Developing Digital Twins for Energy Applications Using Modulus

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Disclaimer

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Introduction/Overview

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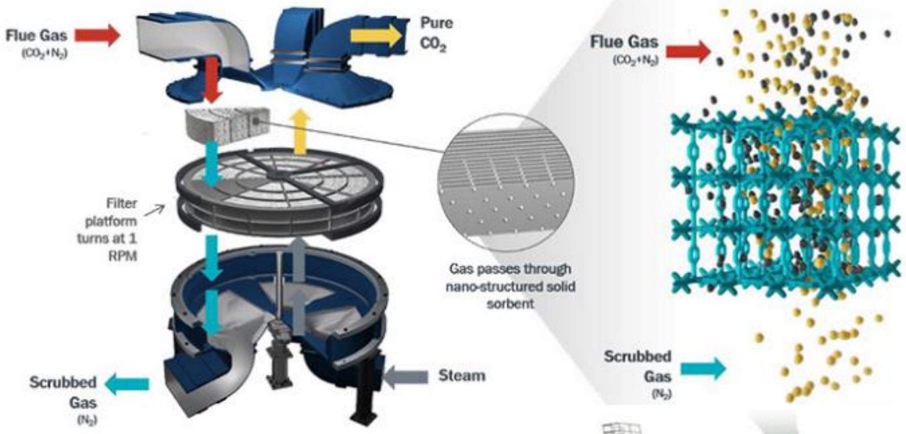
DOE Earthshots: Innovations using AI

★ **Towards net-zero energy economy**

- Reduce emission of greenhouse gases
- Design more energy-efficient systems (industrial/domestic)
- Capture CO_2 from point sources and air
- Enhanced oil recovery (EOR)
- Geological storage of CO_2
- All the above require fast development cycles

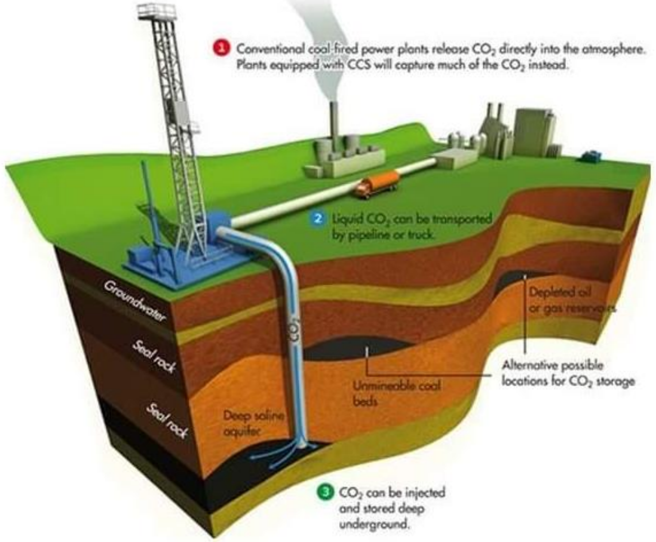
★ **Developing AI-based digital twins of engineering devices**

- Digital replica of engineering process/device
- Greatly accelerate the transition to net-zero
- Efficiently handle a large design space
- Develop and scale CCS devices
- Develop fuel efficient systems



Flue gas capture

Direct air capture



Underground carbon storage

Image sources: NETL Communications/Multimedia Services

Physics Informed Neural Networks

Physics guided deep learning approach using Modulus from NVIDIA

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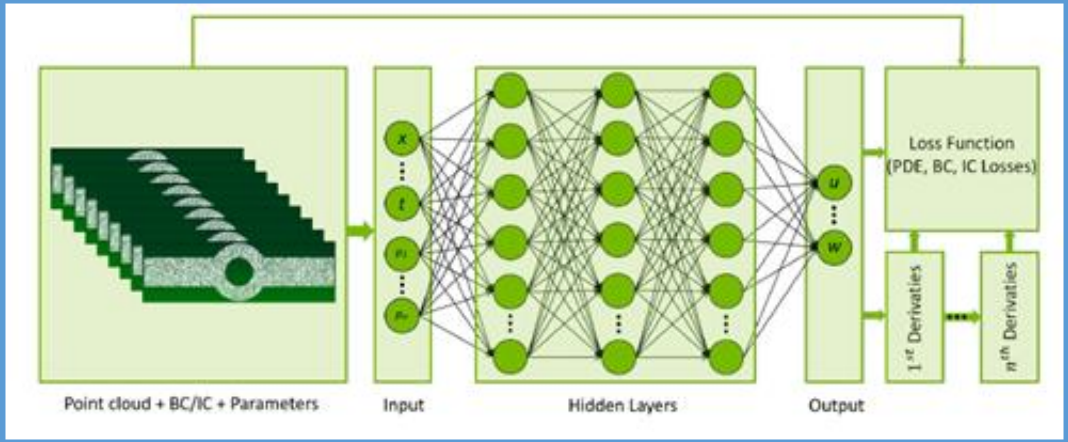
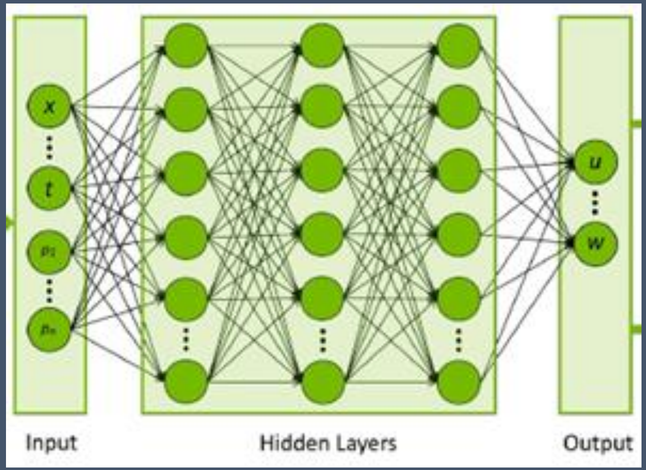
- Relates spatial & temporal coordinates (*x, y, z, t*) to physical fields (e.g., velocity, pressure, temperature)
- NNs trained to minimize the residual form of the same physical equations as in CFD
- Parameterized system representation can solve for multiple configurations simultaneously
- Near-instantaneous inference
- Orders of magnitude faster than CFD for UQ/design optimization problems

