Towards solving high Reynolds number reacting flows in SimNet

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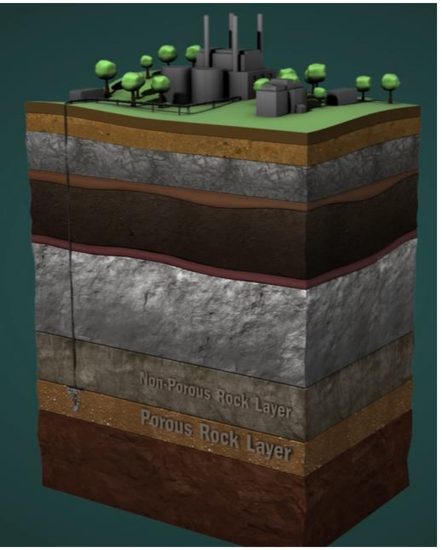
Solutions for Today | Options for Tomorrow

Grand Challenge: Net zero carbon emissions

Achieving net-zero emission goal using PINNs

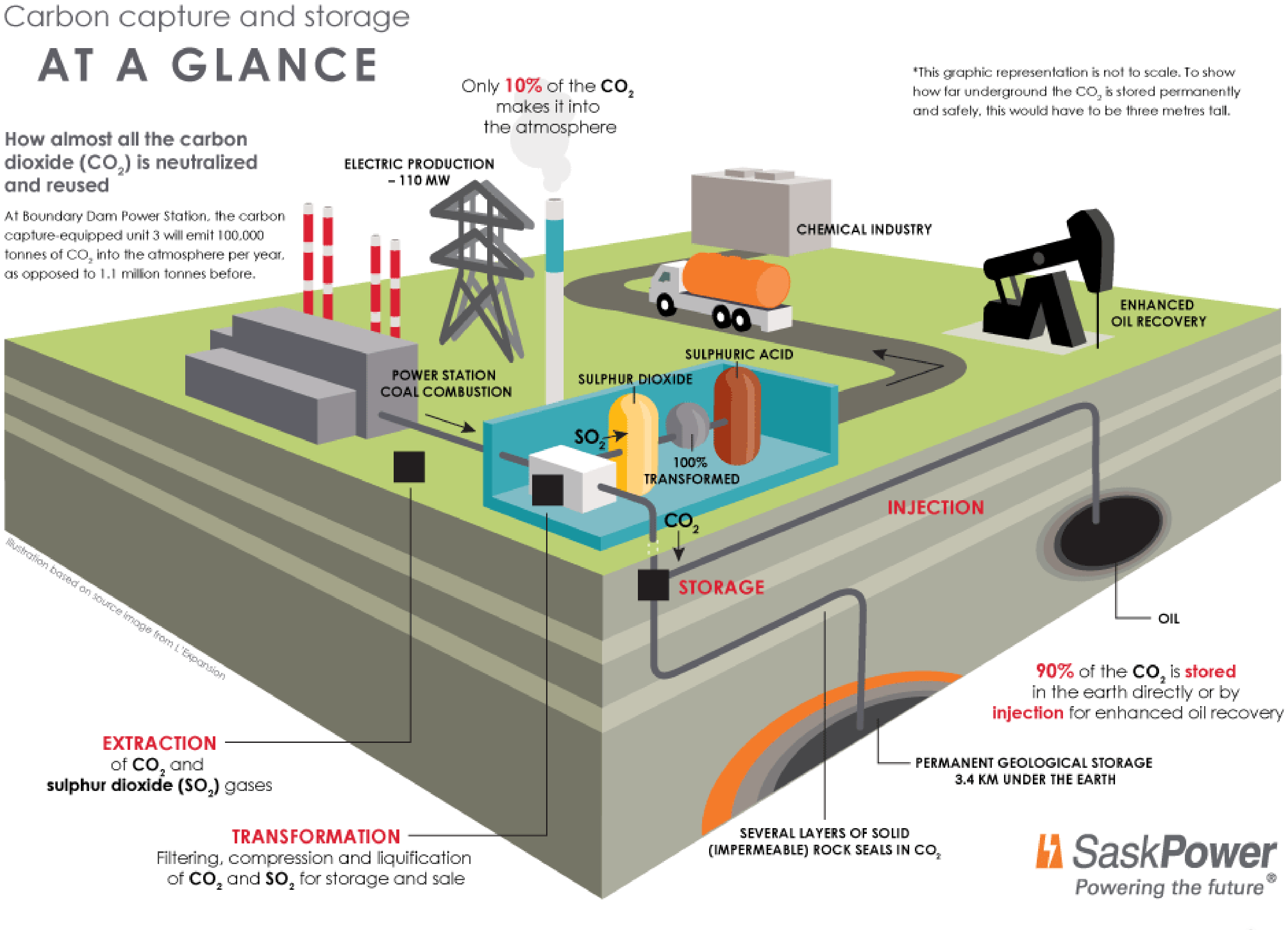
- PINNs necessary for rapid development cycles to meet net-zero grid carbon emission by 2035
- Develop and scale CCS devices
- Develop fuel efficient systems



Carbon storage

Fig source: NETL media team

Direct air capture of CO_2 (DAC)



/https://www.futuretimeline.net/blog/2014/10/21.htm

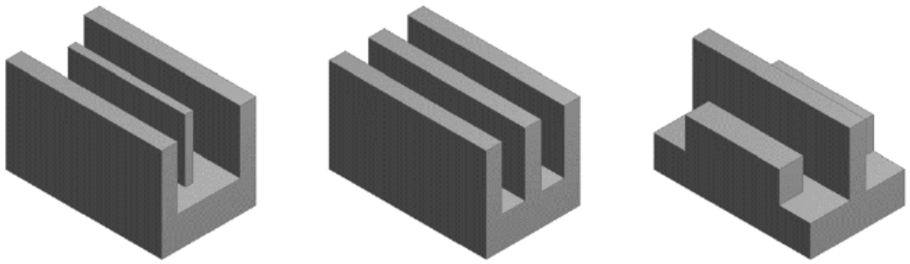
Motivation

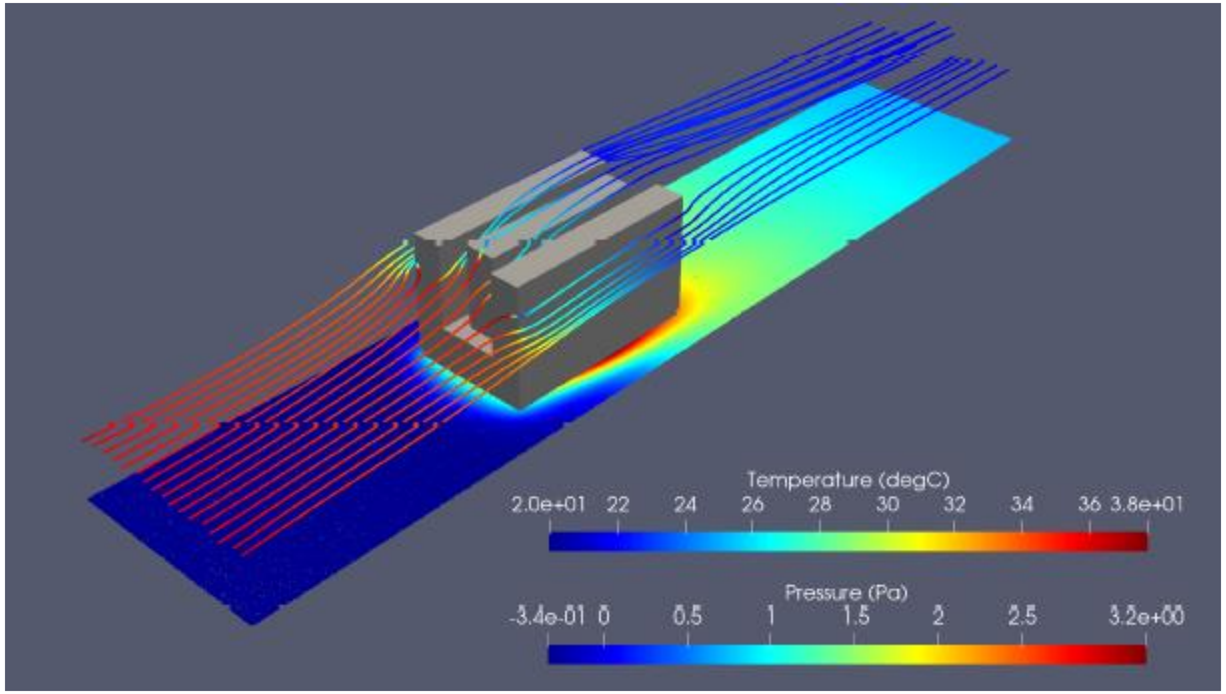
Suitability for product development cycle

- High resolution CFD can be expensive for large parameter space
- Not efficient for UQ and design optimization purposes

$$
\begin{aligned}
h_{centralfin} &= (0.0, 0.6),\\
h_{sidefins} &= (0.0, 0.6),\\
l_{centralfin} &= (0.5, 1.0)\\
l_{sidefins} &= (0.5, 1.0)\\
t_{centralfin} &= (0.05, 0.15)\\
t_{sidefins} &= (0.05, 0.15)
\end{aligned}
$$

