, retrofit existing plants/components, and optimization of new or existing plants.

These tools can reduce risk, cost, accelerate deployment and provide the fidelity and confidence to eliminate the need to build and test at increasingly larger scales.

Engineering software companies do not have the ability to provide "out of the box" high fidelity, fast-running proxy models which can be deployed in the field as a digital twin.



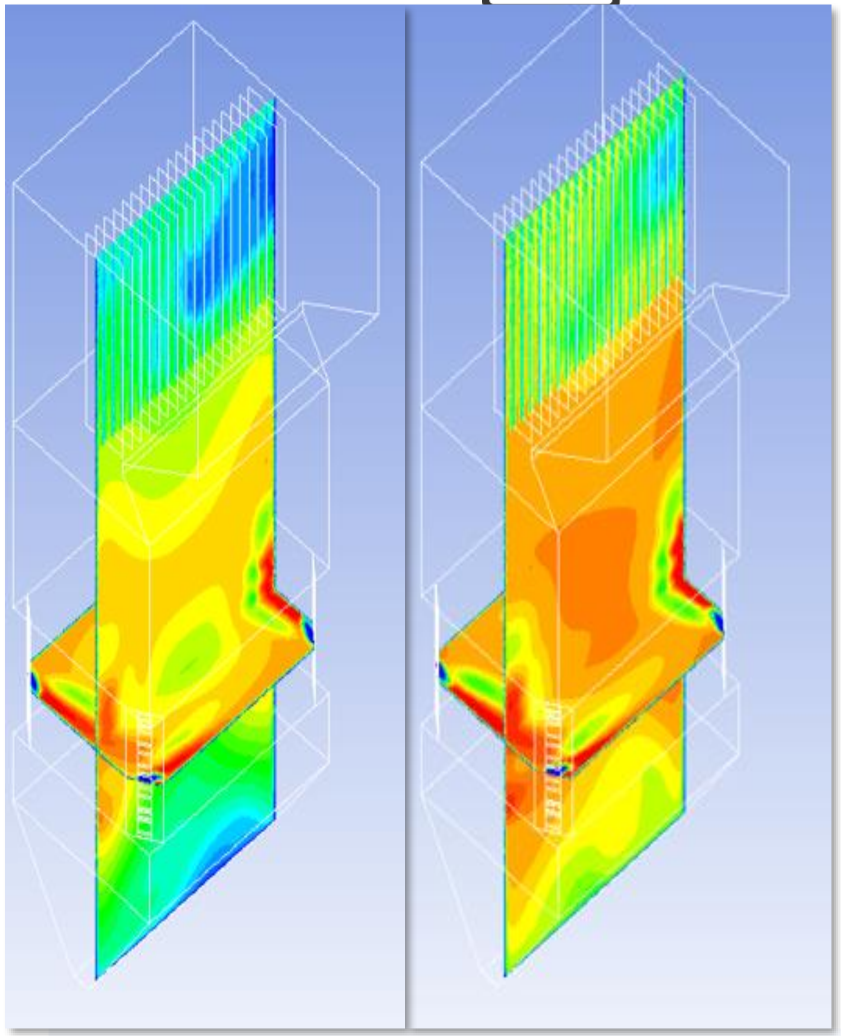
Temperature contour in the Tri-State boiler CFD prediction (left) and Digital Twin prediction (right)

Motivation

Are There Existing Tools To Do The Job?

Commonly accepted that Computational Fluid Dynamic (CFD) models can provide high fidelity information at a device scale level. However, widespread use of these results in industry is limited and rarely used in the field.

- In general industry lacks CFD with AI/ML expertise and has limited computational resources
- Steep learning curve
- Large computational resources and time
- Difficult to quantify uncertainties in model predictions
- Difficult to disseminate modeling results
- Never deployed or used directly in the field



