2024 UTSR & Advanced Turbines Program Review Meeting
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Phy-ChemNODE: Physics-enhanced Neural ODE Enabled Fast and Robust Chemistry Solver for Reacting Flow Simulations

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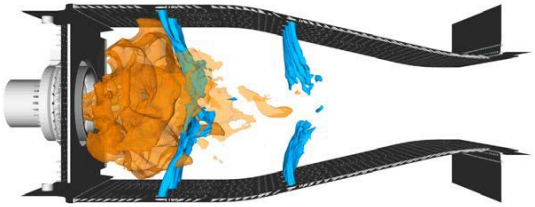
Argonne LCRC

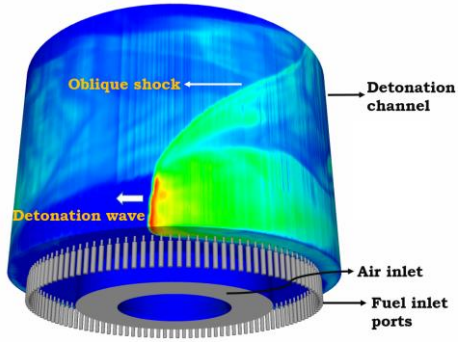
Argonne NATIONAL LABORATORY

MOTIVATION

- Advanced gas turbine and pressure gain combustion systems operating on zero-carbon fuels can play a critical role in the decarbonization of power generation sector
- Computational fluid dynamics (CFD) simulation-driven virtual design analysis can aid the development of these advanced combustion systems, while saving costs associated with experimental prototyping
- CFD simulations of full-scale combustor configurations with detailed fuel kinetics are compute-intensive due to large number of grid points and transport equations with stiff chemical source terms for multiple reactive species evolving over disparate spatio-temporal scales
- Solving for detailed chemistry presents a major bottleneck in the application of combustion CFD for comprehensive parametric analysis and results in prolonged design cycles



Gas turbines



Rotating detonation engines

TCF PHASE 1 PROJECT GOALS

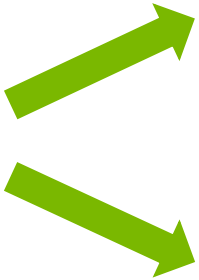
- Advance and demonstrate **ChemNODE**, a novel deep learning (DL) framework developed at Argonne to accelerate detailed chemistry computations, for reacting flow CFD simulations
  - Mature ChemNODE software technology by incorporating algorithmic enhancements to make the DL framework more efficient and robust
  - Perform proof-of-concept demonstration studies by coupling ChemNODE with a CFD solver (CSI's CONVERGE CFD code) for simulations of practical combustion engines

- The ultimate goal is to transition ChemNODE software technology from TRL 2 (technology concept and/or application formulated) to TRL 4 (technology validation in lab environment)
- The project seeks to deliver a self-contained ChemNODE software package that can be readily integrated into CFD solvers for accelerated simulation-driven analysis and design of combustion energy systems; this will facilitate technology transfer to industry

ACCELERATING CHEMICAL KINETICS

$$\rho \frac{DY_k}{Dt} = -\nabla \cdot \mathbf{j}_k + \dot{\omega}_k$$

Reacting flow CFD typically uses operator splitting schemes



Mechanism Reduction

- Classical graph-based reduction methods (DRG, DRGASA, DRGEP, etc.)
- Principal Component Analysis (PCA)
- Reduced-order flamelet models

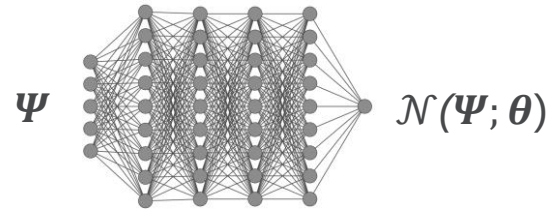
Accelerate Detailed Kinetics

- Sparse stiff ODE solvers
- ML-based computation
  - Readily amenable to GPUs
  - $Y(t+\Delta t) = NN(Y(t), \theta)$ → Δt dependent
  - $\boldsymbol{\dot{\omega}} = NN(\boldsymbol{Y}(t), \boldsymbol{\theta})$ → can handle variable Δt

ChemNODE: BASIC APPROACH

A chemically reacting system (with no diffusion or convective transport) is given by:

$$\frac{d\boldsymbol{\Psi}}{dt} = \dot{\boldsymbol{\omega}}_{\Psi}(\boldsymbol{\Psi}), \qquad \boldsymbol{\Psi} = [T, H_2, O_2, \ldots]^T$$



We can replace the computation of $\dot{\boldsymbol{\omega}}_{\Psi}$ using a neural network, $\mathcal{N}(\boldsymbol{\Psi};\boldsymbol{\theta})$, which learns to predict the source terms as functions of the thermochemical state of the system → **Amenable to variable time-stepping**

Conventional Data-driven Learning Approach

Train a neural network to minimize the difference between the predicted and actual source terms:

$$\mathcal{L} = \left\| \dot{\boldsymbol{\omega}}_{\Psi} - \mathcal{N}(\boldsymbol{\Psi};\boldsymbol{\theta}) \right\|_2^2$$ → **Prone to unstable solution during deployment**

ChemNODE Approach

Train a neural network to obtain a source term that leads to small difference between actual and predicted ODE solutions:

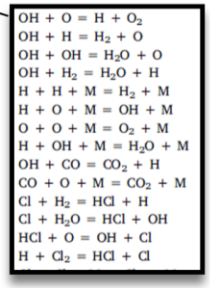
$$\mathcal{L} = \left\| \boldsymbol{\Psi} - \widehat{\boldsymbol{\Psi}} \right\|_2^2$$ → **Combines data-driven learning and numerical validation phases in a robust integrated framework ("a-posteriori" learning)**