Solver	OpenFOAM
Compute Time (hrs)	4099



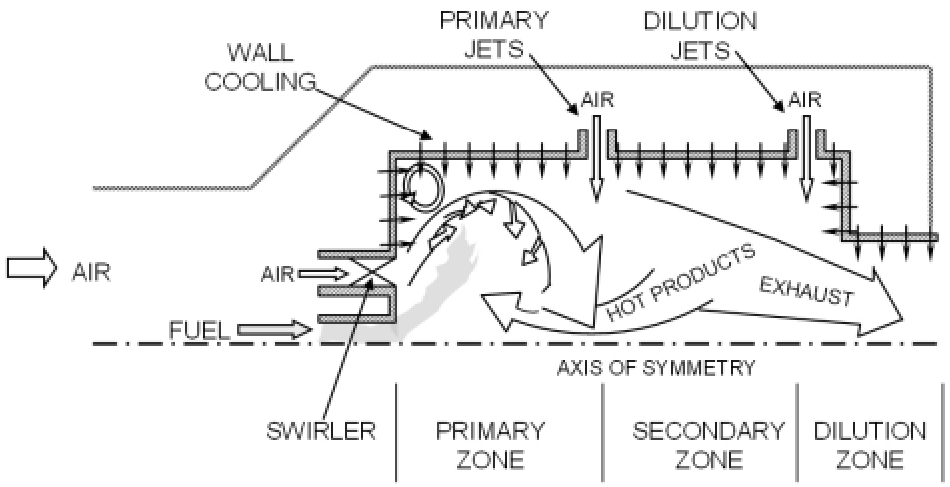


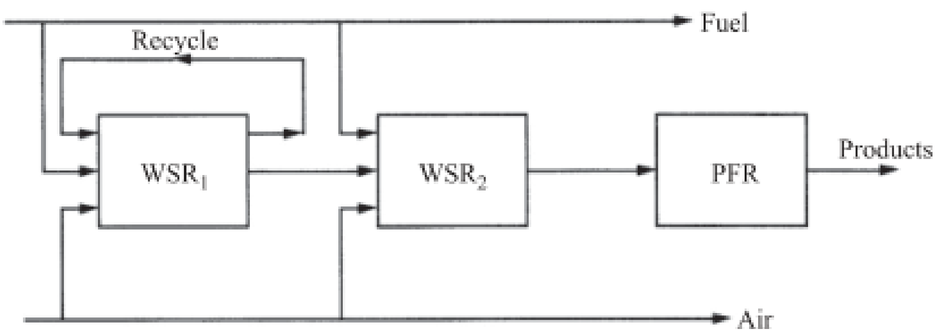
Source: SimNet user guide, version 2106

Motivation

Predictions over a parameterized space

- Reduced ordered models (ROMs) preferred for UQ/design optimization purposes
- Fast but don't capture the accurate physics
- Not robust w.r.t. parameter changes[a]





A reduced order model of a gas turbine combustor using two well-stirred reactors and a plug flow reactor

a. https://web.stanford.edu/group/frg/active_research_themes/reducedmodel.html

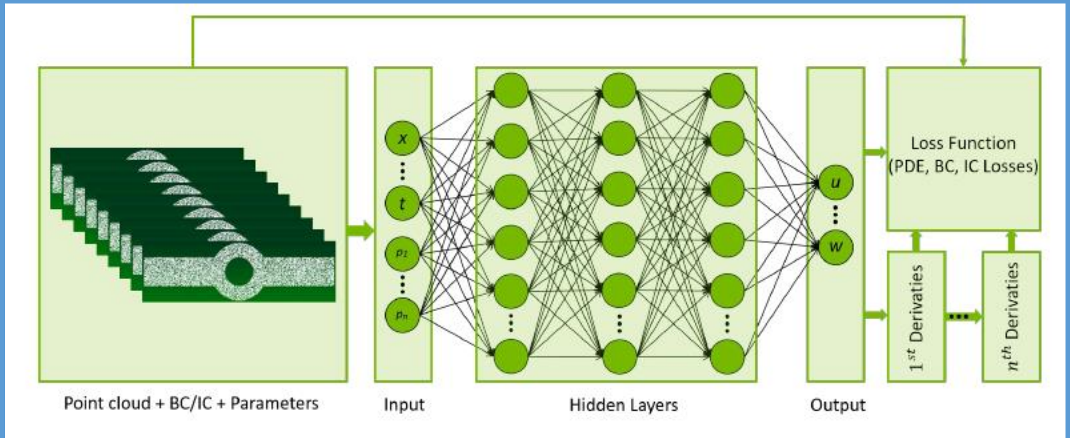
Fig sources: https://www.netl.doe.gov/sites/default/files/gas-turbine-handbook/3-2-1-1.pdf, Turns S, "An Introduction to Combustion: Concepts and Applications"

Physics informed neural network (PINN)

Predictions over a parameterized space

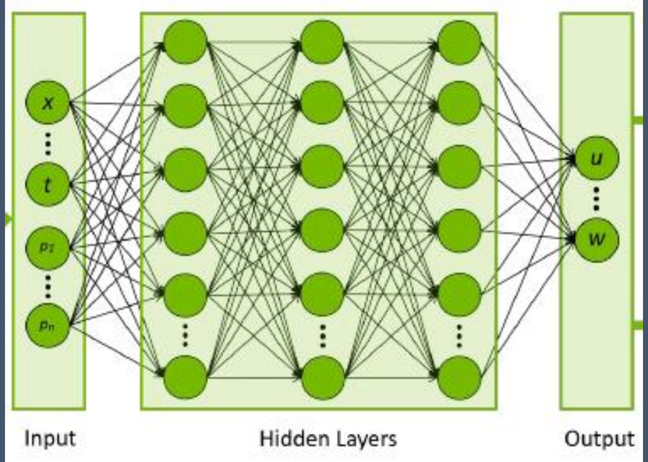
- Near-instantaneous inference for a large parameter space at arbitrary points
- Can have accuracy comparable to CFD
- Applications: 1) digital twins (real time control, cybersecurity, machine health monitoring)
  2) design optimization and UQ

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)

PINNs: Reduced compute time

Predictions over a parameterized space

- High resolution CFD can be expensive for large parameter space
- CFD not efficient for UQ/design optimization purposes

$$
\begin{aligned}
h_{centralfin} &= (0.0, 0.6), \\
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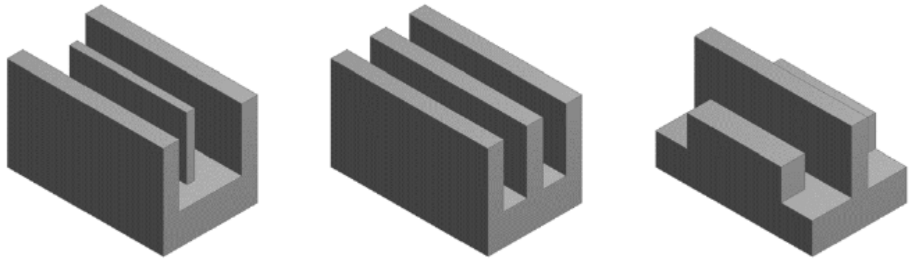
l_{sidefins} &= (0.5, 1.0) \\
t_{centralfin} &= (0.05, 0.15) \\
t_{sidefins} &= (0.05, 0.15)
\end{aligned}
$$

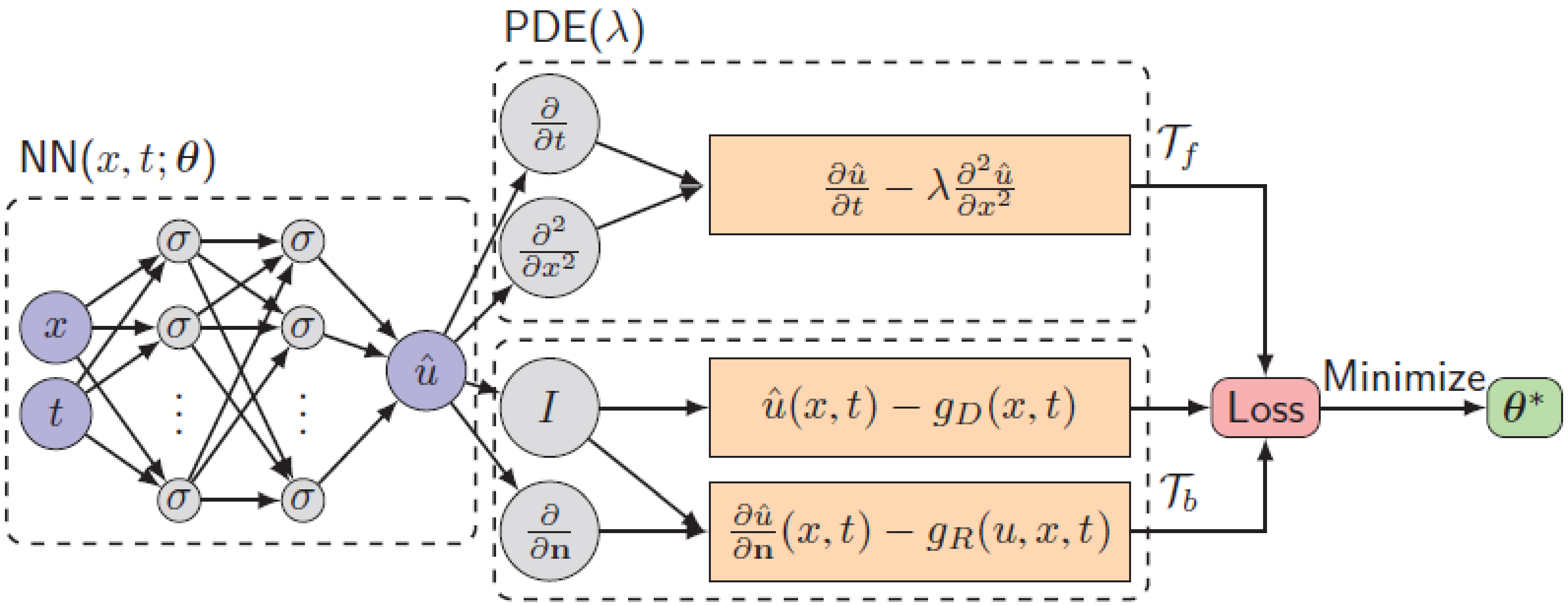
Solver	OpenFOAM	SimNet
Compute Time (hrs)	4099	120