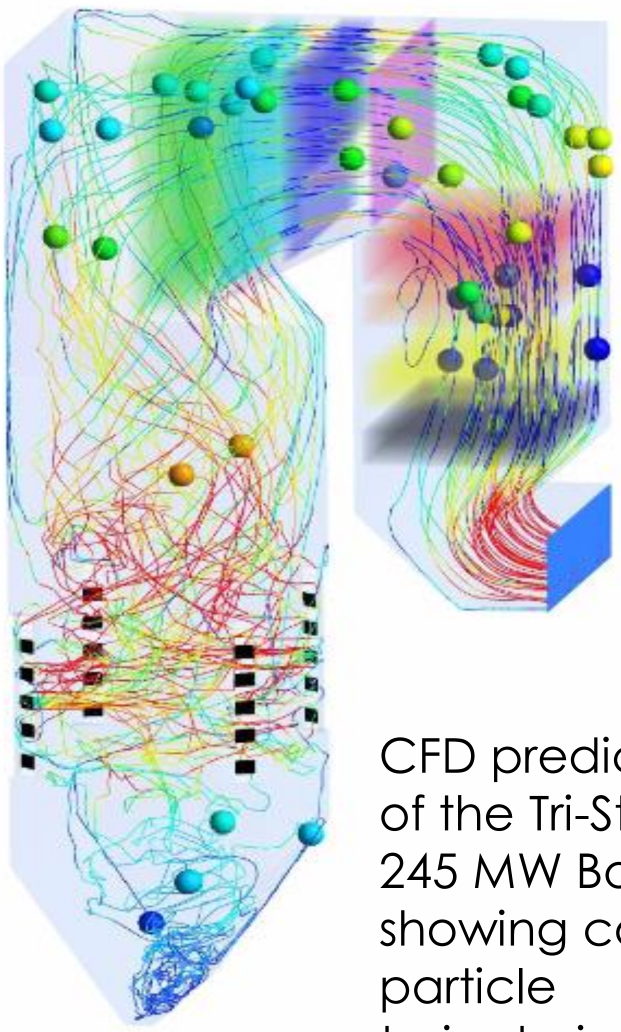
Escalante Tri-State Boiler 40% Full Load (left) and Full Load (right): Gas Temperature CFD Predictions

Research Objective

Success Criteria

Goal: Leverage the fidelity of CFD to develop a fast-running high fidelity proxy model which can be exercised as a digital twin for field deployment.

- Once deployed expertise in CFD not required, fast running almost real time
- Field ready information during complex operations (e.g. turn down)
- Deployment on basic operating systems (desktop, laptop, tablet, phone)
- Easy to use by engineers in the field allowing 3-D field variable information during complex operations in just seconds
- Generalizable to multiple industrial areas and uses (cybersecurity, digital ghosts, virtual sensing, cyber-physical modeling etc.)
- Ability to dynamically update the proxy model with new parameters or increased ranges



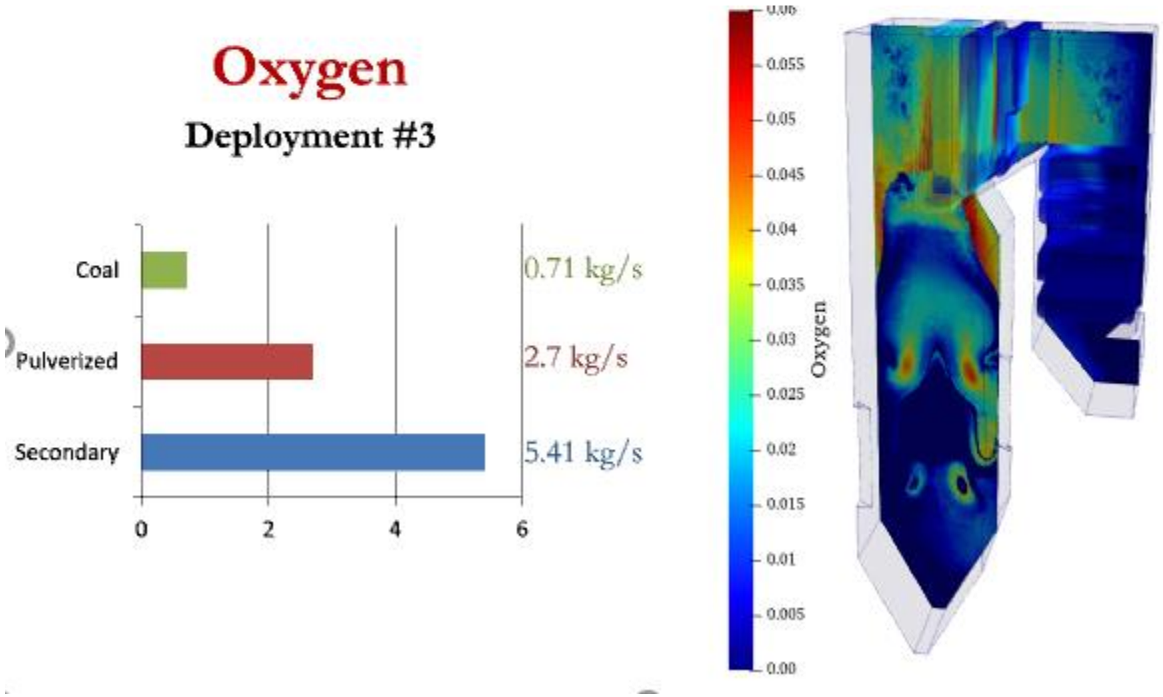
CFD predictions of the Tri-State 245 MW Boiler showing coal particle trajectories