Owoyele & Pal, *Energy and AI*, 2021

NEURAL ODEs

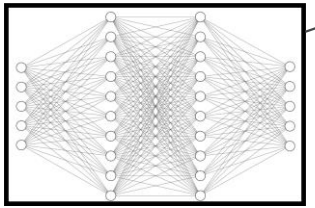
Original system

$$\boldsymbol{\Psi}(t_f) = \boldsymbol{\Psi}(t_0) + \int_{t_0}^{t_f} \mathbf{F}(\boldsymbol{\Psi})\Delta t_{\text{chem}}$$



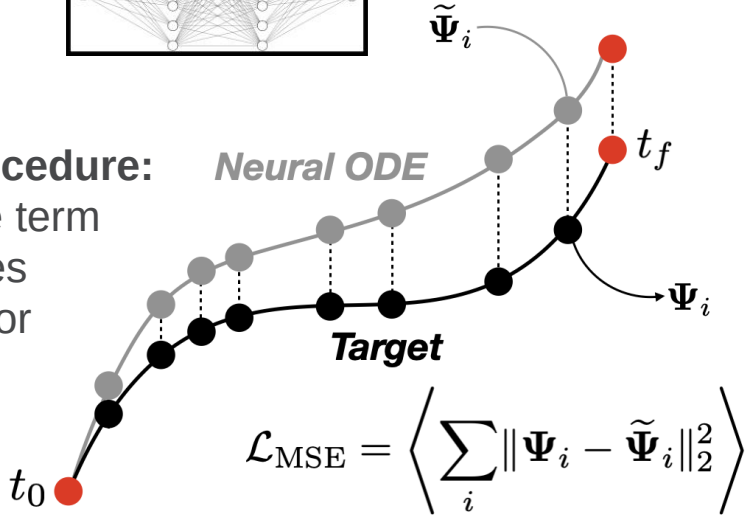
Neural ODE

$$\boldsymbol{\Psi}(t_f) = \boldsymbol{\Psi}(t_0) + \int_{t_0}^{t_f} \mathcal{A}(\boldsymbol{\Psi})\Delta t_{\text{nn}}$$



- **Advantages:**
  - ✓ Trajectory-based training
  - ✓ Adaptive time step integration
  - ✓ Jacobian-free during inference
  - ✓ Can provide stiffness reduction
  - ✓ Non-intrusive ML

Training procedure:
Learn source term that minimizes trajectory error



Owoyele & Pal, *Energy and AI*, 2021

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CASE STUDY: H_2-AIR AUTOIGNITION

- Ground truth data was generated from 0D homogenous constant pressure hydrogen-air reactor simulations at 1 atm using Cantera
- Baseline detailed kinetic mechanism with 9 species and 19 reactions [O'Conaire *et al*. 2004]
- Initial temperature (T_i) range of 1000-1200K and equivalence ratio (Φ) range of 0.5-1.5 considered; 50 points were sampled from each time series; 30 time series in total
- Single NN with two hidden layers (48 neurons each); 9 inputs/outputs; *tanh* activation function for each hidden layer; NN outputs were scaled by the maximum source term values from the dataset
- An implicit–explicit solver available in Julia used for ODE integration during training
- 2nd order Levenberg-Marquardt (L-M) optimizer used to minimize loss function:

$$L_{data} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\mathbf{y} - \hat{\mathbf{y}}}{\boldsymbol{y_{max}} - \boldsymbol{y_{min}}}\right)^2 \quad \mathbf{y} = \left[\log(T), \log(Y_{H_2}), .., \log(Y_{H_2O_2})\right]^T$$

PHYSICS-ENHANCED LOSS FUNCTION

- Adding error in elemental mass fractions to the loss function improves training efficiency

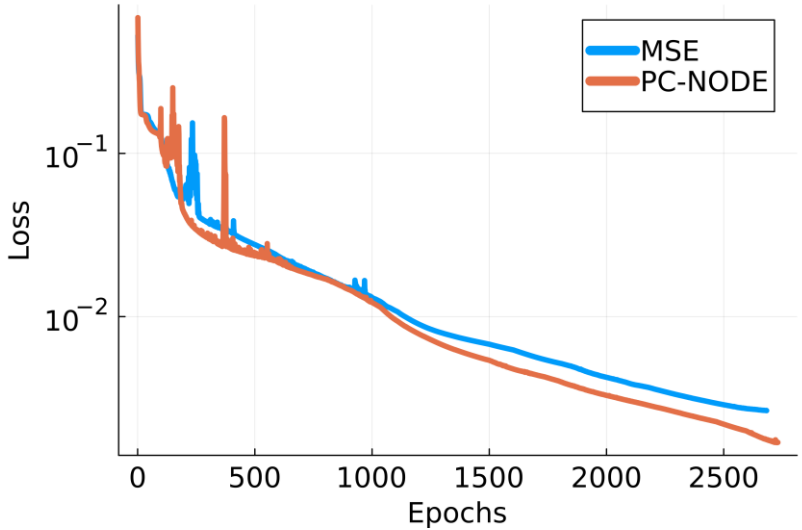
$$L_{Phy-ChemNODE} = L_{data} + \lambda_1 L_{ele-H} + \lambda_2 L_{ele-O}$$

$$L_{data} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\boldsymbol{\Psi_i} - \widehat{\boldsymbol{\Psi_i}}}{\boldsymbol{\Psi_{max}} - \boldsymbol{\Psi_{min}}}\right)^2$$

$$L_{ele-H} = \sum_{i=1}^{N}\left(\log\left(1 + \left|\sum_{k}^{N_s}\frac{N_H^k MW_H}{MW_k}\left(Y_{k,i} - \widehat{Y_{k,i}}\right)\right|\right)\right)^2$$

$$L_{ele-O} = \sum_{i=1}^{N}\left(\log\left(1 + \left|\sum_{k}^{N_s}\frac{N_O^k MW_O}{MW_k}\left(Y_{k,i} - \widehat{Y_{k,i}}\right)\right|\right)\right)^2$$