OFFLINE TRAINING over a parameter space



TRAINABLE NETWORK

ONLINE prediction for arbitrary conditions



FROZEN NETWORK

Figure source: Hennigh et al., "NVIDIA SimNet: An AI-accelerated multiphysics simulation framework" (2020)

Modulus: Salient Features

Modulus Model Training

- Uses TensorFlow 1.x but is being ported to PyTorch
- Exact differentiation
- Soft constraints on governing equations and BCs
- No requirement for structured grid format or grid connectivity information
- Can utilize advanced NN architectures like Fourier Network/SiReN
- Options for dynamic loss weighting (being tested now)

$$Loss(\boldsymbol{\theta}) = \Sigma w_i Loss_{interior} + \Sigma w_b Loss_{boundary}$$

Hyperparameters

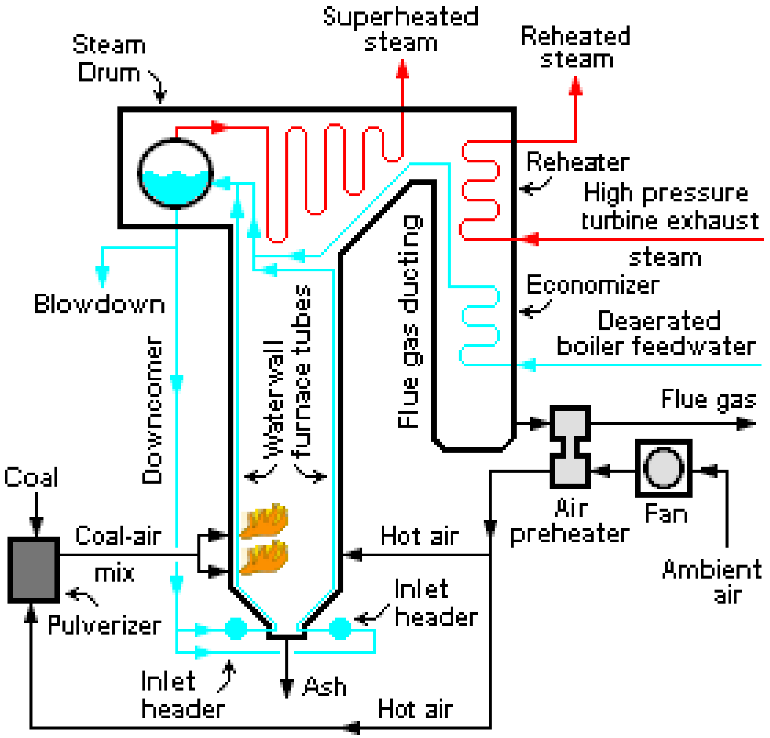
$Loss_{interior} = |LHS_{gov} - RHS_{gov}|^{order}$ $Loss_{boundary} = |LHS_{BC} - RHS_{BC}|^{order}$

PINN for Reacting Flows

Formulation and PINN vs CFD

- **Aim:** Create a digital twin of an industrial scale boiler
- Simplified methane oxidation
- Implemented reacting flow transport equations for kinetics-controlled combustion
- No requirement for training data

★ Single PINN model for a range of input conditions
★ Fidelity and accuracy comparable to CFD
★ Trained PINN can provide near-instantaneous inference for any input condition



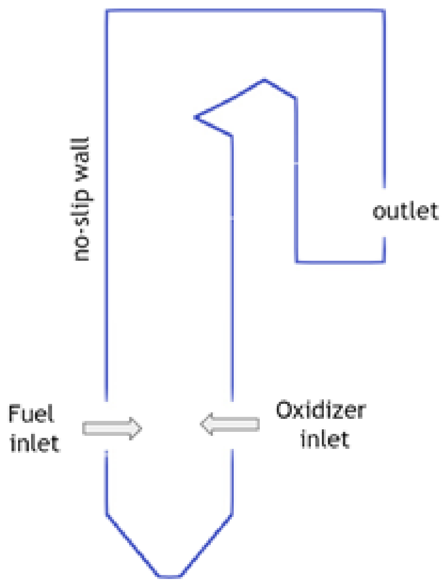


Figure source: https://commons.wikimedia.org/wiki/File:Steam_Generator.png

Towards a Reacting Flow Solver

Governing Equations: Strongly Coupled PDEs

- Single species
- Turbulent
- Steady state
- 2D

→

- **Multiple species**
- Turbulent
- Steady state
- 2D

→

- Multiple species
- **Reacting**
- Turbulent
- Steady state
- 2D

→

- Multiple species
- Reacting
- Turbulent
- **Transient**
- 2D

→

- Multiple species
- Reacting
- Turbulent
- Transient
- **3D**

- Continuity: $\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0$
- Species mass fraction: $\rho \frac{\partial Y_k}{\partial t} + \rho u_i \frac{\partial Y_k}{\partial x_i} = \dot{\omega}_k + \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right)$
- Momentum: $\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$
- Temperature: $\frac{\partial T}{\partial t} + \frac{\partial}{\partial x_i}(u_j T) = \frac{\dot{\omega}_T}{\rho c_p} + \frac{\partial}{\partial x_i}\left(\alpha \frac{\partial T}{\partial x_i}\right)$
- Kinetics-controlled single step irreversible reaction: $CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2$
- Species source/sink terms: $\dot{\omega}_{CH4} = -MW_{CH4} k_f \left(\frac{\rho Y_{CH4}}{MW_{CH4}}\right) \left(\frac{\rho Y_{O2}}{MW_{O2}}\right)$ etc
- Temperature source term: $\dot{\omega}_T = -\sum_{k=1}^{N} h_k \dot{\omega}_k = -\sum_{k=1}^{N} h_{sk} \dot{\omega}_k - \sum_{k=1}^{N} \Delta h_{f,k}^0 \dot{\omega}_k$