Project Approach

NATIONAL ENERGY TECHNOLOGY LABORATORY

Overall Approach

- NETL is recognized as a world leader in reacting multiphase flow simulations and at the forefront in advancing the state-of-the-art.
- Leverage NETL's expertise in reacting multiphase flow simulations, high performance computing and capabilities in AI and Machine Learning.
- Generate high fidelity CFD data of an industrial scale boiler to demonstrate the feasibility and applicability of developing a data driven proxy model from the CFD simulation results over a given parameter space.
- Using AI and machine learning techniques (deep neural networks) to train the model and validate results through blind tests and deployment of the proxy model over the parameter space it was trained
- Demonstrate the utility of the proxy model or digital twin and wide range of potential uses through industrial collaboration



Sensitivity analysis using the proxy model to predict oxygen levels thru the boiler as coal, primary and secondary air is varied

Project Approach

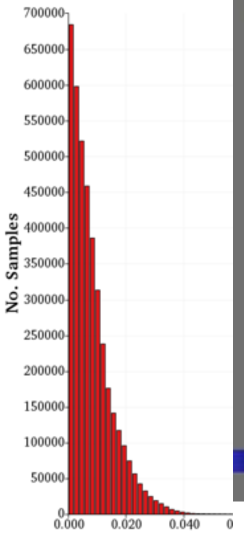
Accomplishments-to-Date

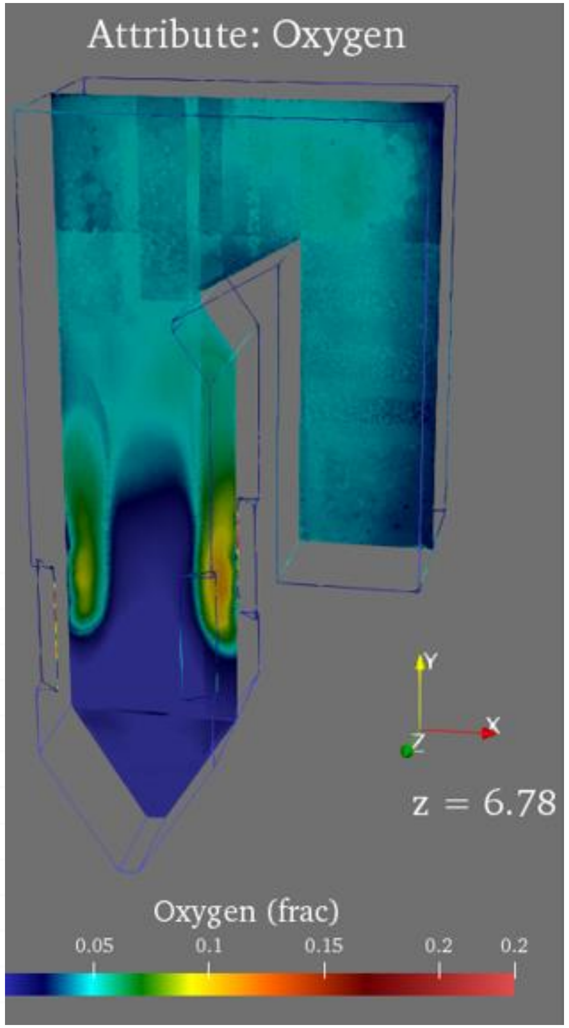
- Develop a CFD and proxy model of the NETL B6 combustion rig (completed)
    - Yong Liu, Mehrdad Shahnam and Chris Guenther, "CFD Simulations of Propane/Natural Gas Blended Fuels Combustion in Gas Turbine," AICHE Annual Meeting, 192d, November 10-15, 2019, Orlando, FL
    - Shahab D. Mohaghegh, Mehrdad Shahnam, Ayodeji Aboaba, Yvon Martinez , Chris Guenther, Yong Liu, Anthony Morrow, and Ashley Konya, "Data-Driven Smart Proxy for Computational Fluid Mechanics," Multiphase Flow Science Workshop, Aug 6-8, 2019, Morgantown WV
- Develop a CFD and proxy model of an industrial scale boiler over multiple parameters(completed)
    - Aboaba, A.; Martinez, Y.; Mohaghegh, S.; Shahnam, M.; Guenther, C.; Liu, Y., Smart Proxy Modeling Application of Artificial Intelligence & Machine Learning in Computational Fluid Dynamics, https://www.osti.gov/biblio/1642460 DOI 10.2172/1642460