PINN formulation

Model training

- Using Neural Networks as function approximators
- Conservation equations and BCs used as regularizers
- Derivatives of any order can be calculated in an exact manner



Lu Lu, Xuhui Meng, Zhiping Mao, George E. Karniadakis, DeepXDE: A deep learning library for solving differential equations (2020). Retrieved from https://arxiv.org/abs/1907.04502

SimNet: Salient Features

SimNet training

- **Exact differentiation:** Can obtain any order derivatives accurately using automatic differentiation
- **Soft constraints** on governing equations and BCs

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

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

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

- Optimal set of NN parameters obtained by **minimizing the loss function**

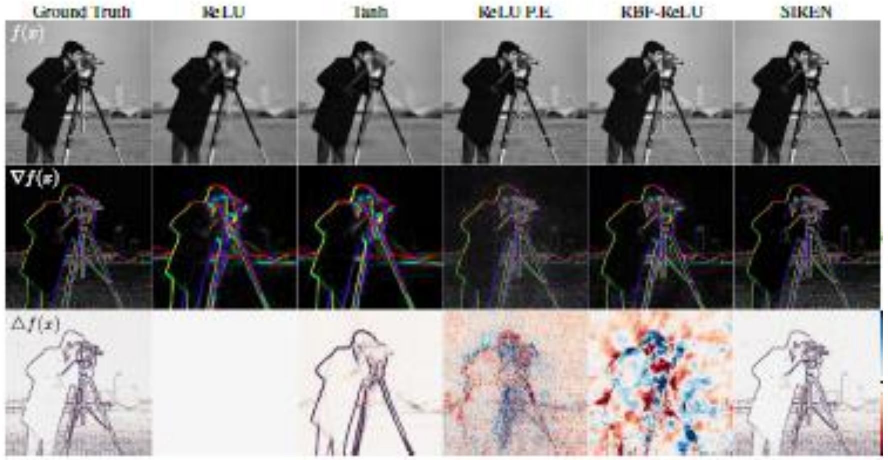
$$\boldsymbol{\theta}^* = [\boldsymbol{w}^*, \boldsymbol{b}^*] = arg \min_{\theta} Loss(\boldsymbol{\theta})$$

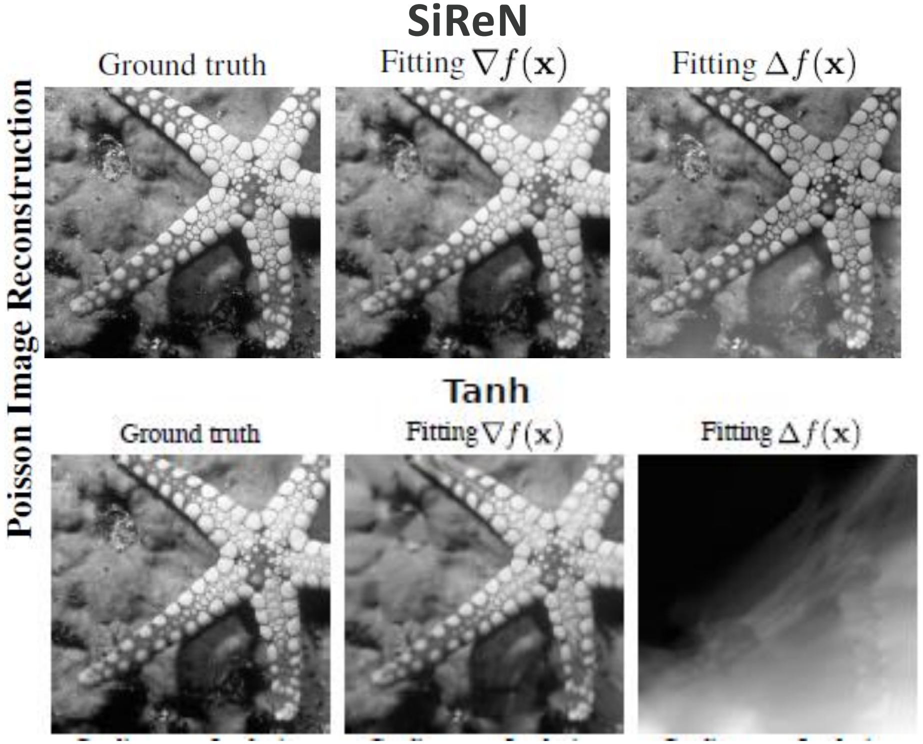
- When loss goes close to zero, the NN manages to memorize the governing equations given adequate training point density

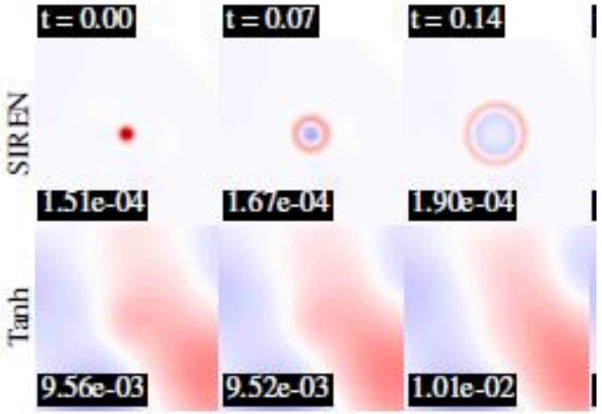
Specialized NNs for SimNet

Sinusoidal Representation Networks: SiReNs

- A specialized NN formulation originally developed for image reconstruction
- Uses sin activation functions with custom weights initialization for reconstructing finer features
- Can learn well implicit representations from derivatives







Sitzmann et al, “Implicit Neural Representations with Periodic Activation Functions” (2020)

Assessing PINN capability

PINN models for powerplant boiler

- Challenging test case for PINNs
- Create digital twin of an industrial scale boiler
- Turbulent multiphase reacting flow
- Boilers operate at different input conditions based on demand
- Generate PINN for predictions across different input conditions
- Need to optimize combustion processes to reduce CO, NO_x and CO_2 emissions

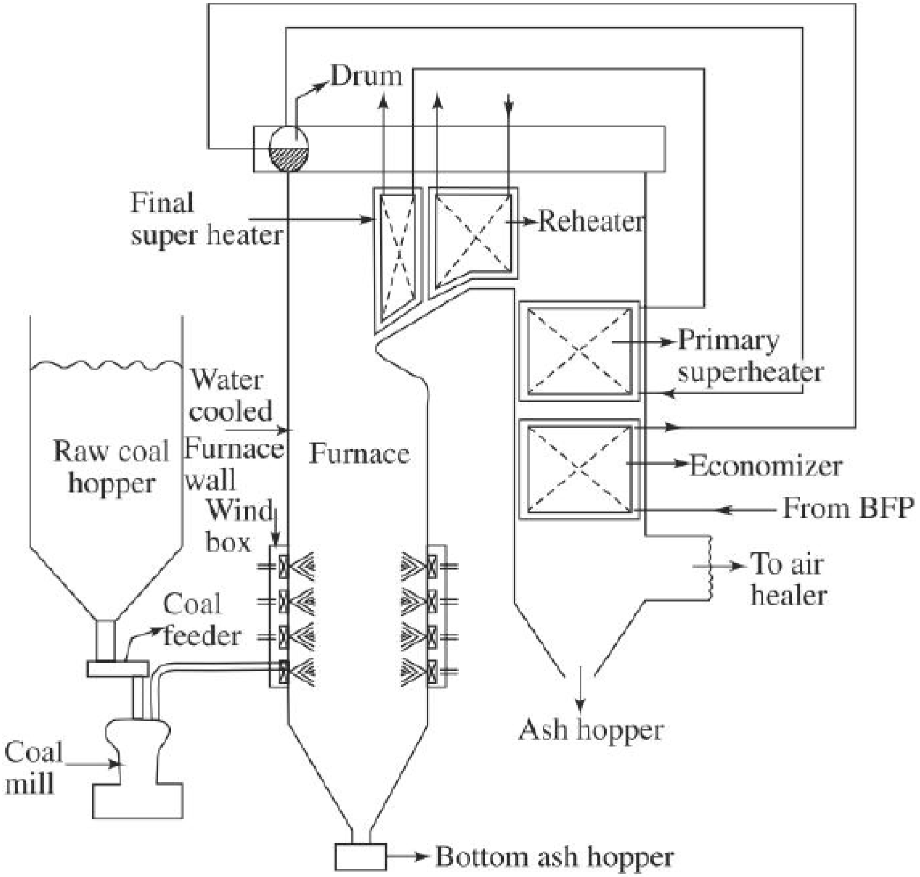
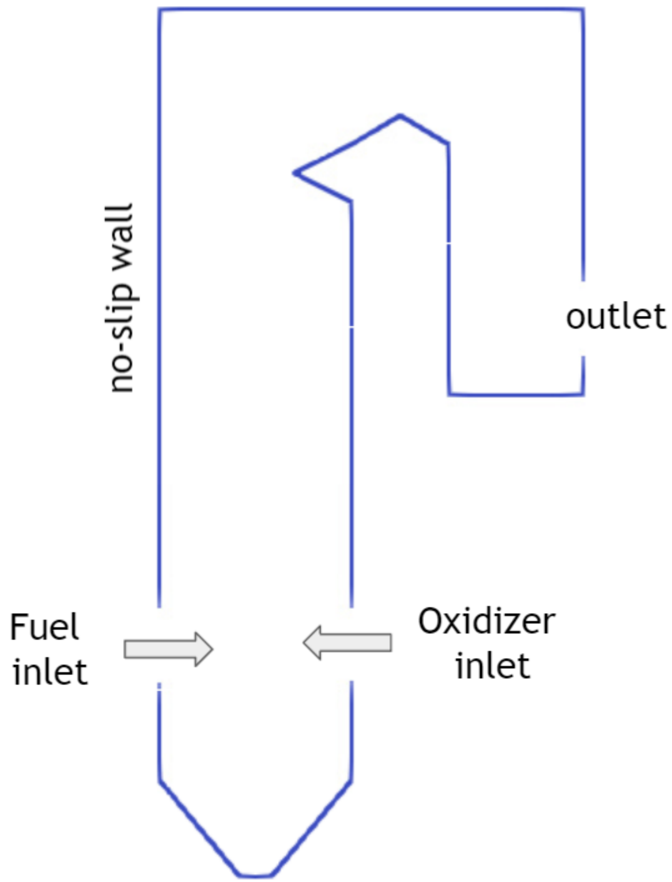