Parametric Boundary Conditions

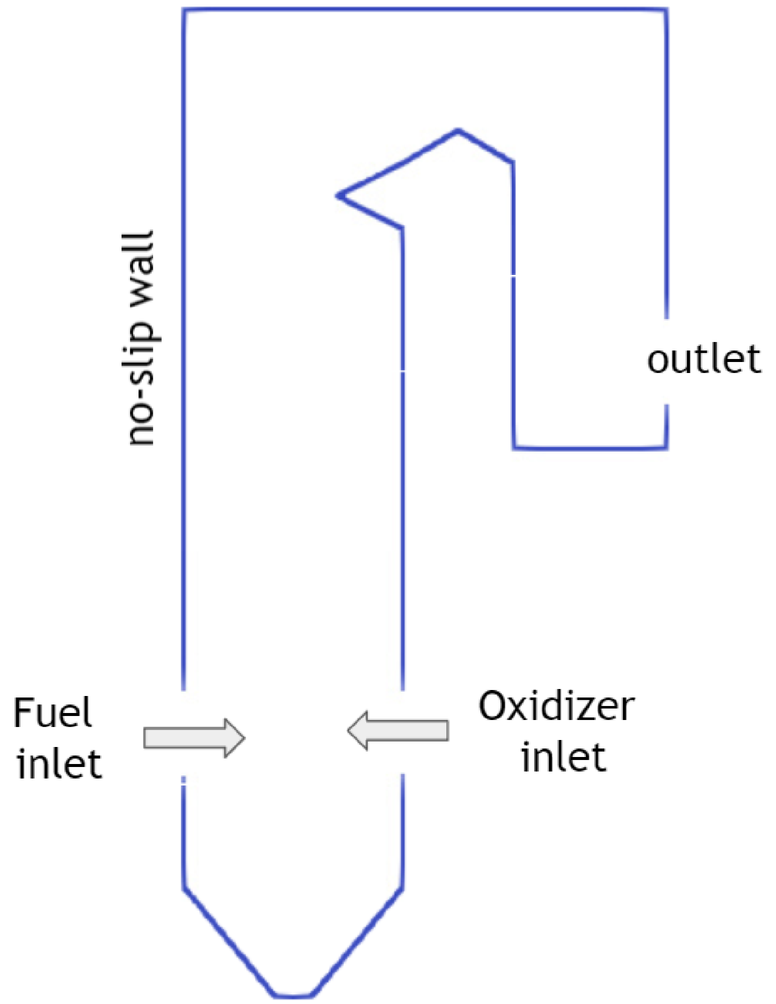
Species Mass Fractions, Velocity and Temperature

Inlet Conditions

	Fuel inlet	Oxidizer inlet
Y_ch4	0.5	0.0
Y_o2	0.0	0.23
Y_co2	0.01	0.01
Y_h2o	0.01	0.01
Y_n2	0.48	0.75
Velocity, m/s	1.0	**1.0 – 5.0**
Temperature, K	650	650

Wall Conditions

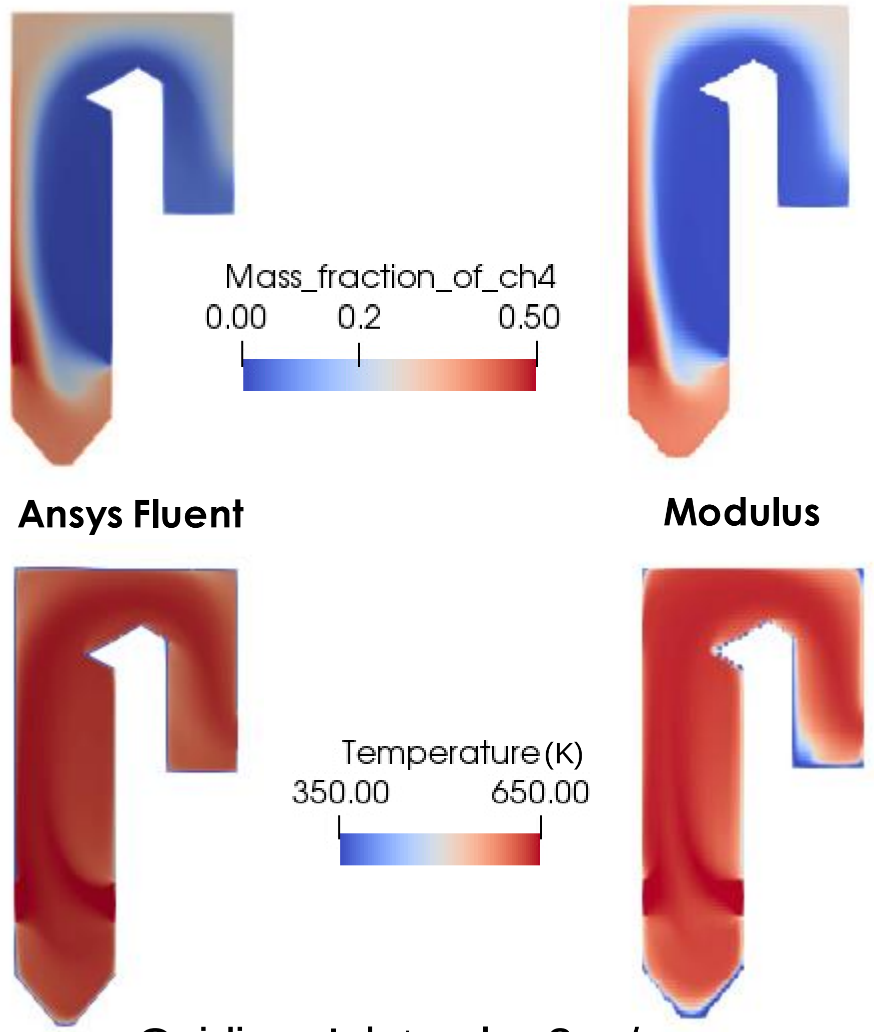
Temperature, K	350.0
Species	Zero flux
Velocity	No-slip