Total Number of Cells = 4,035,275

	Number of Cells	Perc. Cells
< 10%	4,034,585	99.98%
10% - 20 %	690	0.02%
20% - 30 %	-	0.00%
30% - 40 %	-	0.00%
40% - 50 %	-	0.00%
50% - 60 %	-	0.00%
60% - 70 %	-	0.00%
70% - 80 %	-	0.00%
80% - 90 %	-	0.00%
> 90%	-	0.00%

Oxygen prediction and error analysis from the digital twin compared to CFD results

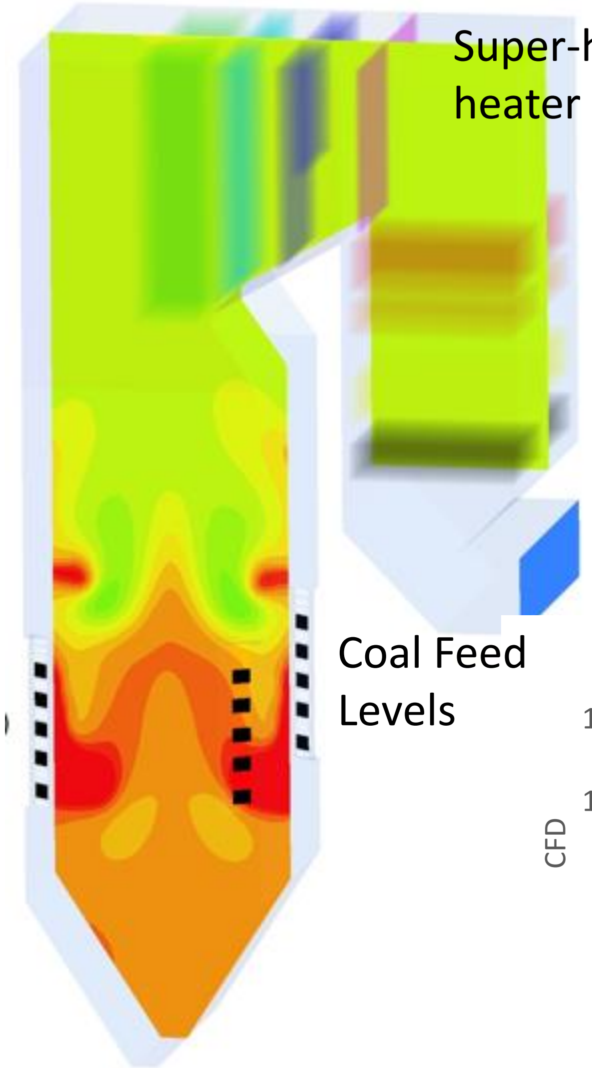




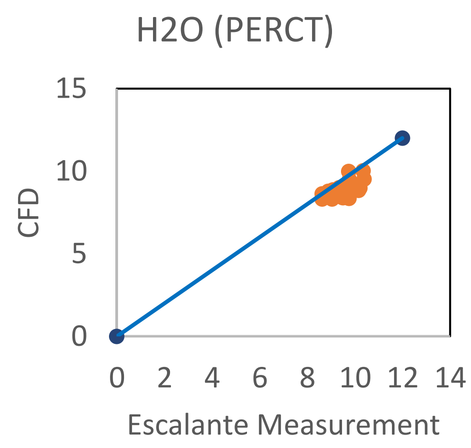
EY21 Project Approach

Research Plan through EY21 and beyond

- Evaluate various methodologies to establish a framework at NETL to generate a high fidelity proxy model of a particular device.
  - NETL In-House Tools
  - Deep XDE
  - NVIDIA's SimNet
- Evaluate in the loop cognitive training development for proxy models or digital twins(in-progress)
  - Allows greater flexibility in the goal of extending this work to include transient data applications
- Submit Power Engineering article (in-progress)
  - "Development of a High Fidelity Digital Twin of a Industrial Scale PC Boiler Under Partial Load Operations "