Figure from Nag PK, “Power Plant Engineering” (2002)

Formulation

Simplified boiler combustion

- Simplified methane oxidation
- One step forward irreversible stoichiometric reaction
- Reynolds number $O(10^4 - 10^5)$
- Zero-equation turbulence model
- Variable density species mass fraction + global momentum + temperature + continuity equations + equation of state



Formulation-No Reactions, Steady State

Governing equations

- Continuity: $$\frac{\partial(\rho u_i)}{\partial x_i} = 0$$

- Species mass fraction: $$\rho u_i \frac{\partial Y_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right) = 0$$

- Momentum: $$\frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

  where τ_{ij} includes the turbulent Reynolds stresses modeled using the Zero-equation model

- Temperature: $$\frac{\partial}{\partial x_i}(u_j T)) = \frac{\partial}{\partial x_i}\left(\alpha \frac{\partial T}{\partial x_i}\right)$$

Parametric Boundary Conditions

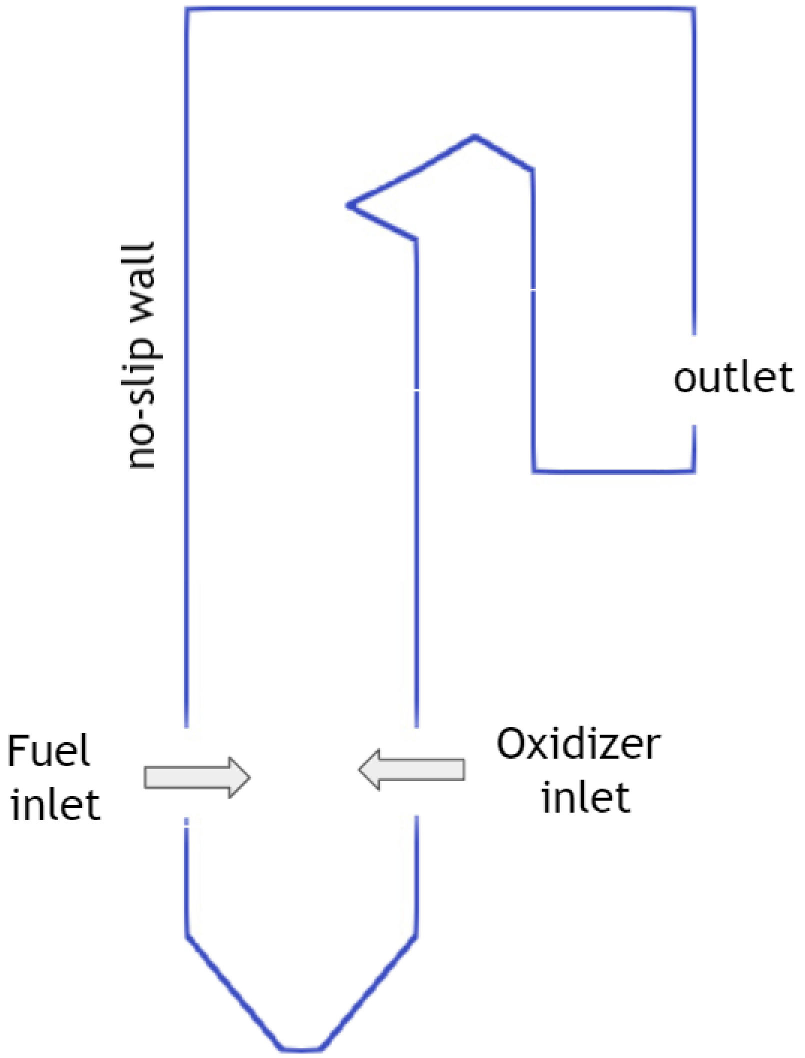
Species mass fractions, velocity and temperature