Multi-Species Nonreacting Flow

CFD vs. PINN

- 3 non-reacting species (CH_4, O_2, N_2)
- Species (Y) and Temperature (T) distributions compare well with ANSYS Fluent
- Improved predictions after normalization of the governing equations and BCs

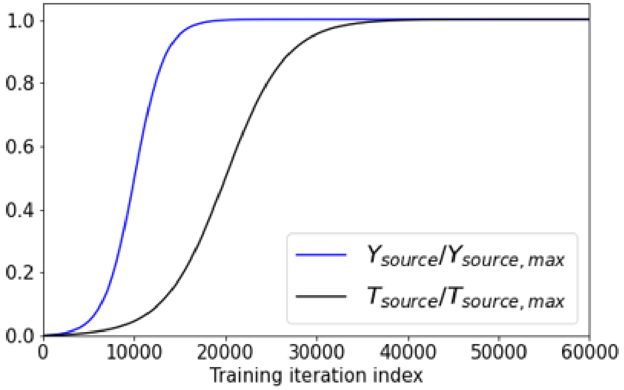


Oxidizer Inlet vel = 2 m/s

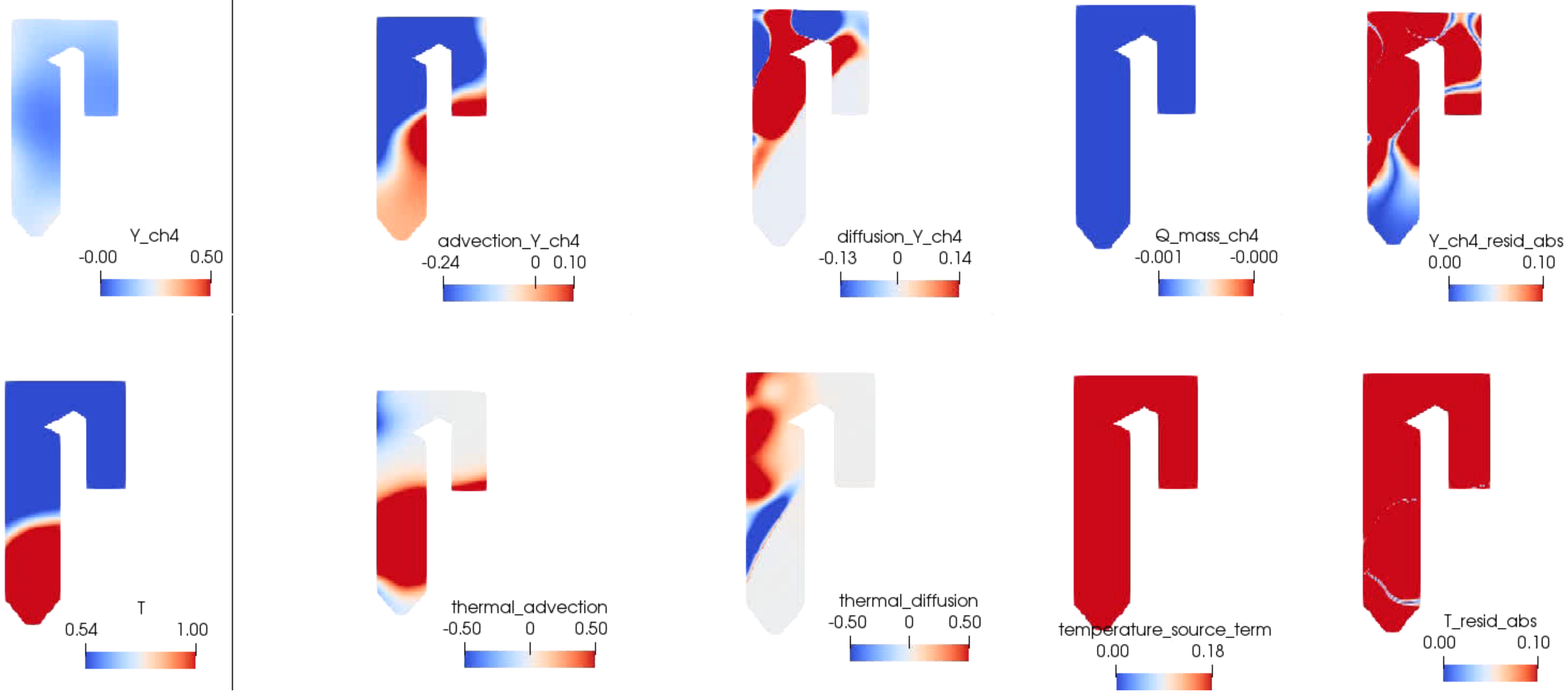
First Attempt at Reacting Flow Solver

Handling Y-T coupling

- Strongly coupled PDEs