- Ensure proxy models can be leveraged by Advance Sensors & Controls Task 82 (dynamic, deployed through cloud services)



Proxy model prediction of Tri-State boiler moistures levels thru the boiler and CFD predictions compared to plant data



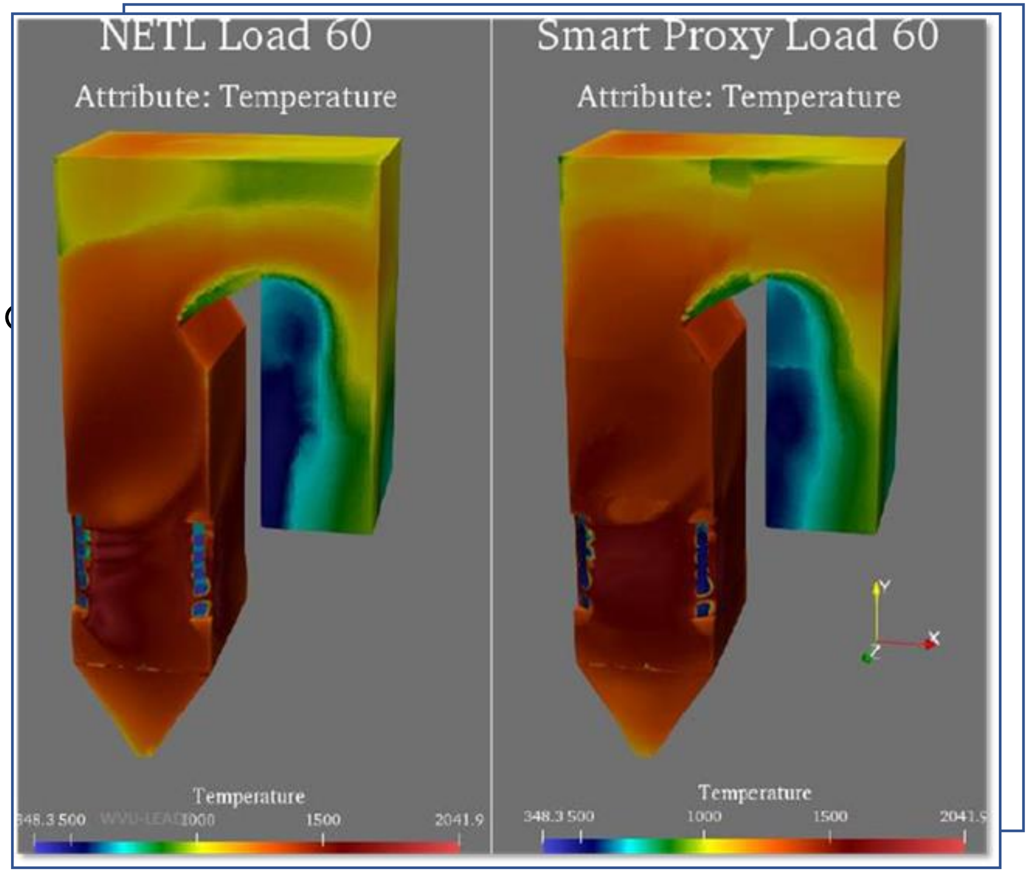
Proxy Model Development

Option A: NETL In-House Tools

- Supervised deep learning framework developed in a NETL + WVU collaboration.
- Requires a set of input features and corresponding CFD solution fields for training.
- Loss functions based on differences between predictions and CFD data (ground truth) at CFD grid point locations.

Pros
- Doesn't need to solve the governing PDEs (difficult for stiff problems)
- Can be easily ported to ANSYS digital twin builders.

Cons
- Requires large CFD data sets for training
- Requires careful crafting of input features for NN training.
- Poor generalizability. Difficult to adapt the framework developed for one engineering device for use in another.