$$\lambda_1 = 3, \quad \lambda_2 = 3$$

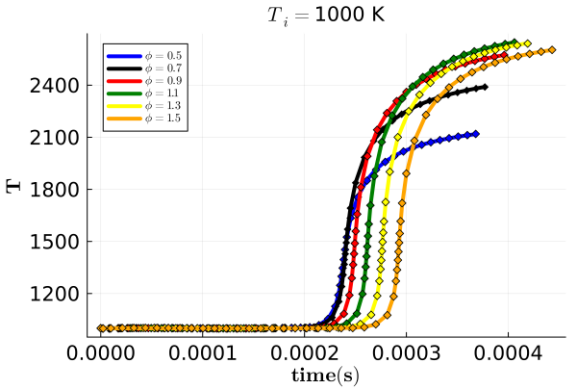


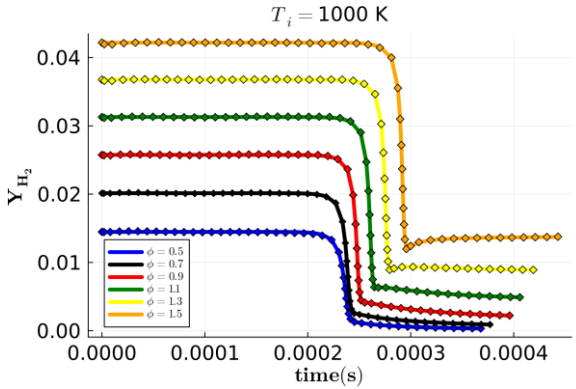
Kumar et al., *NeurIPS ML for Physical Sciences*, 2023

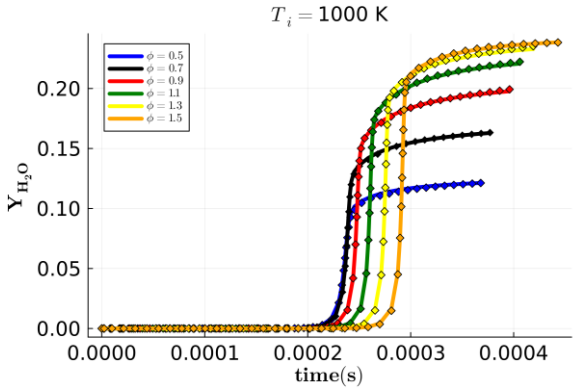
Phy-ChemNODE: H_2-AIR AUTOIGNITION

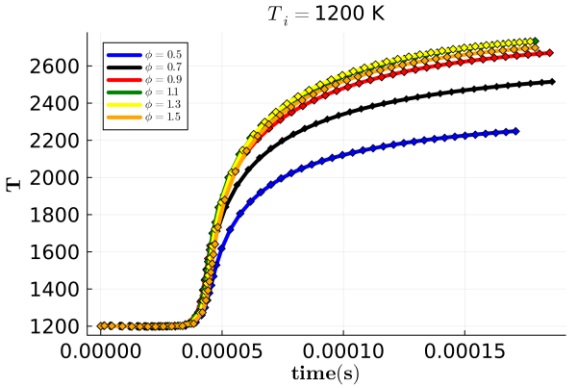
A-posteriori studies: In-sample Initial Conditions

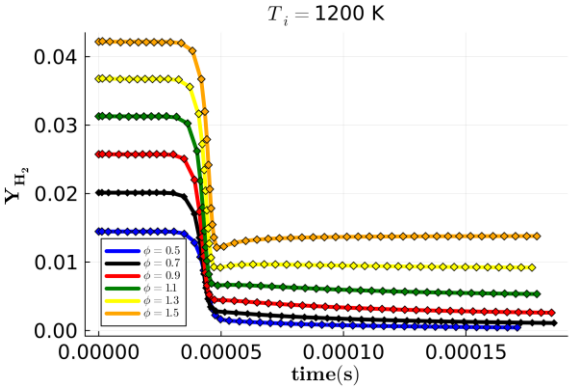
Markers: Cantera-PhyChemNODE
Solid lines: Ground truth (Cantera)

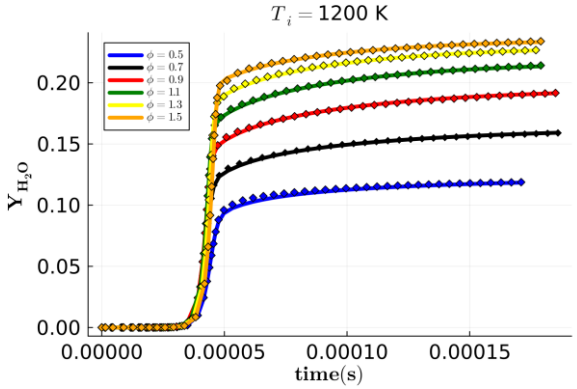










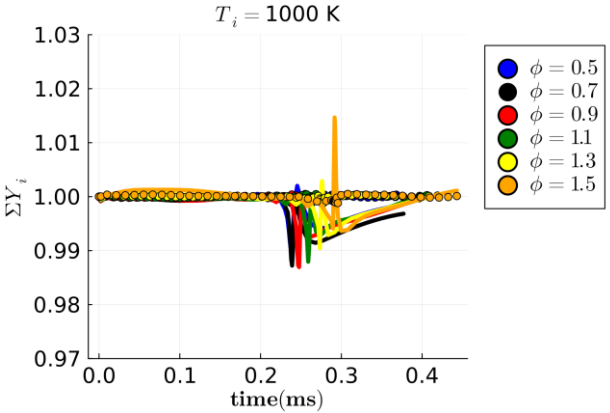


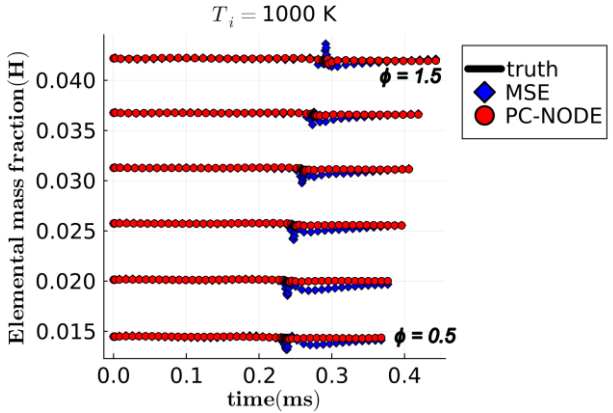
Inference speedup : ~3X over H_2/air detailed chemical mechanism