- Y and T source terms allowed to increase gradually



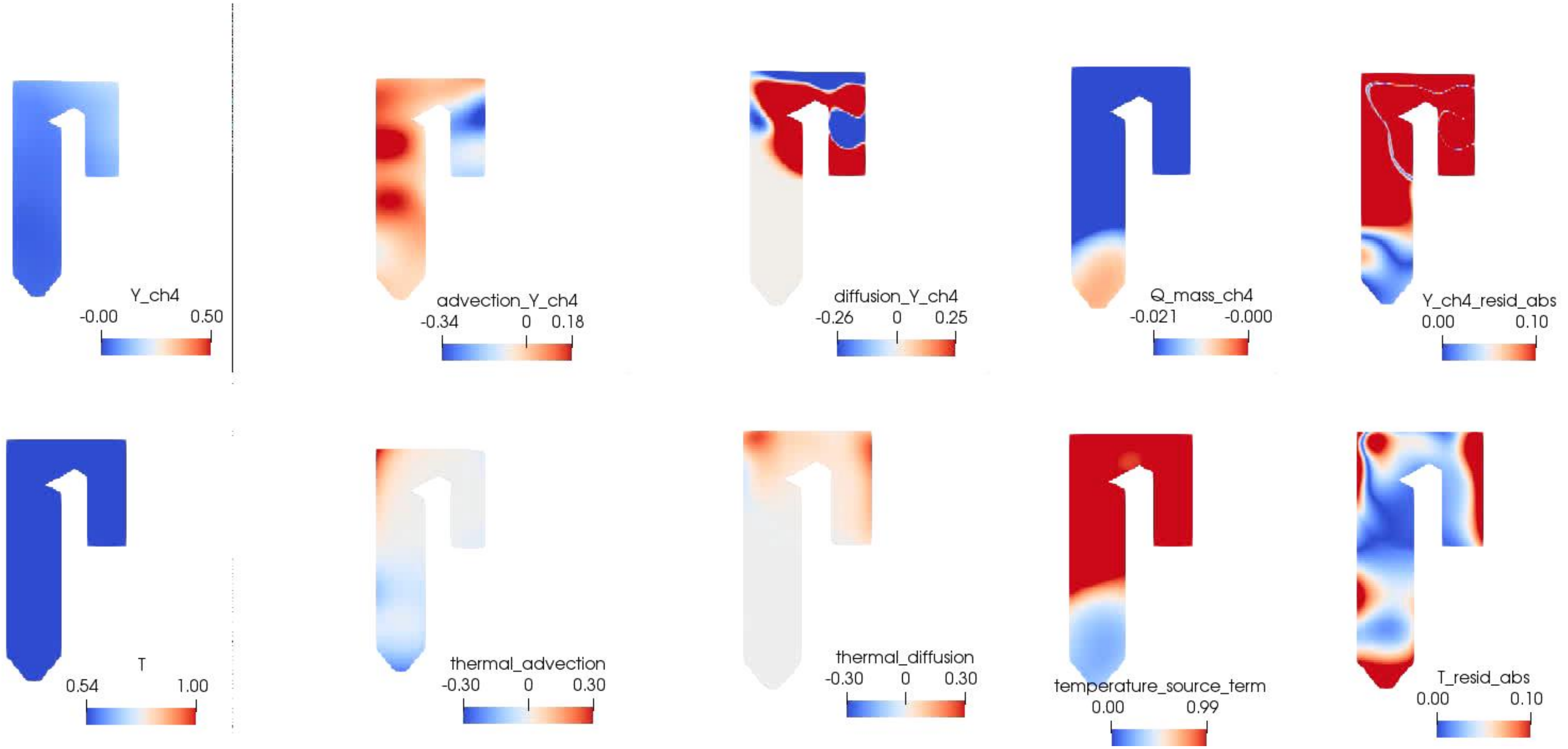
- Y distribution goes unphysical after initial increase
- Unphysical Y distribution affects the T field



Without T-Source

Simplified system

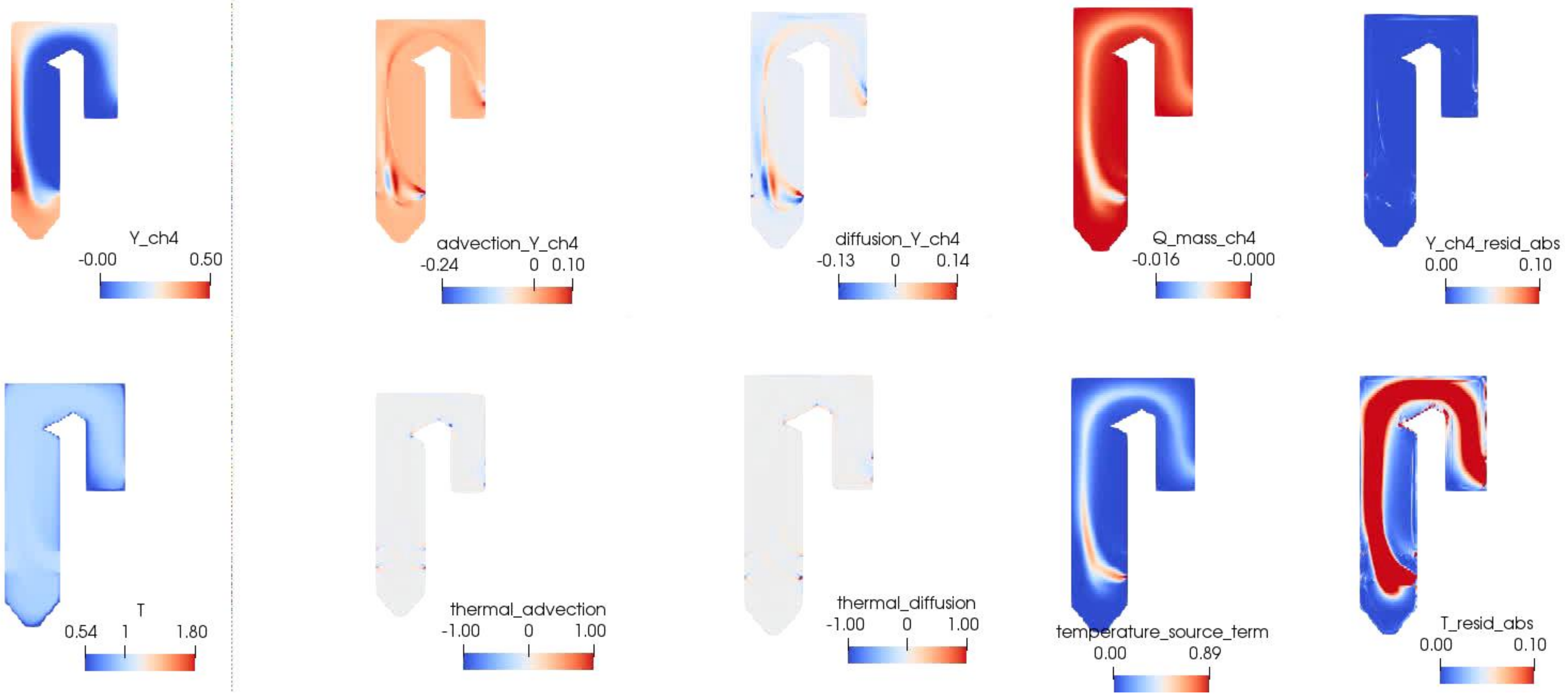
- T source removed from the system for the time being
- The reactant and product distributions are reasonable
- This field is used as IC for subsequent cases