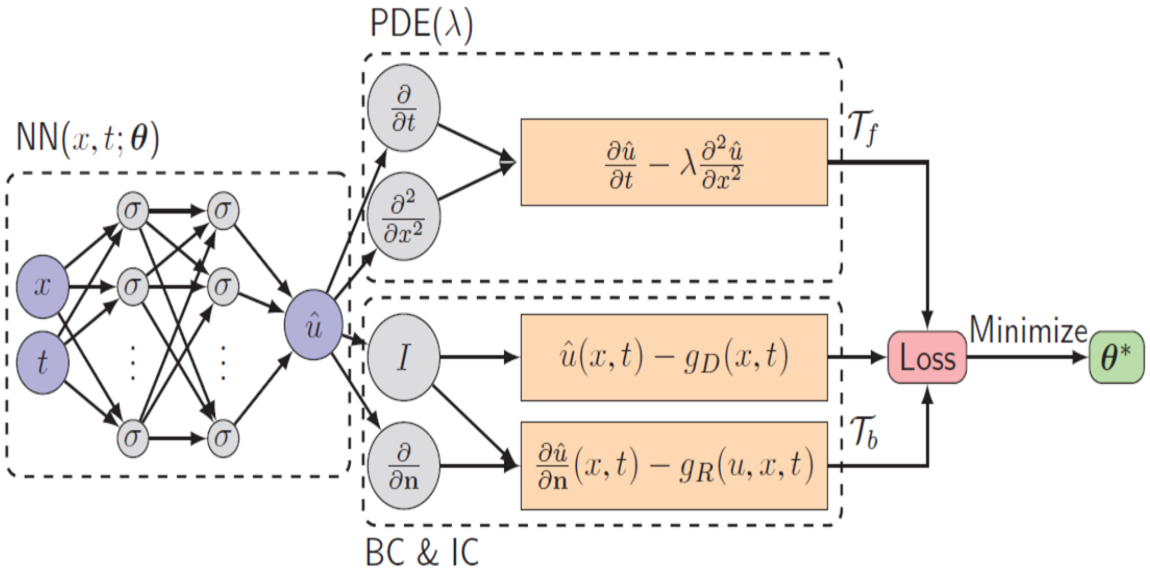


CFD and Proxy Model Predictions of a Boiler Under Turn-Down

Proxy Model Development

Option B: Deep XDE

- Unsupervised physics-informed deep learning framework developed at Brown University.
- Takes spatial coordinates & time as inputs to generate & momentum equation satisfying flow fields.
- Loss functions based on the residuals of the governing equations at arbitrary points.



DEEP XDE TRAINING PROCEDURE

Pros

- Does not require any CFD data for training.
- Generalizable. Can be easily adapted for any geome
- Can be integrated with ANSYS tools.

Cons

- Requires solving the governing PDEs
- Limited features. Requires significant development work to make it usable by engineers for a broad range of problems.
- Development required to allow for reacting flows & parametric studies.