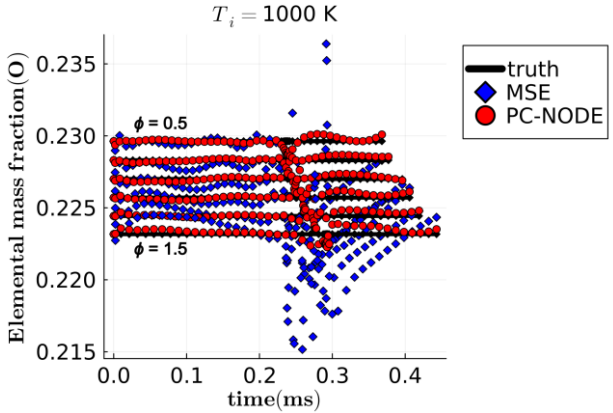
Kumar et al., *NeurIPS ML for Physical Sciences*, 2023

Phy-ChemNODE: H_2-AIR AUTOIGNITION

A-posteriori studies: In-sample Initial Conditions







- Better total and elemental mass conservation for Phy-ChemNODE

Kumar et al., *NeurIPS ML for Physical Sciences*, 2023

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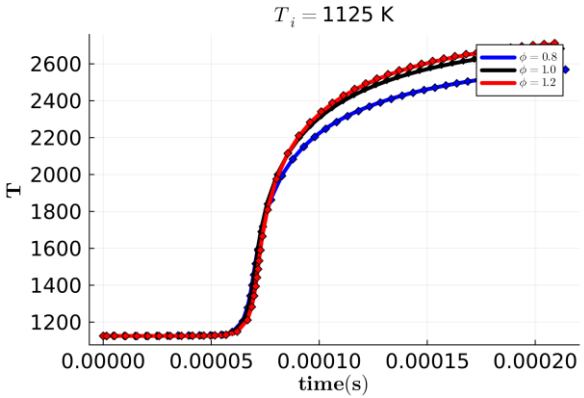
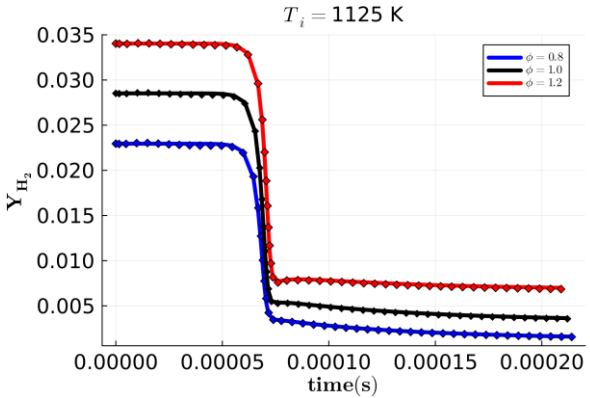
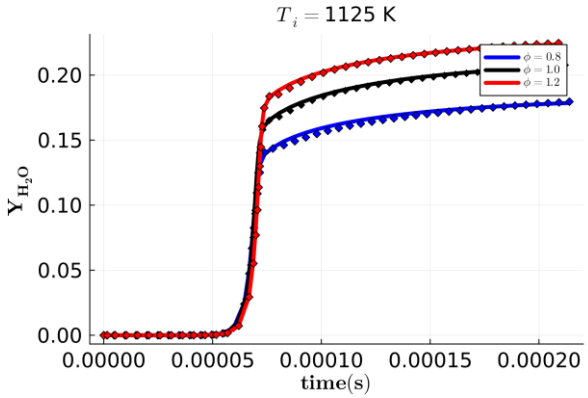
Phy-ChemNODE: H_2-AIR AUTOIGNITION

A-posteriori studies: Out-of-sample Initial Conditions

Markers: Cantera-PhyChemNODE
Solid lines: Ground truth (Cantera)