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

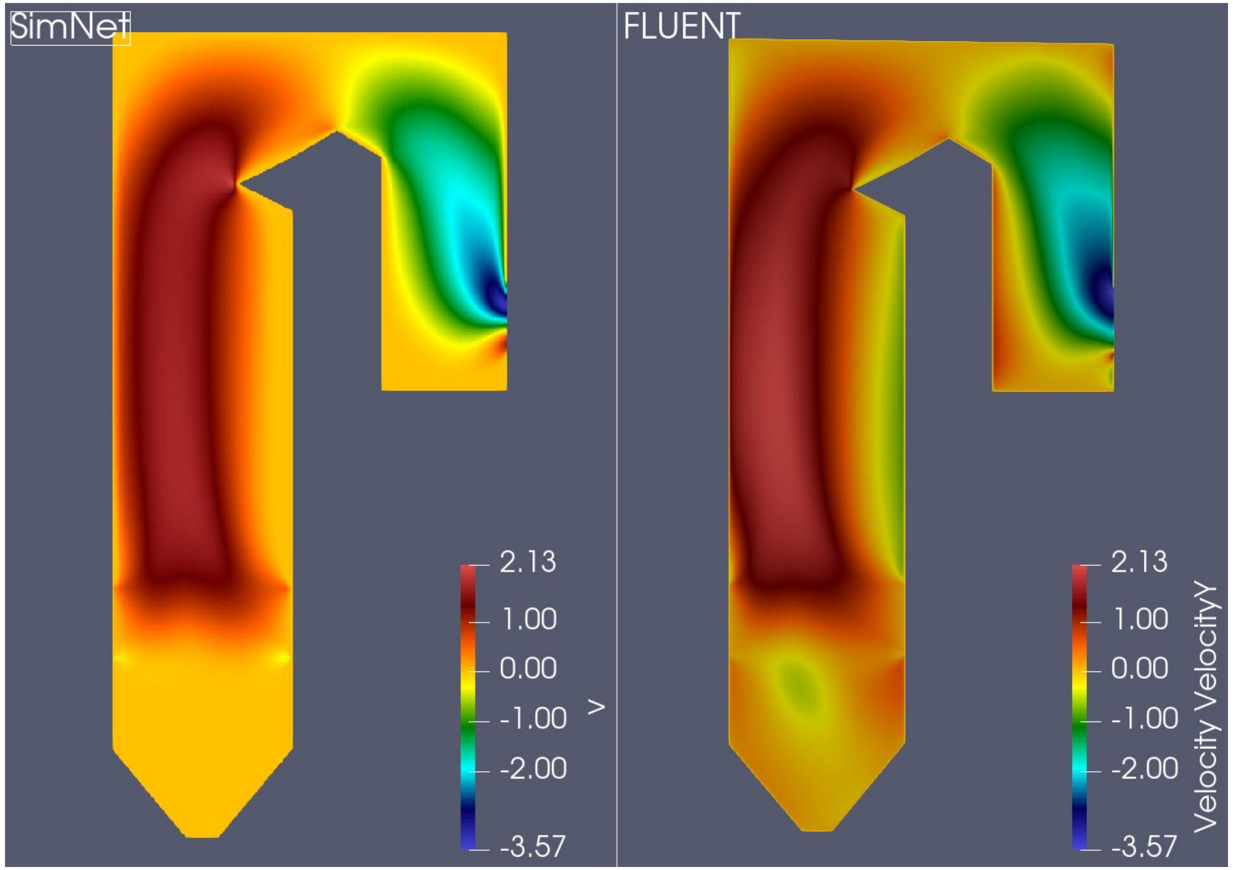
Wall Conditions

Temperature, K	350.0
Species	Zero flux
Velocity	No-slip

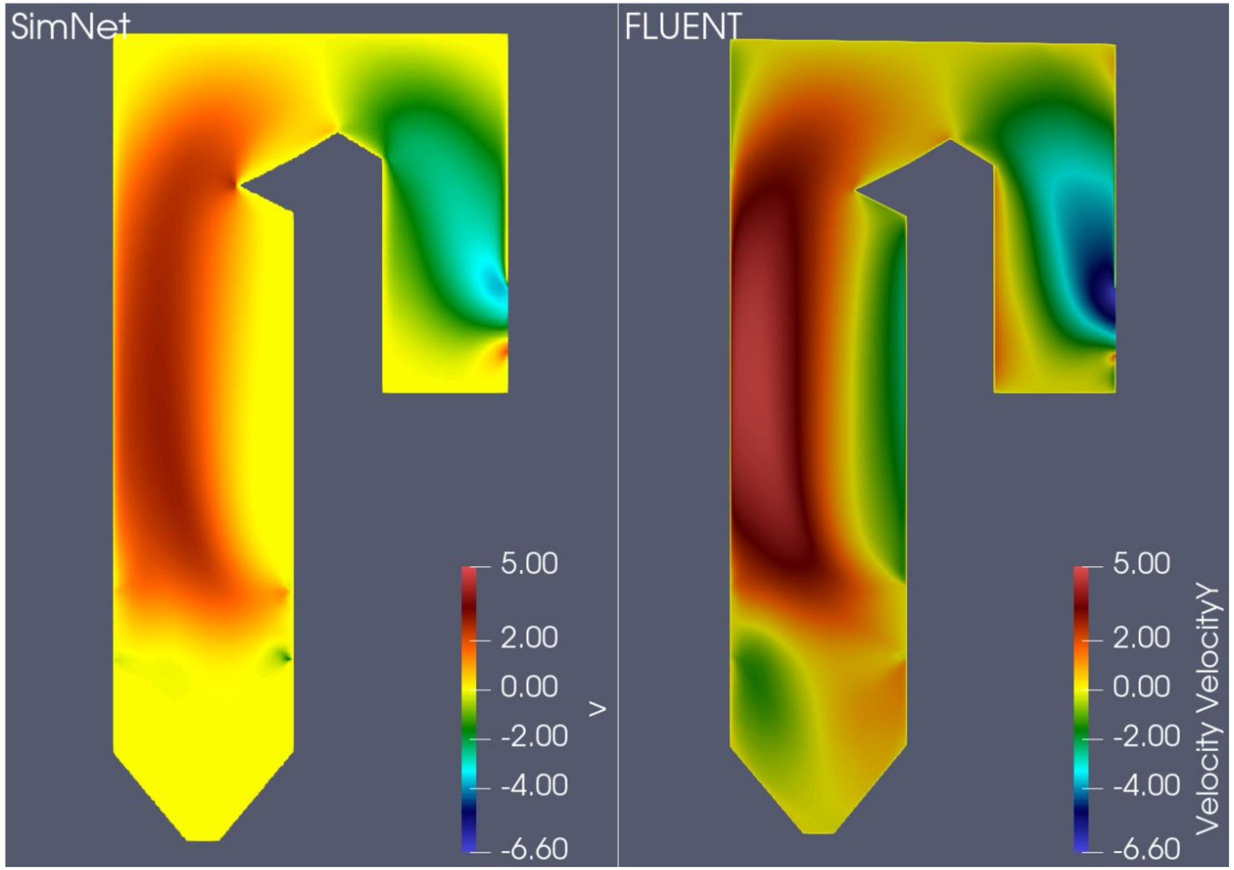


Results - No Reactions

Vertical Velocity Field



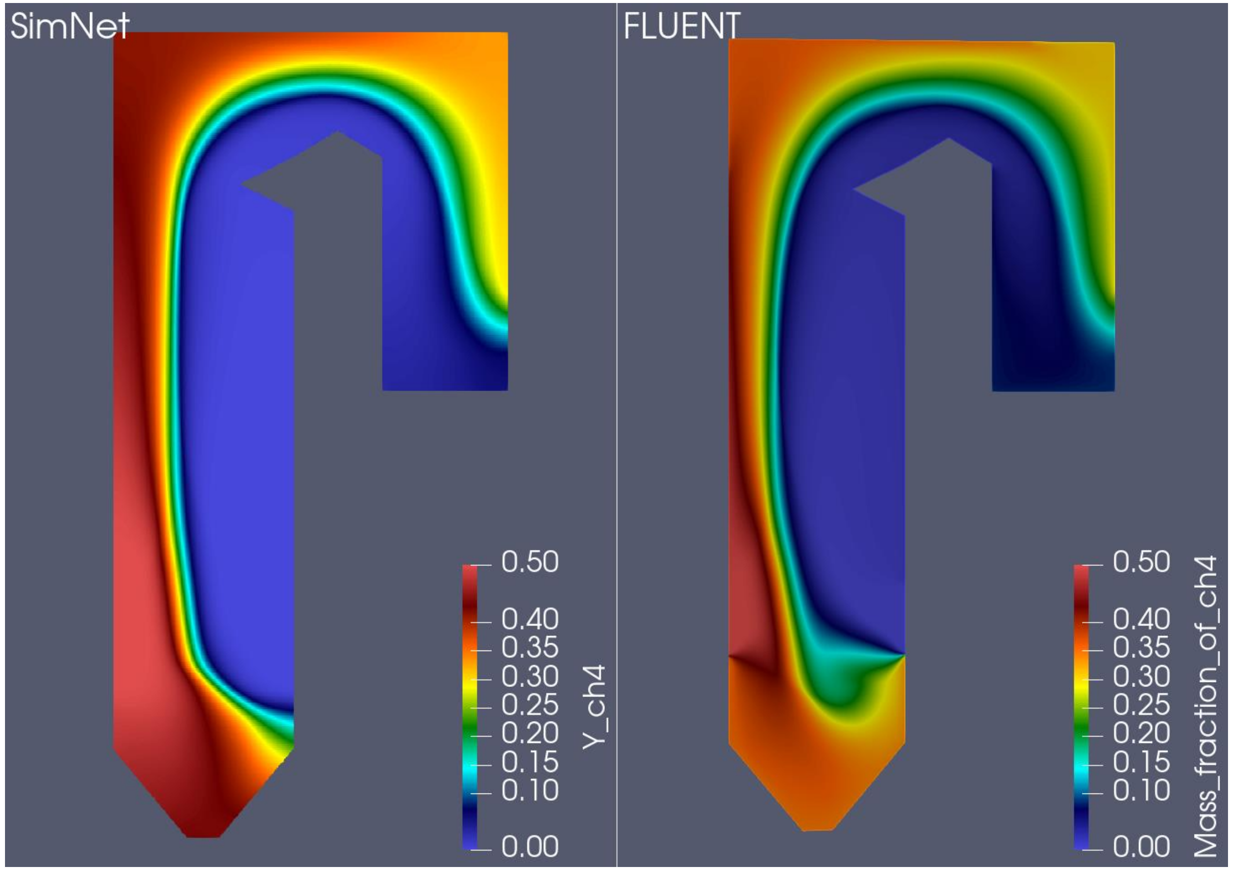
Oxidizer inlet velocity: 1.53 m/s



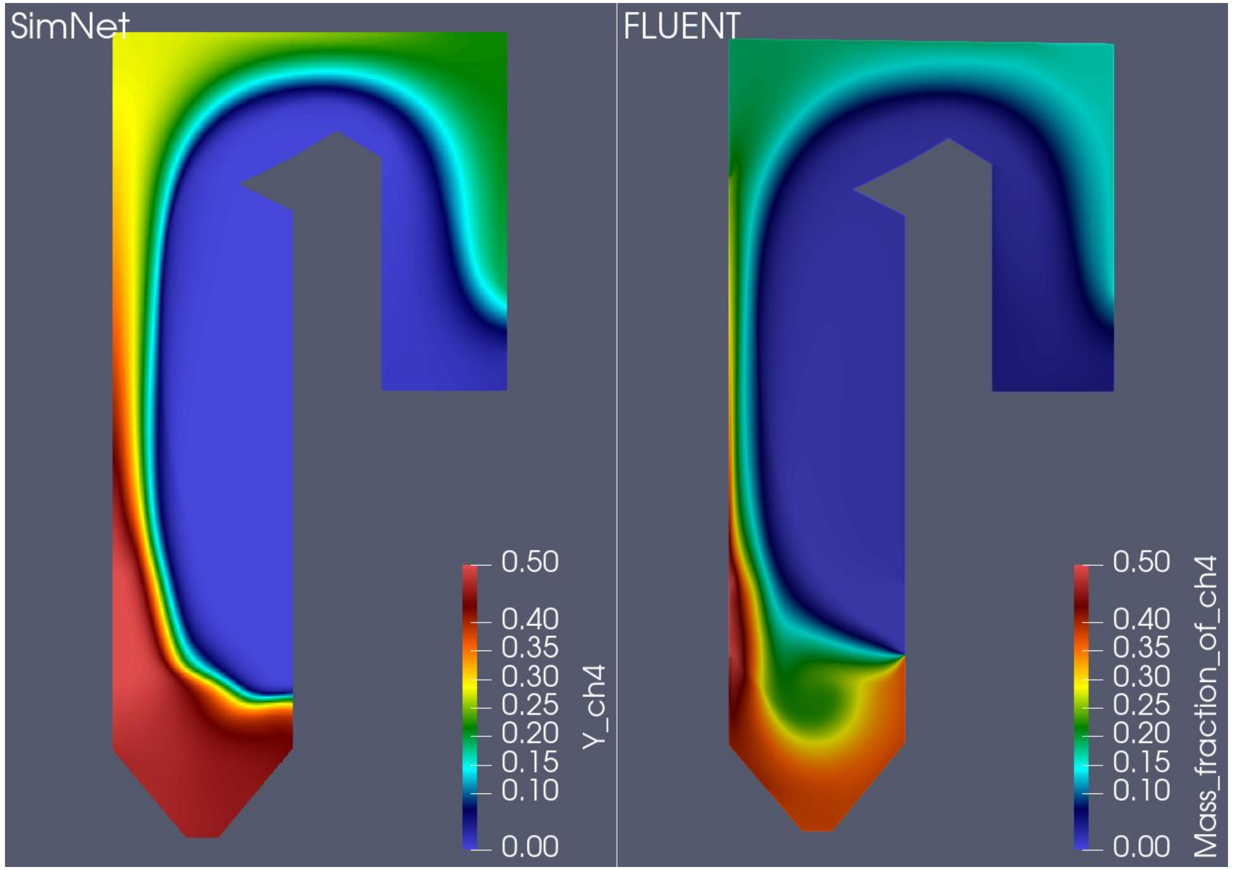
Oxidizer inlet velocity: 3.67 m/s

Results - No Reactions

Methane mass fraction



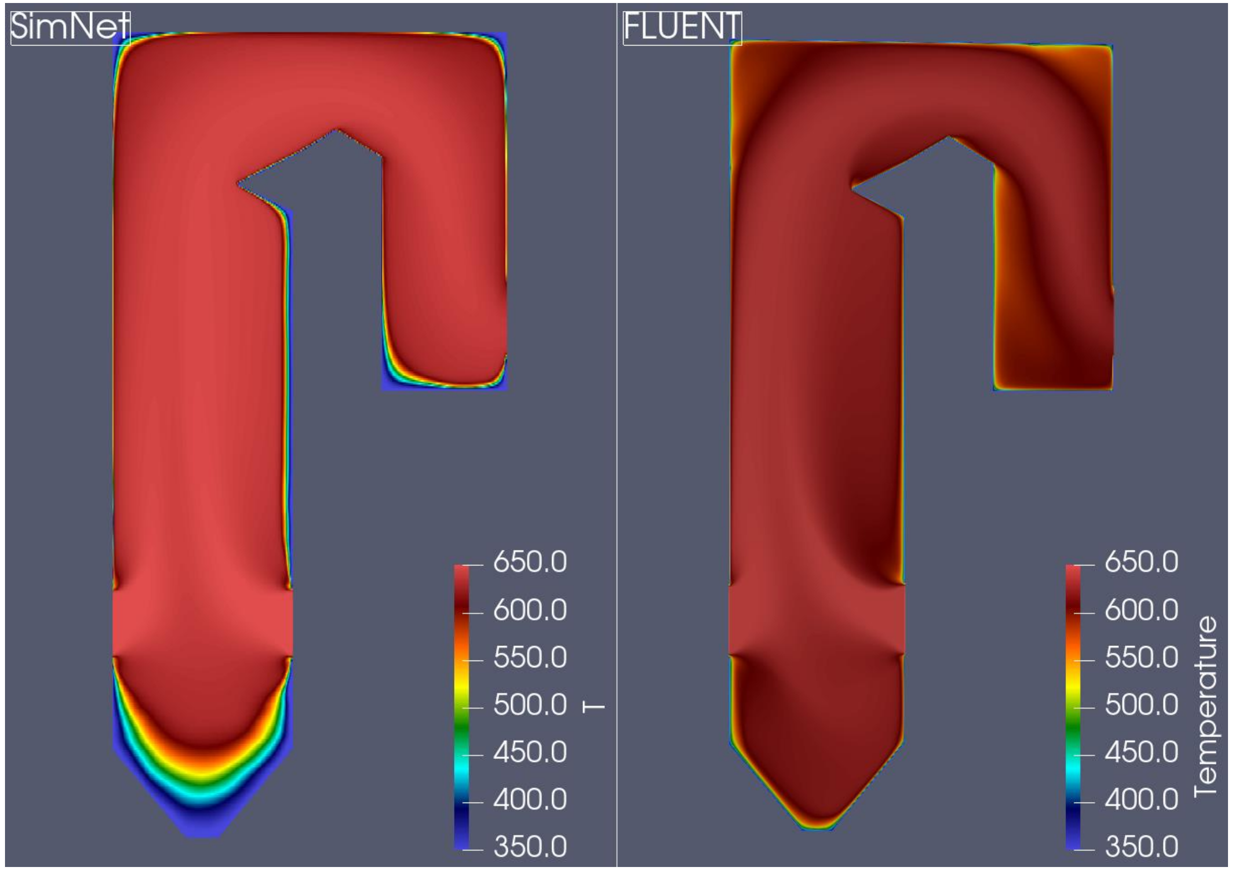
Oxidizer inlet velocity: 1.53 m/s



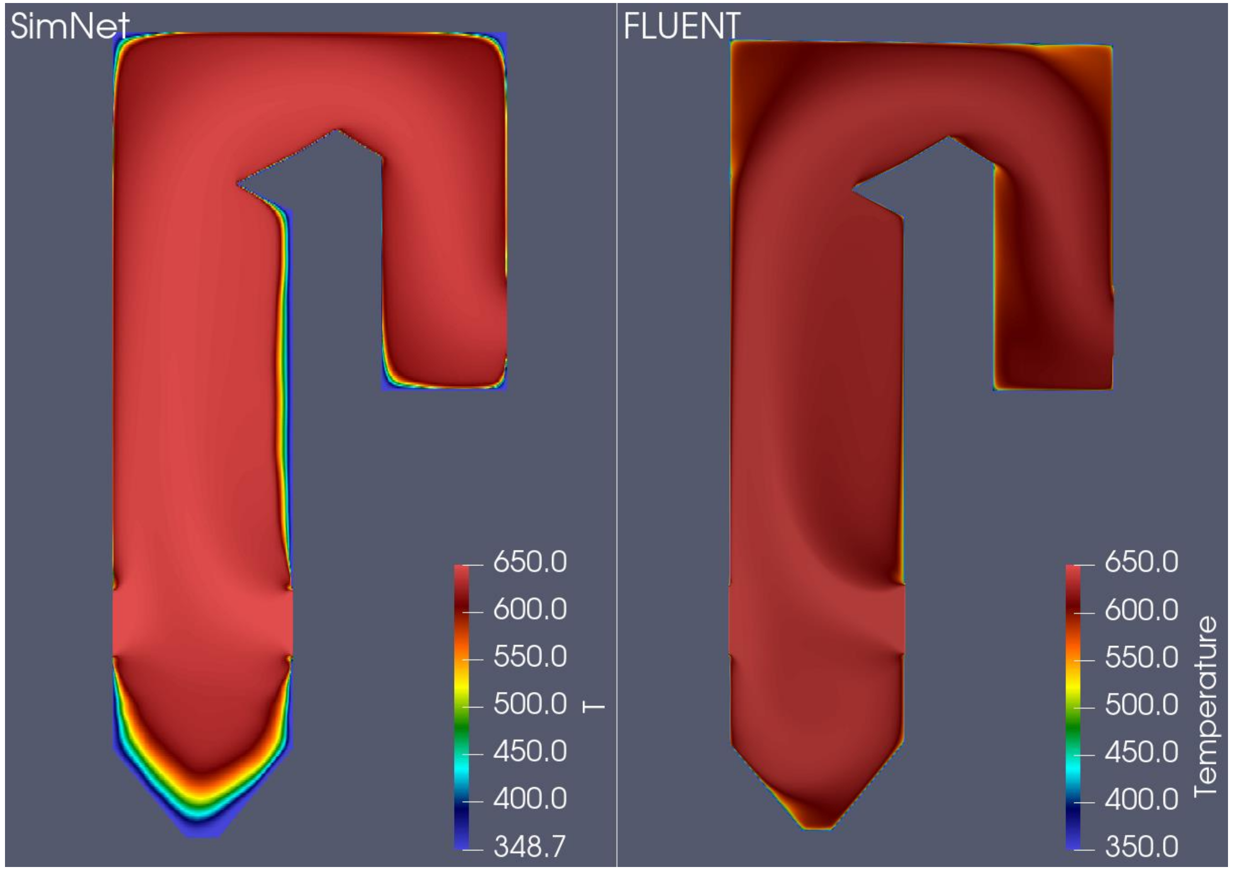
Oxidizer inlet velocity: 3.67 m/s

Results - No Reactions

Temperature field



Oxidizer inlet velocity: 1.53 m/s



Oxidizer inlet velocity: 3.67 m/s

Results – 3D steady state, no reactions

3D steady state compressible two species turbulent flow, parametric inlet

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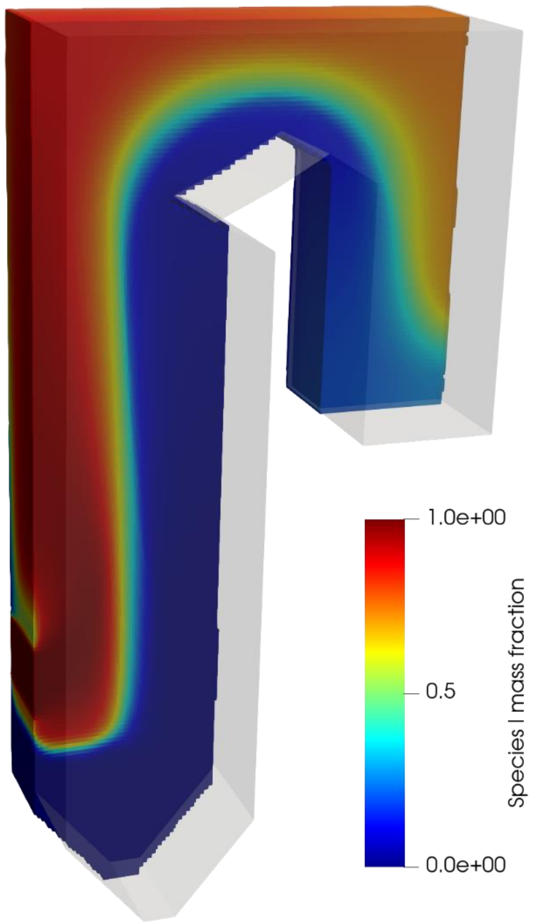