One Way Y-T Coupling

Frozen Species Field

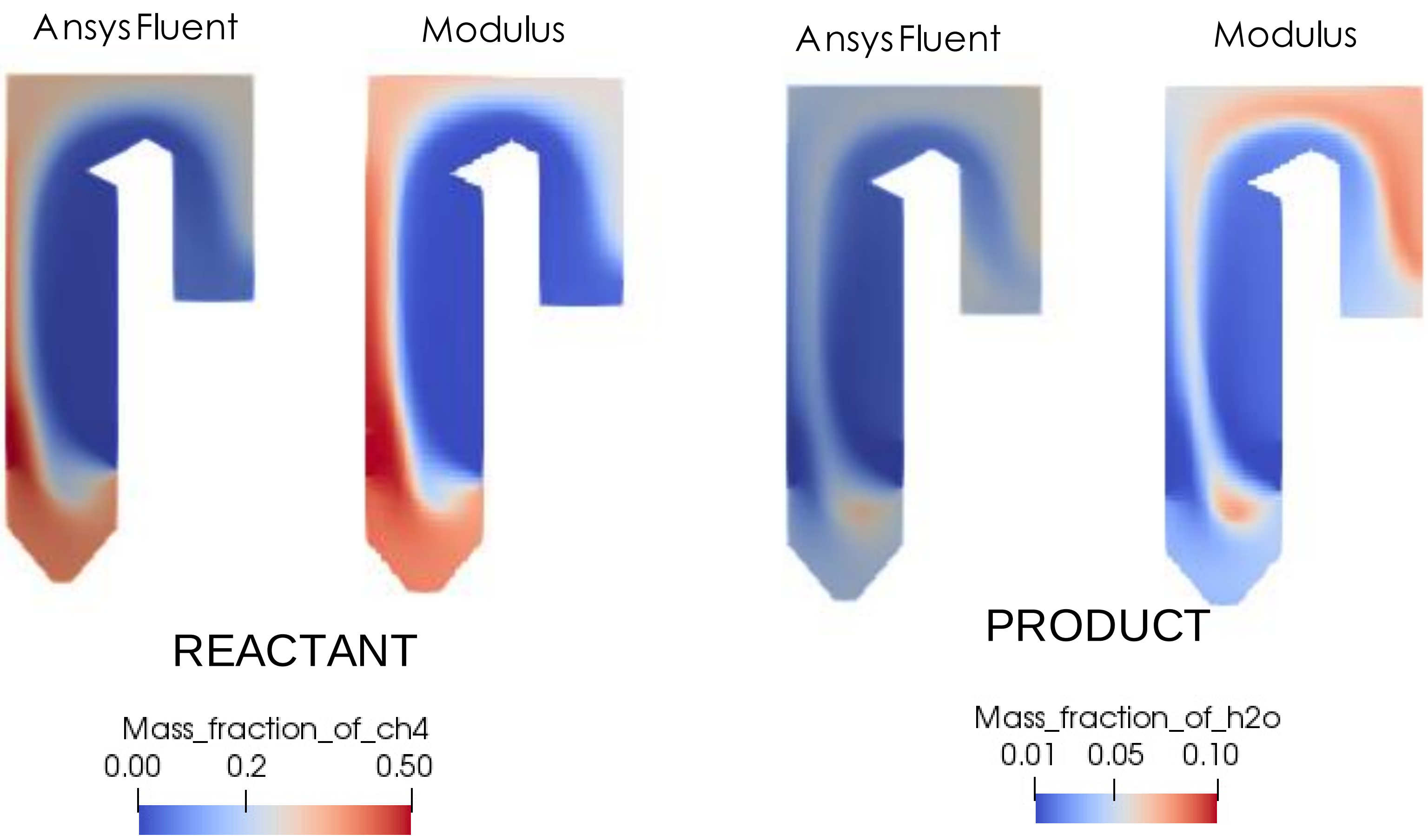
- Species not allowed to evolve from the IC
- T-source reasonably developed at the reaction zone
- Decoupled T and Y fields can lead to severe errors