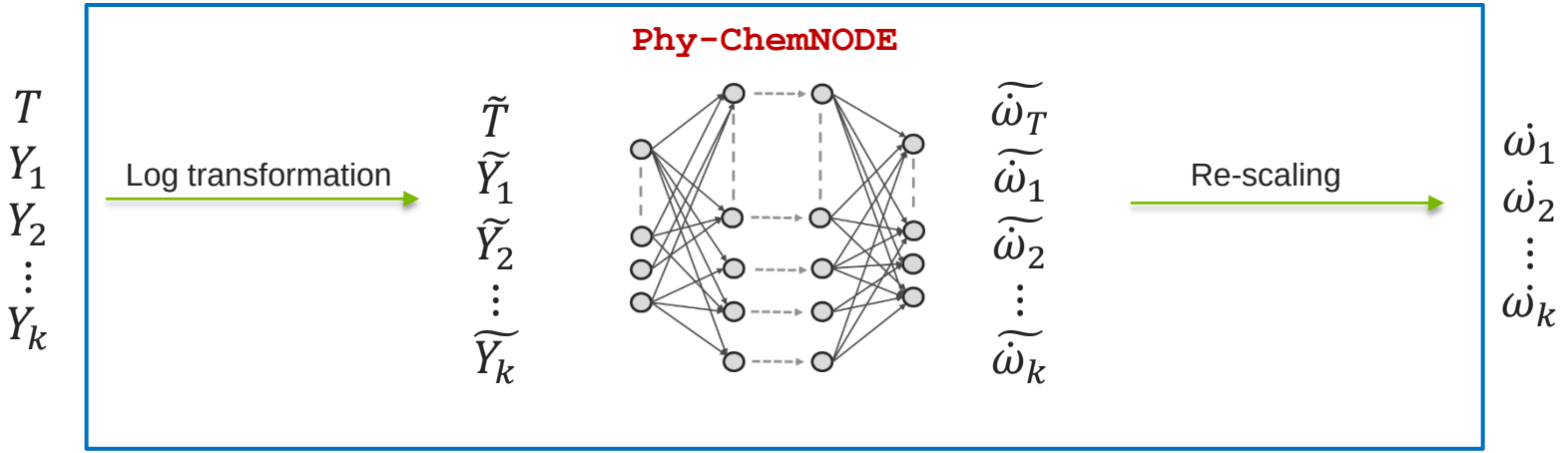






- $T_i = 1125$K and $\phi = [0.8,1.0,1.2]$ are within the bounds of training initial conditions, but were not used for training the network

CFD SOLVER INTEGRATION



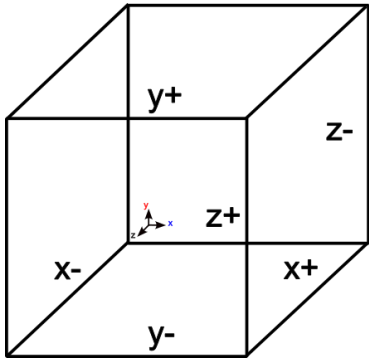
`sage_molefrac`

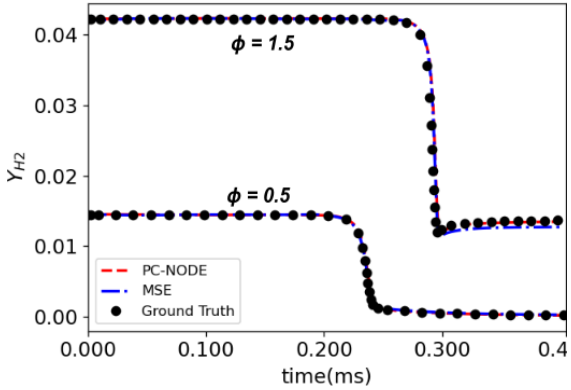
CONVERGE UDF

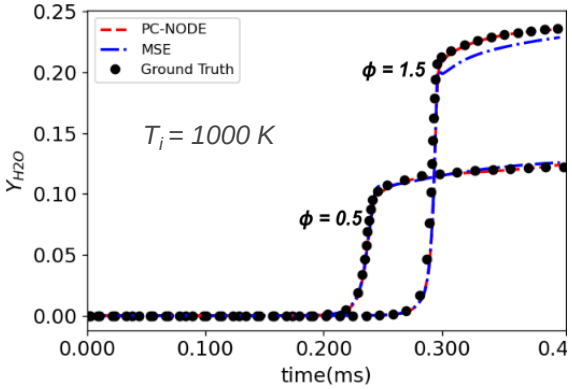
`sage_molefrac_dot`

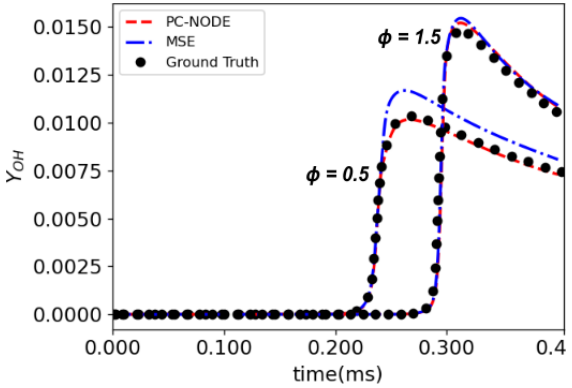
A-POSTERIORI Phy-ChemNODE+CFD TESTS

Hydrogen-air case









- 0D constant pressure autoignition mimicked in CONVERGE CFD solver as a 3D single cell problem with edge length $l = 100\ \mu m$
- Homogeneous temperature and species mass fractions are specified as initial conditions in the box
- Boundary conditions:
  - x^+: Dirichlet for pressure, zero gradient for temperature, species and velocities
  - x^-, y^+, y^-, z^+, z^-: Symmetry boundary conditions for pressure, temperature, species, and velocities