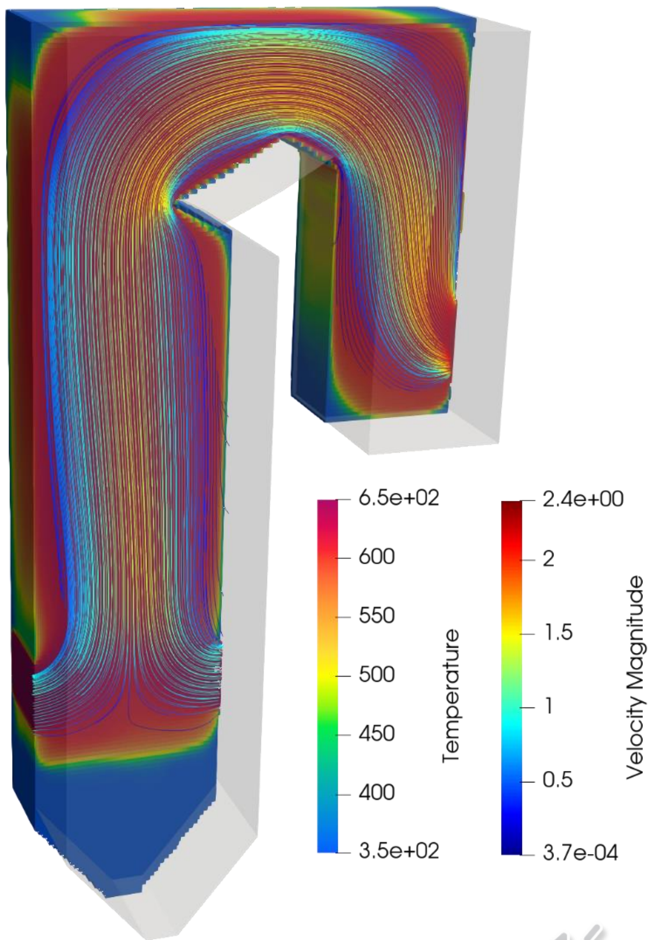
Challenges moving from 2D to 3D

- Training complexity increases in general
- Need higher representation capacity
- Increased number of loss terms
- Need larger batch size that can be limited by the GPU memory
- Increased training time to convergence

Species I mass fraction



Streamlines (m/s) & Temperature (K)



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Formulation – Towards Reacting Flow

Governing equations

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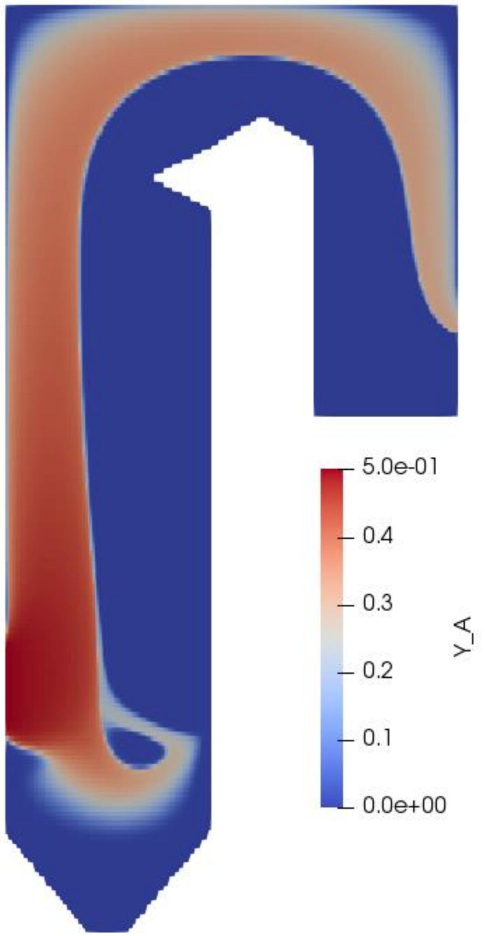
- Simplified reaction: $A \rightarrow B$
- Continuity: $$\frac{\partial(\rho u_i)}{\partial x_i} = 0$$
- Species mass fraction: $$\rho u_i \frac{\partial Y_k}{\partial x_i} - \cancel{\frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right)} = constant \times Y_k$$
- Momentum: $$\frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$