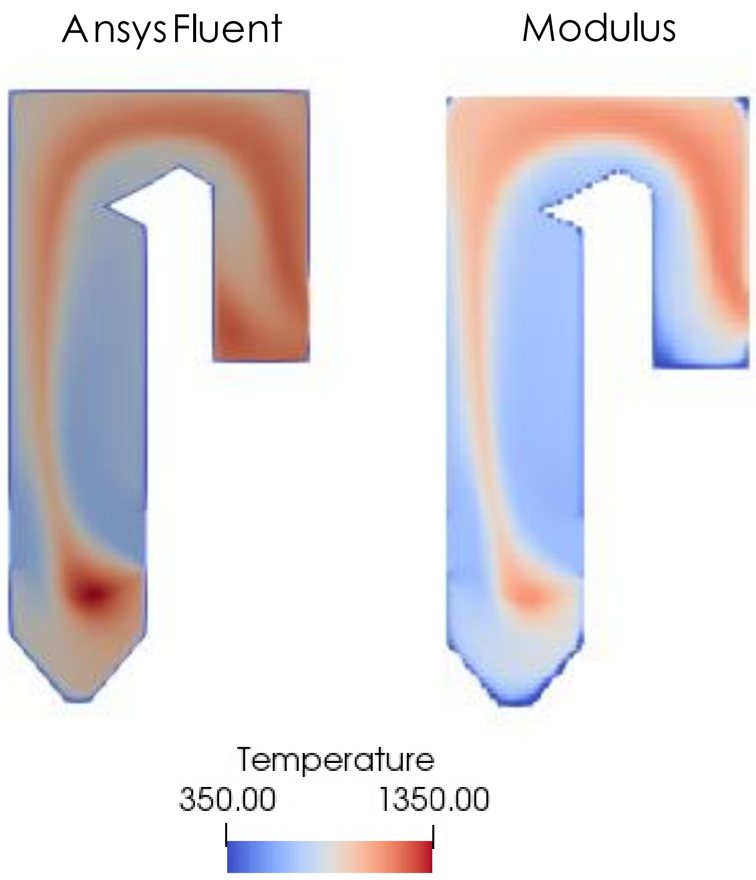
Simplified Systems

PINN vs. CFD

Species distributions for case without T source term

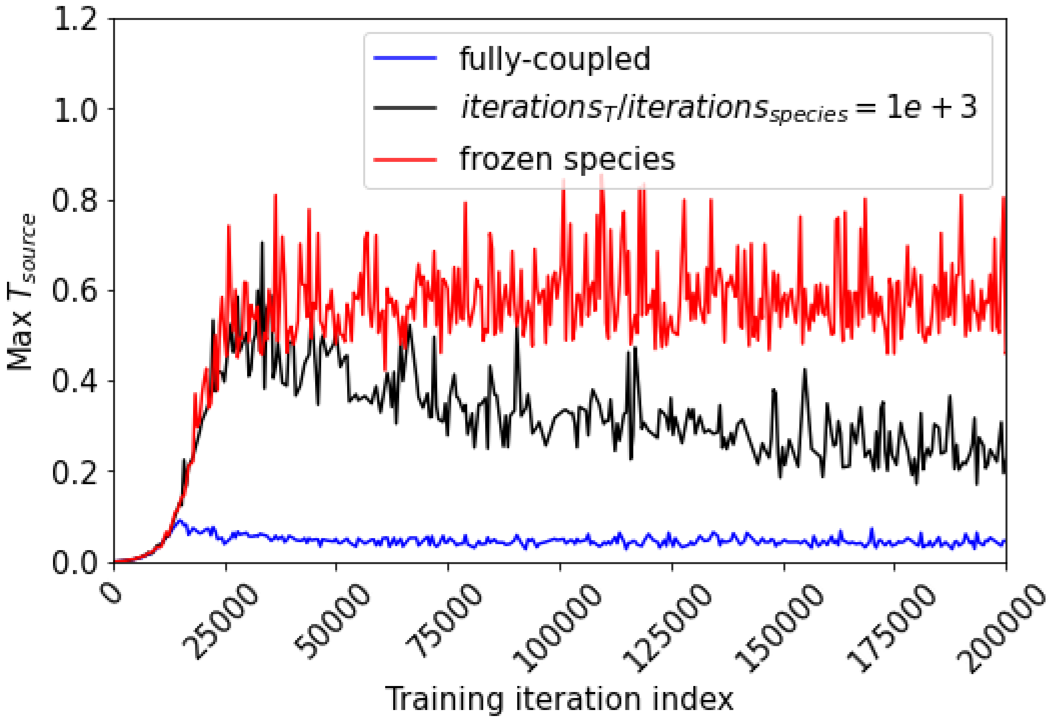


Temperature distribution with frozen species



Increasing Y-T Coupling

- To increase the Y-T coupling, Y solved for every 100-1000 T iterations
- Issue persists: T-source drops off