Kumar et al., arXiv:2312.00038, 2023

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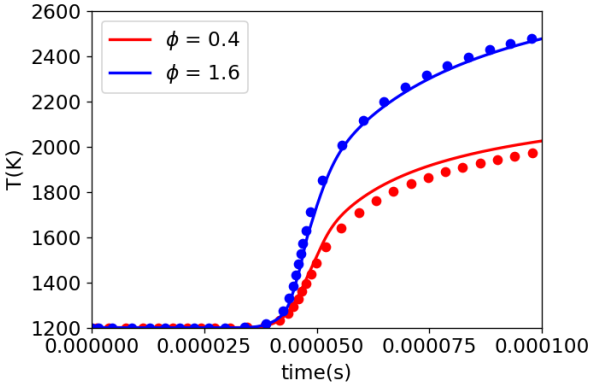
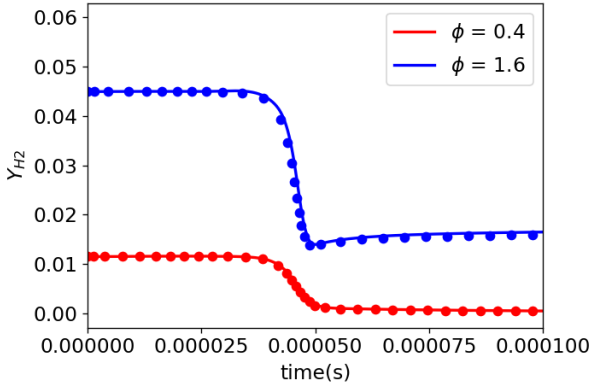
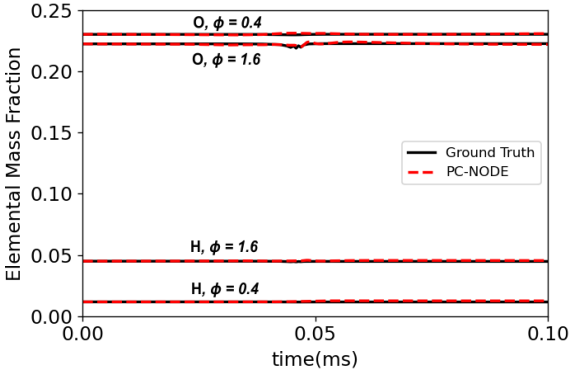
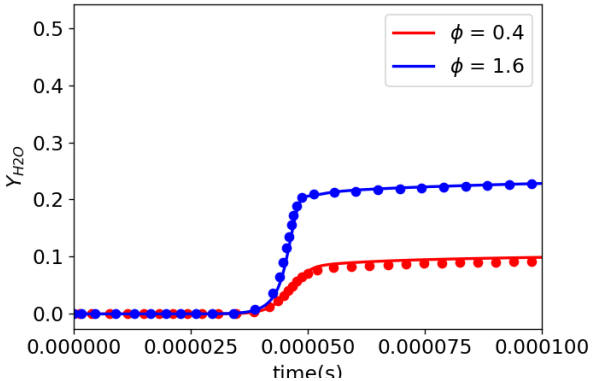
A-POSTERIORI Phy-ChemNODE+CFD TESTS

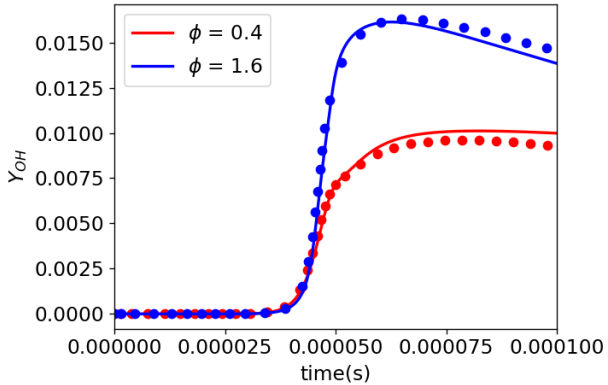
Extrapolation tests (hydrogen-air case)











Kumar et al., arXiv:2312.00038, 2023

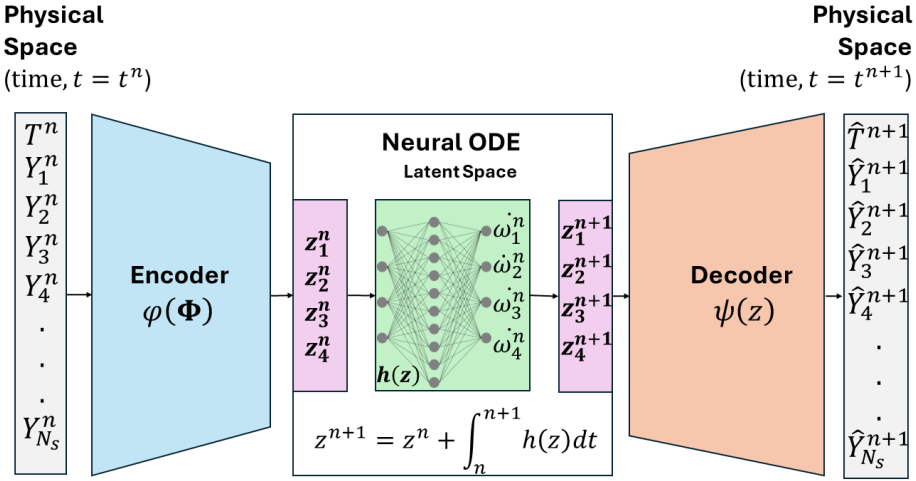
EXTENSION TO HYDROCARBON CHEMISTRY

Learning Dynamics in Latent Space using Autoencoder-NeuralODE

- Combining dimensionality reduction with latent space dynamics learning
  - **Encoder-Decoder** for mapping to and from latent space
  - **NeuralODE** to capture dynamics in the reduced latent space
- Trained by combining the prediction loss, mapping loss, and element conservation loss

$$L = \left|\left|\hat{y} - y\right|\right|_1 + \left|\left|\psi(\phi(y)) - y\right|\right|_1$$

$$L_{total} = L + \lambda_1 L_{ele-1} + \lambda_2 L_{ele-2} \ldots + \lambda_3 L_{ele-n}$$



Kumar et al., CSSCI 2024

Kumar et al., AIAA SciTech 2025 (accepted)

Kumar et al., *NeurIPS ML for Physical Sciences*, 2024

EXTENSION TO HYDROCARBON CHEMISTRY

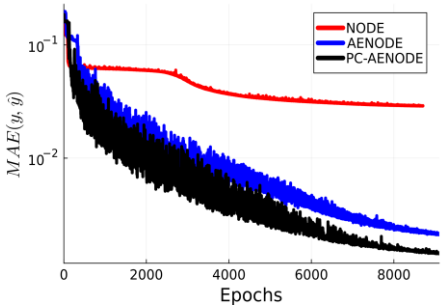
Phy-ChemNODE demonstration for methane combustion kinetics