Proxy Model Development

Option C: SimNet

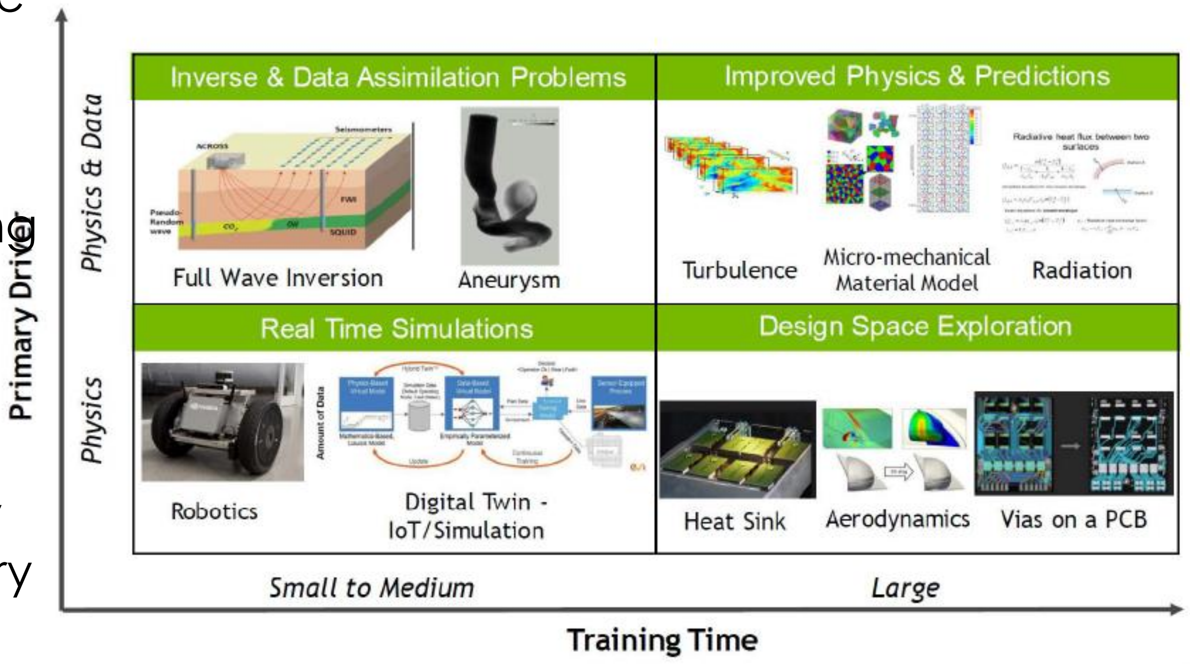
- Unsupervised physics-informed deep learning framework from NVIDIA.
- Takes spatial coordinates, time and parameter range as inputs to generate mass, momentum & energy equation satisfying flow fields for a wide range of parameters.
- Loss functions based on the residuals of the governing equations at arbitrary points.

Pros

- Does not require any CFD data for training.
- Allows for parametric studies (e.g. for UQ)
- Highly generalizable. Can be easily adapted for any flow configuration with arbitrary changes in geometry and physics.

Cons

- Requires solving the governing PDEs
- Development required for reacting flows
- Has some licensing requirements



SIMNET CAPABILITIES

Engagements & Technology Maturation

Engagement Activities

Partners

Outreach & Engagement Activities

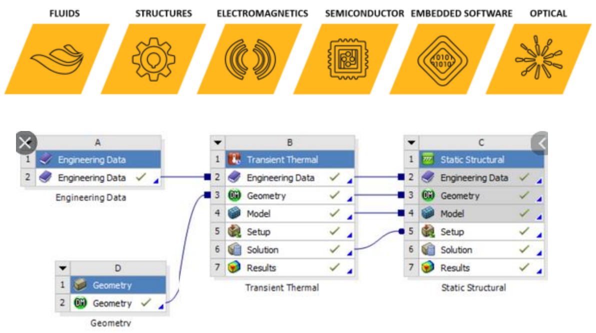
- Escalante/Tri-State Power Plant (CRADA Location New Mexico)
- Longview Power Plant (CRADA Location West Virginia)
- NTPC-NETRA (MOU Location India)
- Ansys/Fluent (CRADA discussions being held Location Canonsburg, PA)
  - Software is being provided to NETL for evaluation to build dynamic digital twins deployed through cloud services