Resolving the issue with large T-source

Handling large T-source

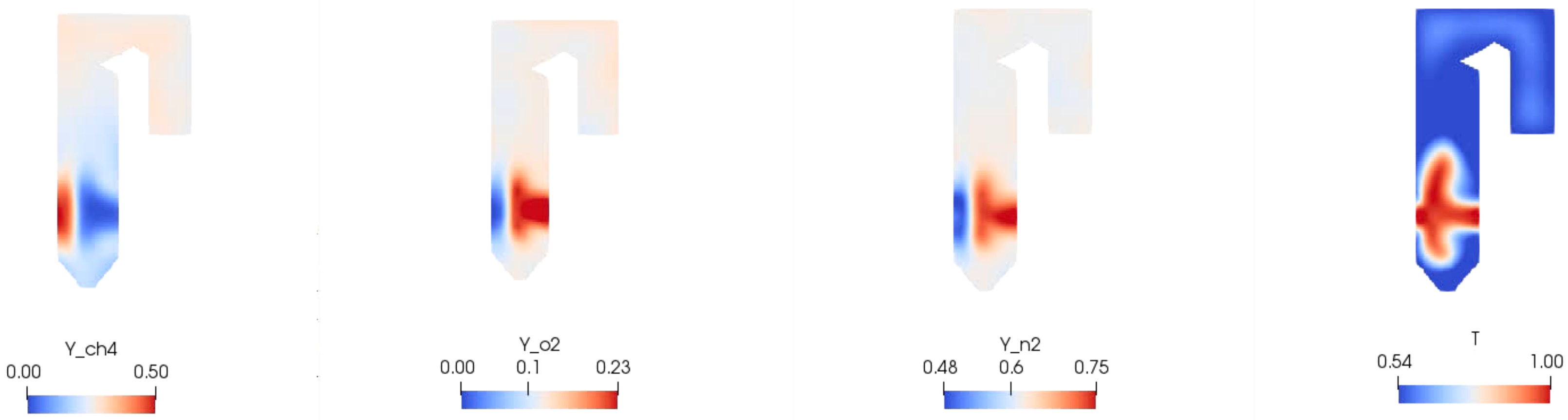
- T-source dominates the Y-source
- This can lead to imbalances between the backpropagated gradients

A) Gradient normalization approach

- Attempts to remove the dominance of any component of the global loss function
- Dynamically assigns weights to different constraints

B) Transient approach

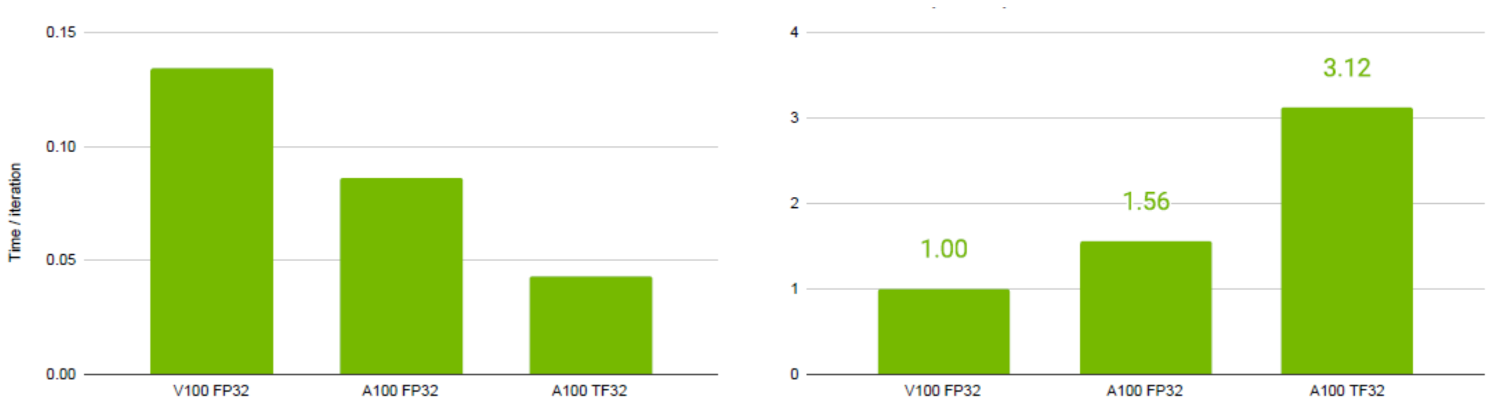
- Handles large source terms by learning the change between states instead of learning everything at once
- Uses a moving time window approach



TF32 vs. FP32 and Scaling Study

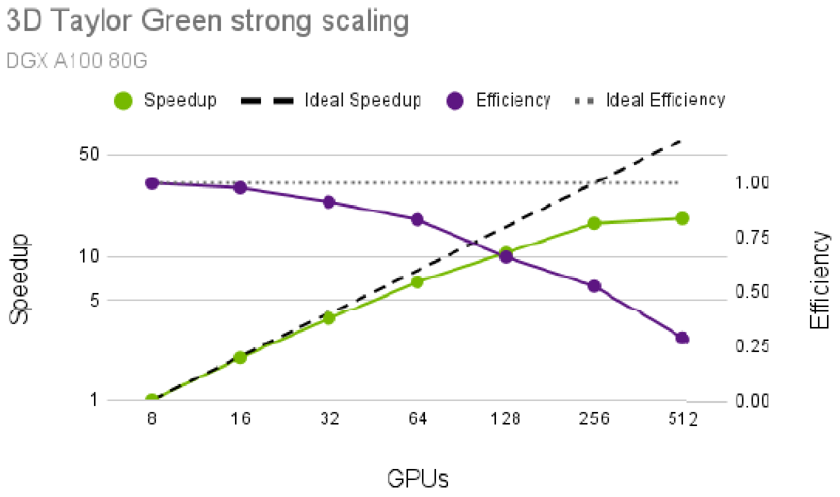
Math Mode & Strong Scaling Performance

- Boiler cases ran on NVIDIA P100 GPUs
- Performance metrics available for sample problems using TF32 on A100 GPUs
- Good multi-node scaling obtained using Horovod for a 3D decaying turbulence case



(a) Time per iteration (b) Speed-up

Accelerated training using TF32 on A100 GPUs



Strong Scaling- Speedup and Scaling Efficiency

Next Steps

Short and Long-Term Goals

- Transition to PyTorch framework from TensorFlow
- Develop a PINN methodology for stiff chemistry
- Develop an RNN-based PINN for transient problems
- Integration with NVIDIA tools for deployment as digital twin

Thank You!

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