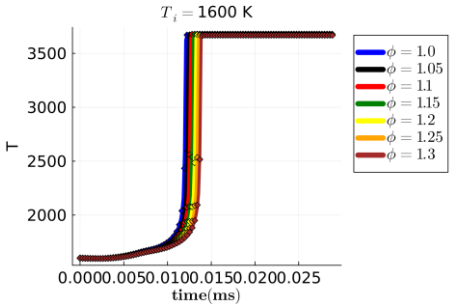
- **32-species, 266-rxns** FFCM-1 mechanism
- Training data based on 0D constant pressure homogeneous autoignition of methane-oxygen mixture at 20 bar for φ = 1-1.3 and T_i = 1600-2000 K
- Ground truth data generated for 63 initial conditions
- **Explicit Solver** used to integrate the NeuralODE, **BackwardAdjoint** sensitivity to calculate the gradients
- **ADAM** optimizer with learning rate decay
- Mean absolute error (MAE) used as the loss function
- **Encoder-Decoder**
  - 5 Hidden layers, 64 Neurons, ELU activation
- **NeuralODE**
  - 4 Hidden layers, 64 Neurons, ELU activation

$$L = \left|\left|\hat{y} - y\right|\right|_1 + \left|\left|\psi(\phi(y)) - y\right|\right|_1$$

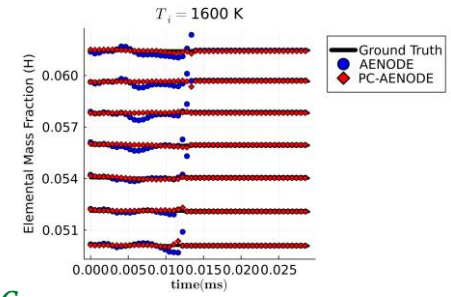
$$L_{total} = L + \lambda_1 L_{ele-H} + \lambda_2 L_{ele-O} + \lambda_3 L_{ele-C}$$

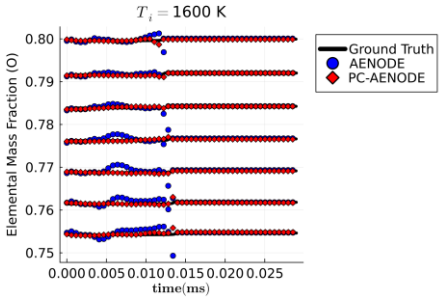
Markers: PC-AENODE
Solid lines: Ground truth (Cantera)





~10X over full chemical mechanism





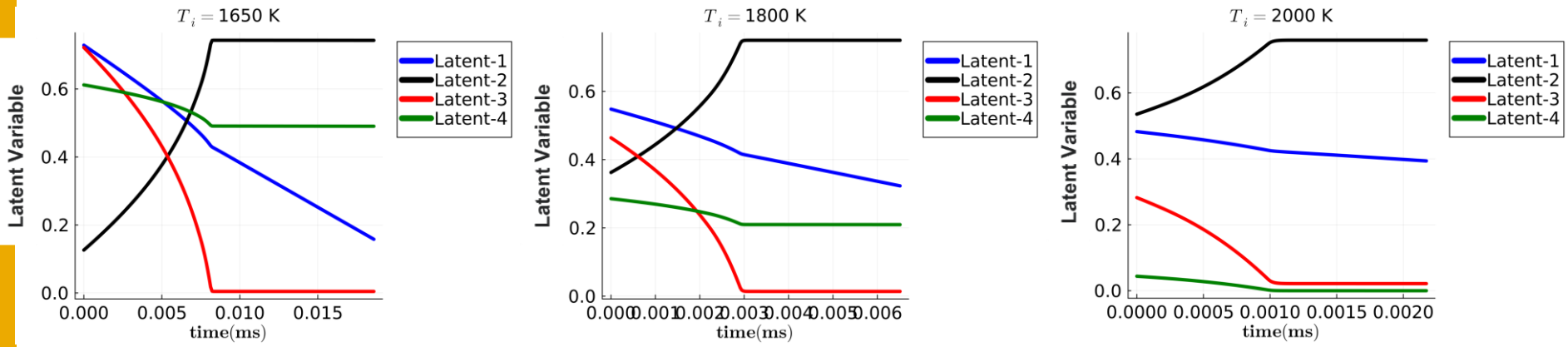
Kumar et al., *NeurIPS ML for Physical Sciences*, 2024

Kumar et al., CSSCI 2024

Kumar et al., AIAA SciTech 2025 (accepted)

EXTENSION TO HYDROCARBON CHEMISTRY

Dynamics in the Latent Space



- Significantly smoother dynamics in the AE latent space learned by Phy-ChemNODE (stiffness reduction)

Kumar et al., AIAA SciTech 2025 (accepted)

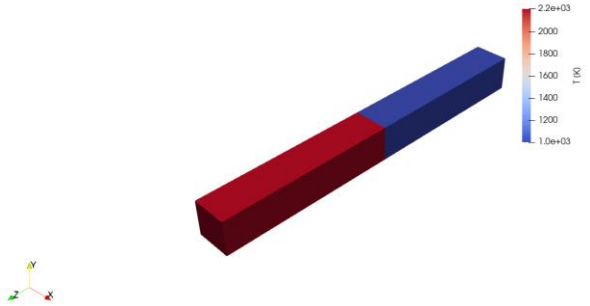
Kumar et al., *NeurIPS ML for Physical Sciences*, 2024

SUMMARY

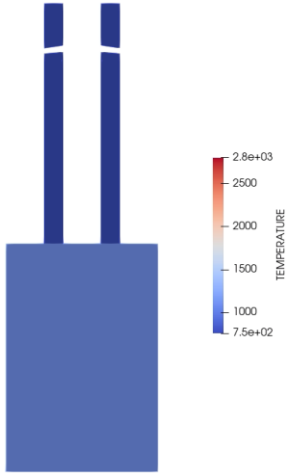
- A novel neural ODE based deep learning approach was developed for accelerating detailed chemical kinetic computations in reacting flow simulations **(ChemNODE)**
- Physics-based constraints pertaining to elemental mass conservation were incorporated within the ML training framework **(Phy-ChemNODE)**
- Phy-ChemNODE demonstration studies were performed for constant-pressure autoignition of hydrogen-air mixtures, showing ~3X speedup over the 9-species detailed mechanism
- Phy-ChemNODE was further extended to larger hydrocarbon combustion kinetics by incorporating an autoencoder framework for learning the dynamics in a lower-dimensional latent space
- Autoencoder-coupled Phy-ChemNODE was demonstrated for methane combustion kinetics with ~10X speedup over a 32-species chemical kinetic mechanism
- In collaboration with Convergent Science Inc., Phy-ChemNODE was embedded within CONVERGE CFD solver via user-defined functions (UDFs)
- Preliminary *a-posteriori* CFD+Phy-ChemNODE demonstration studies were performed showing robust performance in both interpolative and extrapolative tests