- Temperature: $$\frac{\partial}{\partial x_i}(u_j T^*) = \cancel{\frac{\partial}{\partial x_i}\left(\alpha \frac{\partial T^*}{\partial x_i}\right)}$$

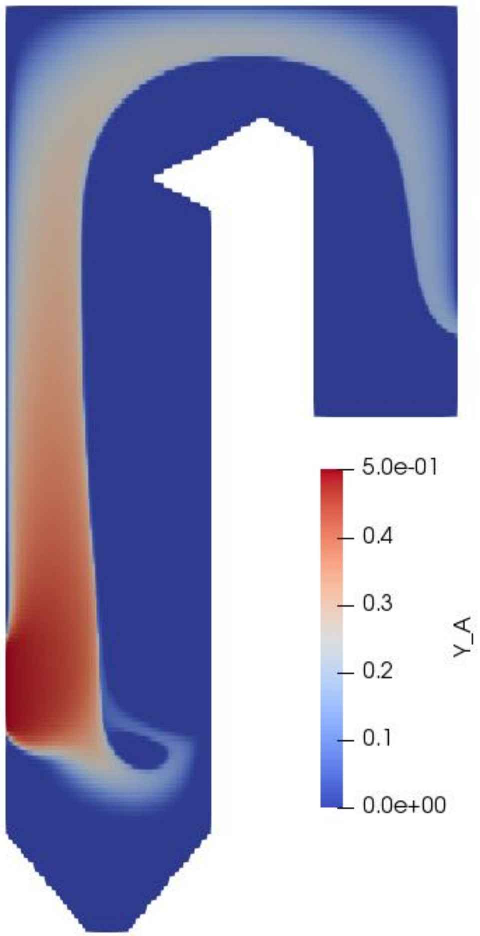
Results - Towards reacting flow

Species mass fraction

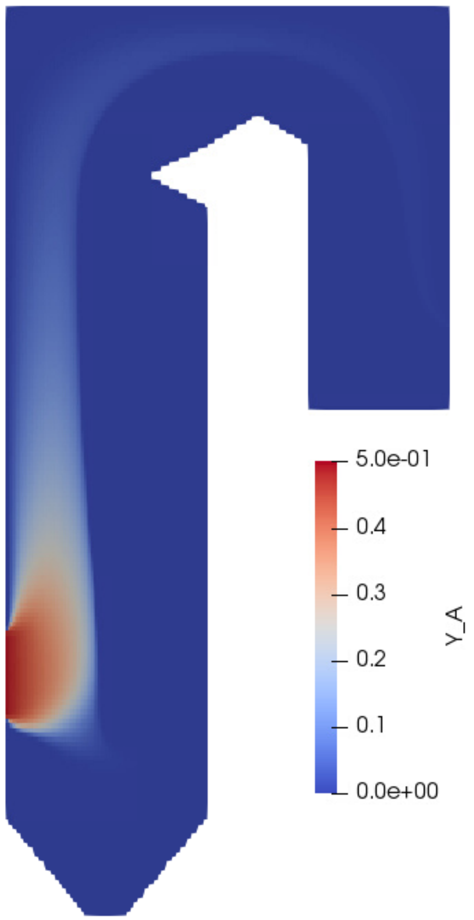
Inlet Y_A = 0.5



$$\frac{dY_A}{dt} = -0.1Y_A$$



$$\frac{dY_A}{dt} = -0.23Y_A$$



$$\frac{dY_A}{dt} = -1.0Y_A$$

Formulation-No Reactions, Transient

Governing equations

- Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0$$

- Species mass fraction:

$$\rho \frac{\partial Y_k}{\partial t} + \rho u_i \frac{\partial Y_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right) = 0$$

- 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:

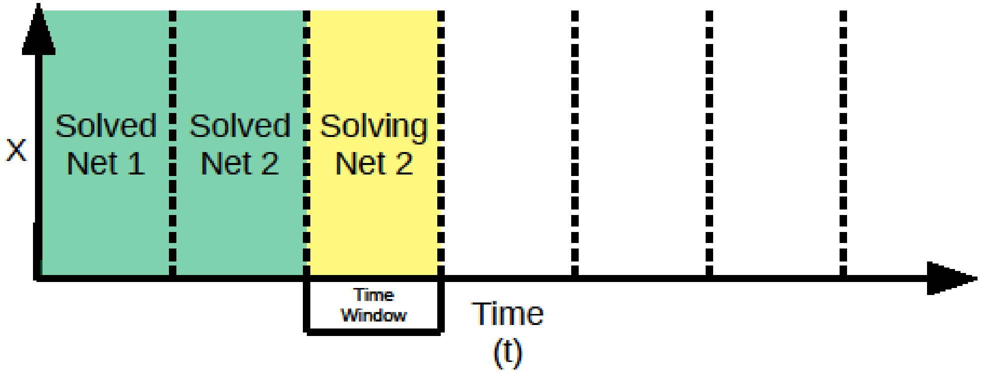
$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x_i}\left(u_j T\right) = \frac{\partial}{\partial x_i}\left(\alpha \frac{\partial T}{\partial x_i}\right)$$