Digital Twin for Field Engineers

Proxy Model Deployment with ANSYS Tools

NATIONAL ENERGY TECHNOLOGY LABORATORY

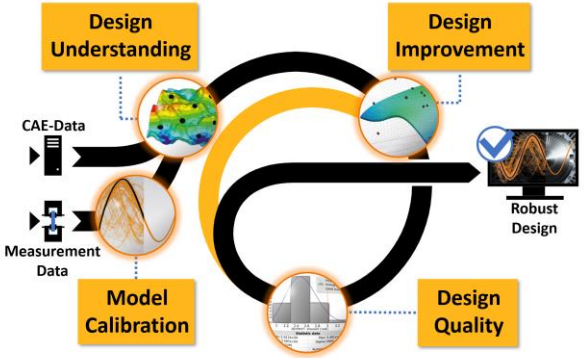
CAPTURE



Capture Multiphysics and Systems

- CFD, data, etc
- External/proprietary Proxy Models

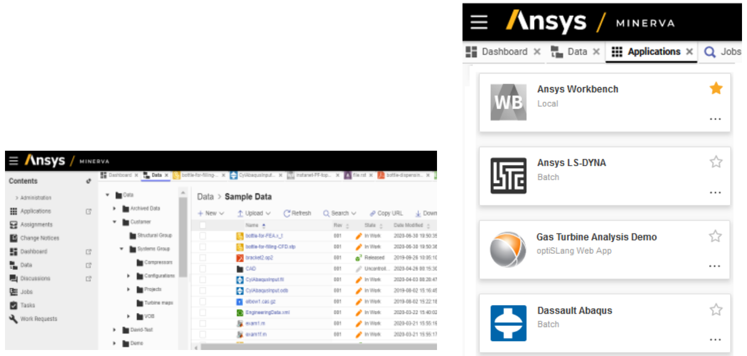
CONNECT



Implement design studies with ANSYS and 3rd party tools

- Process Integration, workflow automation
- Connect Python based Proxy Models and postprocessing

DEPLOY

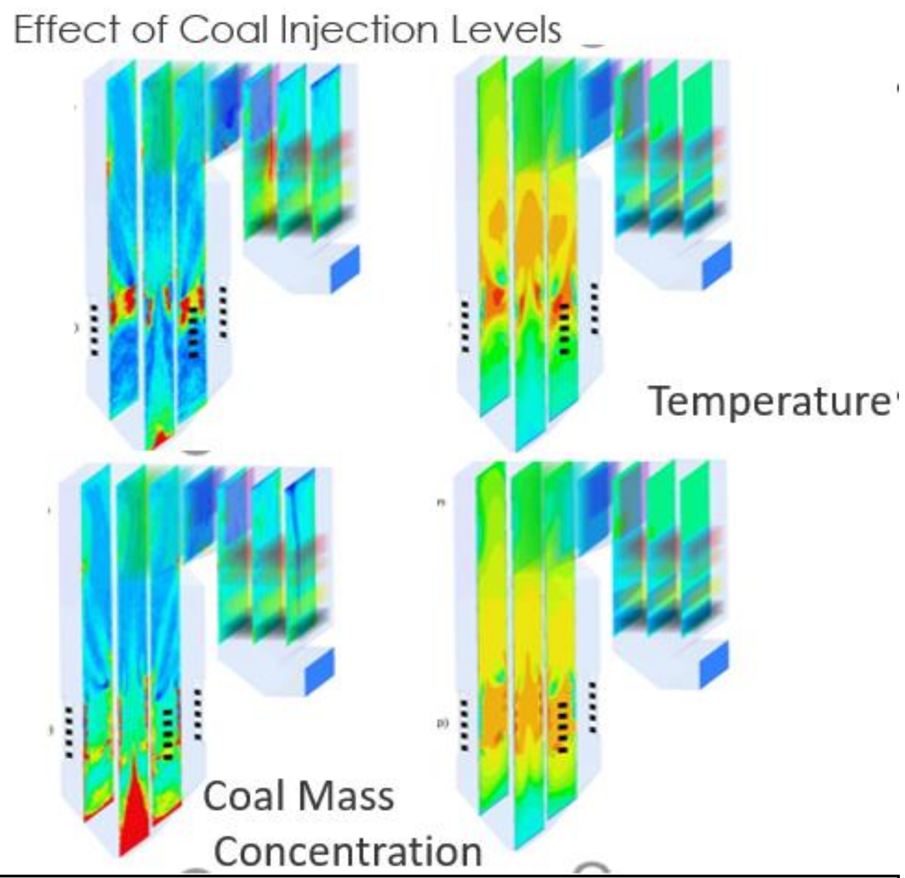


Deploy simulations across the enterprise

- Field deployment through webinterface
- Manage real-time access

Summary

- Industry does not typically have in-house or commercially available tools to deploy proxy model based digital twins.
  - Efficiency, optimization, guide complex operations, cyber security etc.
- NETL has successfully demonstrated the ability to develop a high-fidelity proxy model based on CFD data which can be deployed as a digital twin
  - Demonstrated the methodology is geometry independent, scale independent, runs in near real-time.
  - Restricted to steady-state CFD data, difficult to train the NN, not generalizable
- Currently in the process of evaluating best approach in developing a proxy model (in-house, Deep XDE, SimNet)
  - Generalizable, steady-state or transient, easily trained.
  - Dynamically updated and served through the cloud.
- Partnered with ANSYS to demonstrate approach to industry and ensure a pathway for technology maturation.



Proxy model predictions during variation in the operation of the coal injection levels.