ONGOING WORK

- Proof-of-concept demonstration studies for 3D combustion CFD simulations



Laminar flame propagation



Combustor flashback

FUTURE WORK

- Efficient scaling of Phy-ChemNODE training to wide range of initial conditions and compositions (including blends)
- Demonstration for larger gas-phase kinetic mechanisms (~60-100 species, ~*O*(1000) reactions)
- Demonstration of emissions (NO_x) modeling with Phy-ChemNODE
- Extension to constant-volume combustion → Relevance to rotating detonation engines (RDEs)
- Demonstration of Phy-ChemNODE coupled full-scale combustor CFD simulations on DOE's GPU-based supercomputers

PUBLICATIONS

- T. Kumar, A. Kumar, and P. Pal, “A physics-constrained autoencoder-neuralODE framework (Phy-ChemNODE) for learning complex fuel chemical kinetics”, *NeurIPS Machine Learning and the Physical Sciences (ML4PS) Workshop*, 2024 (under review).

- T. Kumar, A. Kumar, and P. Pal, “A physics-constrained autoencoder-neuralODE framework for learning complex hydrocarbon fuel chemistry”, *AIAA SciTech Forum*, 2025 (accepted).

- T. Kumar, A. Kumar, and P. Pal, “A physics-constrained neural ordinary differential equations approach for robust learning of stiff chemical kinetics”, *Combustion Theory and Modelling*, 2024 (under review).

- T. Kumar, A. Kumar, and P. Pal, “A physics-constrained autoencoder-neuralODE framework for learning complex hydrocarbon fuel chemistry: Methane combustion kinetics”, *Spring Technical Meeting of the Central States of the Combustion Institute*, Cleveland, USA, 2024.

- T. Kumar, A. Kumar, and P. Pal, “A posteriori evaluation of a physics-constrained neural ordinary differential equations approach coupled with CFD solver for modeling of stiff chemical kinetics”, ArXiv, 2023. *https://arxiv.org/abs/2312.00038v3.*

- T. Kumar, A. Kumar, and P. Pal, “A physics-constrained neuralODE approach for robust learning of stiff chemical kinetics”, *NeurIPS Machine Learning and the Physical Sciences (ML4PS) Workshop*, New Orleans, USA, 2023.

- P. Pal, “Machine learning tools for accelerating simulation-driven engine design and optimization”, *20th International Conference on Flow Dynamics (ICFD)*, Sendai, Miyagi, Japan, 2023.

- O. Owoyele and P. Pal, “ChemNODE: A neural ordinary differential equations framework for efficient chemical kinetics solvers”, *Energy and AI*, Vol. 7, 2021.

INVITED TALKS

- P. Pal, T. Kumar, and A. Kumar, “Phy-ChemNODE: A physics-enhanced neural ordinary differential equations approach for accelerating stiff chemical kinetic computations”, *NETL Multiphase Flow Science Workshop*, 2024.
- T. Kumar, A. Kumar, and P. Pal, “Physics-constrained neural ordinary differential equations for robust learning of stiff chemical kinetics”, *Artificial Intelligence for Robust Engineering & Science (AIRES) 5 Workshop*, 2024.
- P. Pal, “Machine learning tools for accelerating simulation-driven engine design and optimization”, *20th International Conference on Flow Dynamics (ICFD)*, Sendai, Miyagi, Japan, 2023.
- T. Kumar, “ChemNODE: A neural ordinary differential equations approach for robust deep learning augmented chemical kinetic solvers”, *AFRL/AFOSR Combustion ROMs Panel Session*, AIAA SciTech, National Harbor, USA, 2023.
- T. Kumar and P. Pal, “ChemNODE: A neural ordinary differential equations approach for accelerating detailed chemistry calculations in reacting flow CFD”, *18th International Conference on Numerical Combustion (ICNC)*, San Diego, USA, 2022.
- P. Pal, “Neural ordinary differential equations approach for time-series prediction of chemical kinetics”, *Artificial Intelligence for Robust Engineering & Science (AIRES) 3 Workshop*, 2022.
- T. Kumar, “ChemNODE: A neural ordinary differential equations approach for accelerating detailed chemistry calculations in reacting flow CFD”, *Sandia Machine Learning & Deep Learning (MLDL) Workshop*, 2022.

CONFERENCE PRESENTATIONS

- T. Kumar, A. Kumar, P. Pal, “Phy-ChemNODE: A physics-enhanced neural ordinary differential equations approach for accelerating stiff chemical kinetic computations”, *APS Division of Fluid Dynamics Meeting*, Salt Lake City, USA, 2024.
- T. Kumar, A. Kumar, P. Pal, “Phy-ChemNODE: A physics-enhanced neural ordinary differential equations approach for accelerating stiff chemical kinetic computations”, *CONVERGE CFD Conference*, 2024.
- T. Kumar, P. Pal, A. Kumar, “A physics-constrained neural ordinary differential equations approach for robust data-driven modeling of chemical kinetics”, *APS Division of Fluid Dynamics Meeting*, Washington, USA, 2023.
- T. Kumar, A. Kumar, P. Pal, “A physics-constrained neural ODE approach for robust data-driven modeling of chemical kinetics”, *CONVERGE CFD Conference*, 2023.
- T. Kumar, P. Pal, O. Owoyele, “ChemNODE: A robust ML framework for efficient chemical kinetic solvers”, *CONVERGE User Conference*, 2022.

THANK YOU

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