Results-No Reactions, Transient

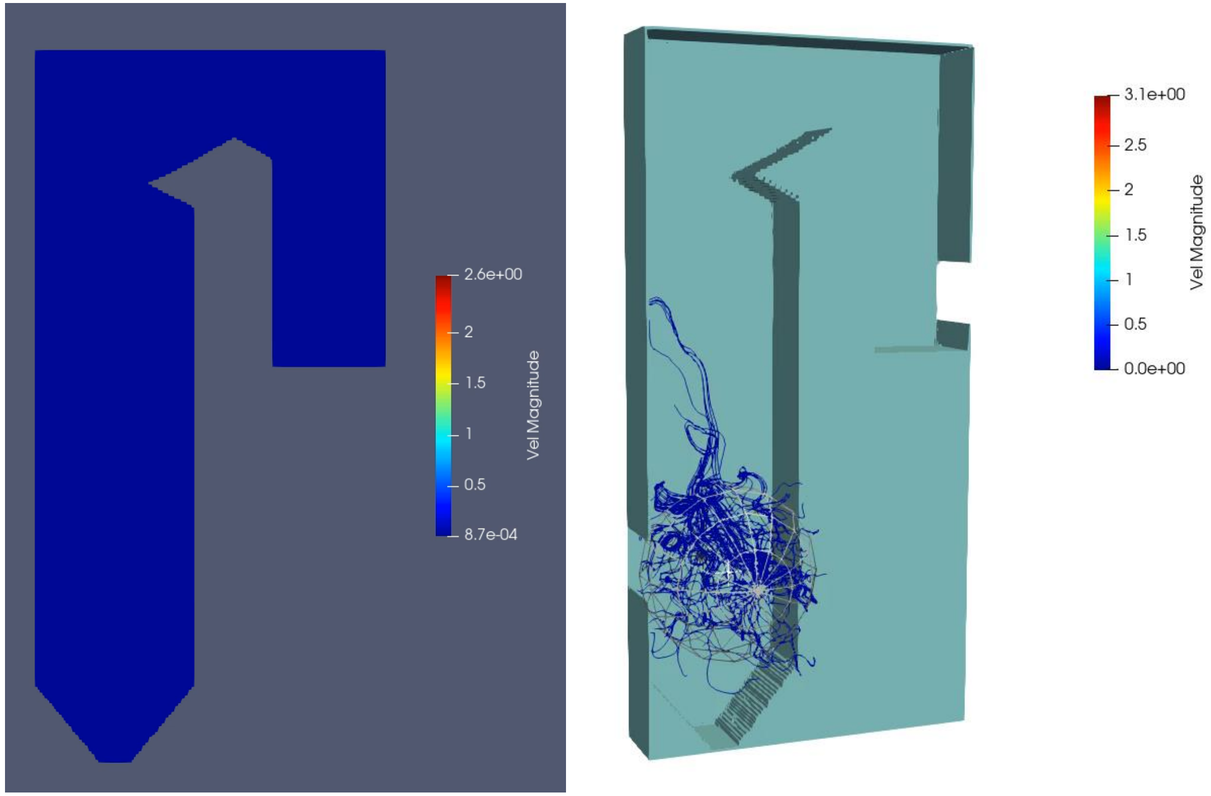
2D & 3D transient compressible laminar single species flow

Moving time window approach

- In standard PINNs, the model is trained at once for the entire space-time (the continuous time method)
- This can be difficult to learn, and the accuracy decreases as the simulation time frame increases
- We use a novel moving time window approach that iteratively solves for small time windows
- The time windows use the previous window as new initial conditions
- The continuous time method is used for solving inside a particular window



Velocity Magnitude, m/s



Lessons learned from initial study

PINNs vs CFD

- We are solving the same equations as in CFD
- The solution procedures in CFD and in PINN training are vastly different
  - CFD is done with iterative linear solvers, with a single equation in each linear solve, with defined tolerances for each equation
  - PINNs attempt to solve all equations in a single minimization procedure using a single weighted loss equation.
- The single weighted loss minimization equation in PINN training can cause difficulties that are not present in CFD
  - A NN will always focus on reducing the largest loss terms in the weighted equation
  - Thus, all loss terms must have the same order of magnitude
  - Increasing focus on one aspect of the simulation may come at a detriment to other parts of the equation set
  - There does not seem to be an objective method to determine the weight factors in the loss equation
  - There does not seem to be a way to ensure that a particular equation will be able to be solved to a predefined tolerance before training begins.

Future work

Near-term plans

- Improve the accuracy of the momentum and continuity equations
  - Normalize all variables
  - Objectively determine the appropriate loss weightings
- Develop a fully reacting flow capability
  - Validate the species decay for the simplified reaction model against exact analytical solutions
  - Couple the reaction equations to the temperature
  - Explore the capability of SimNet to handle stiff chemistry where the source terms can be orders of magnitude larger than the other terms in the advection diffusion equations
    - Could possibly require us to use the time variant solver
- Find the most optimal way to serve trained models for inference

Future work

Long term development

- Validate the implementation of the k-ϵ turbulence model
- Explore multiphase capabilities
  - Eulerian Eulerian formulation (high probability of success)
  - Einstein Vlasov Eulerian Lagrangian formulation (lower probability of success)
- Assist NVIDIA to develop & test a version of the transient solver using RNNs
- Extend SimNet for use in other areas of interest in CCS by adding capabilities to handle other important phenomena like adsorption, absorption & flow through porous media

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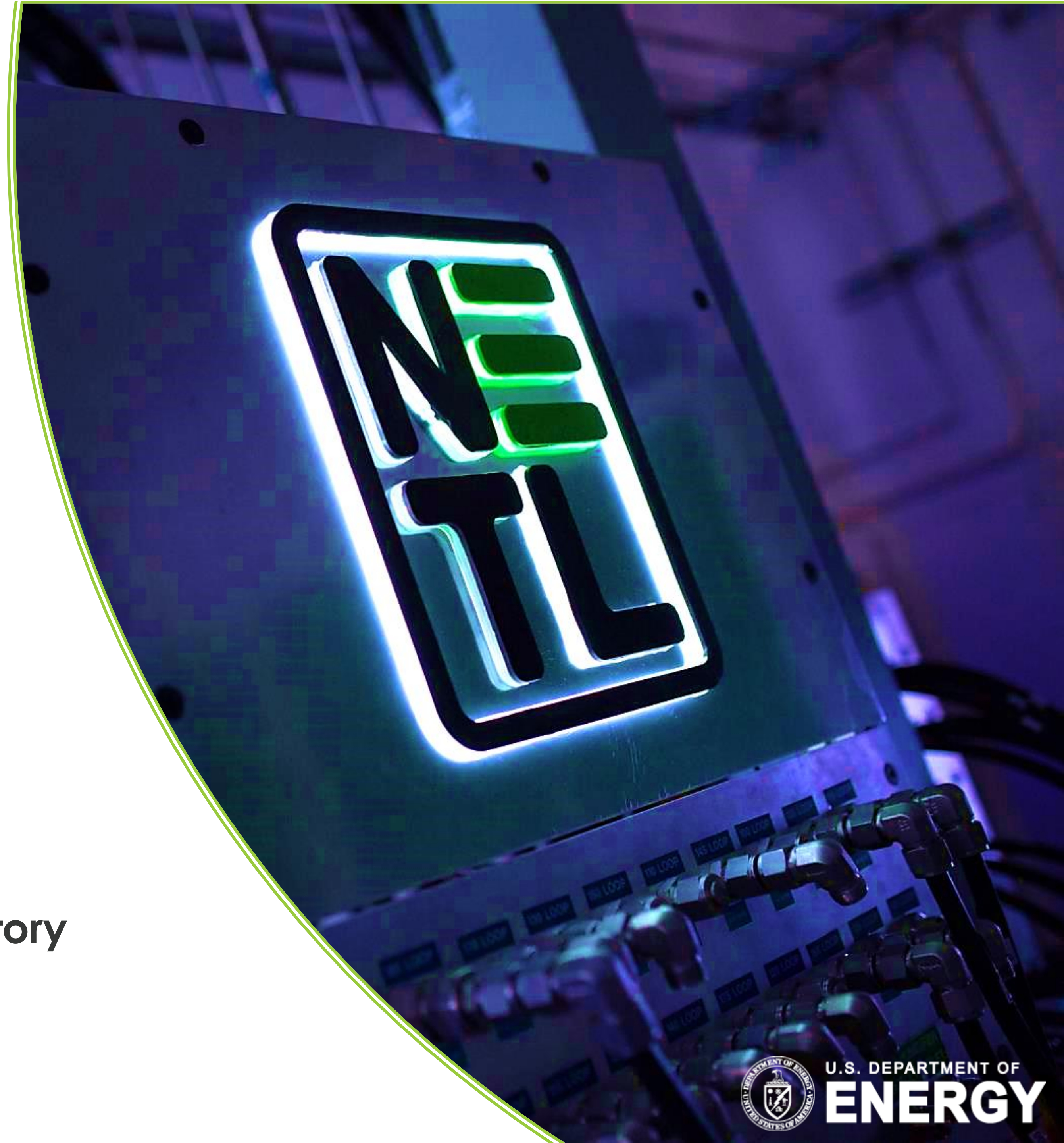

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Question?