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Phy-ChemNODE: A Physics-enhanced Neural Ordinary Differential Equations Approach for Accelerating Stiff Chemical Kinetic Computations

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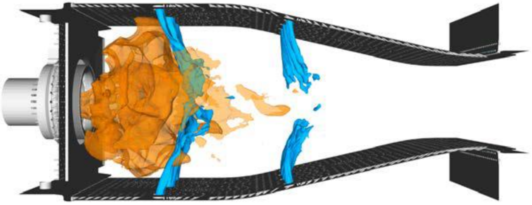
MOTIVATION

- Chemically reacting flows are prevalent in a wide range of reactors employed in a variety of applications: gas turbines, IC engines, gasification systems, etc.

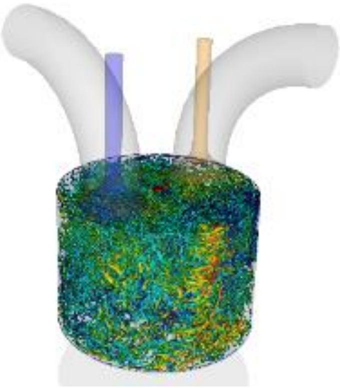
- Computational fluid dynamics (CFD) simulation-driven virtual design analysis can aid the development of these advanced reactors, while saving costs associated with experimental prototyping

- CFD simulations of full-scale reactor 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

- <u>Solving for detailed chemistry presents a major bottleneck in the application of combustion CFD for comprehensive parametric analysis and results in prolonged design cycles</u>



Gas turbines

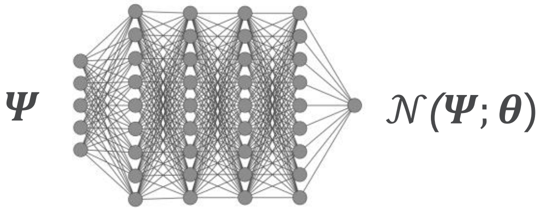


IC engines

ChemNODE: BASIC APPROACH

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

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



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**

Owoyele & Pal, *Energy and AI*, 2021

ChemNODE: BASIC APPROACH

Governing equations

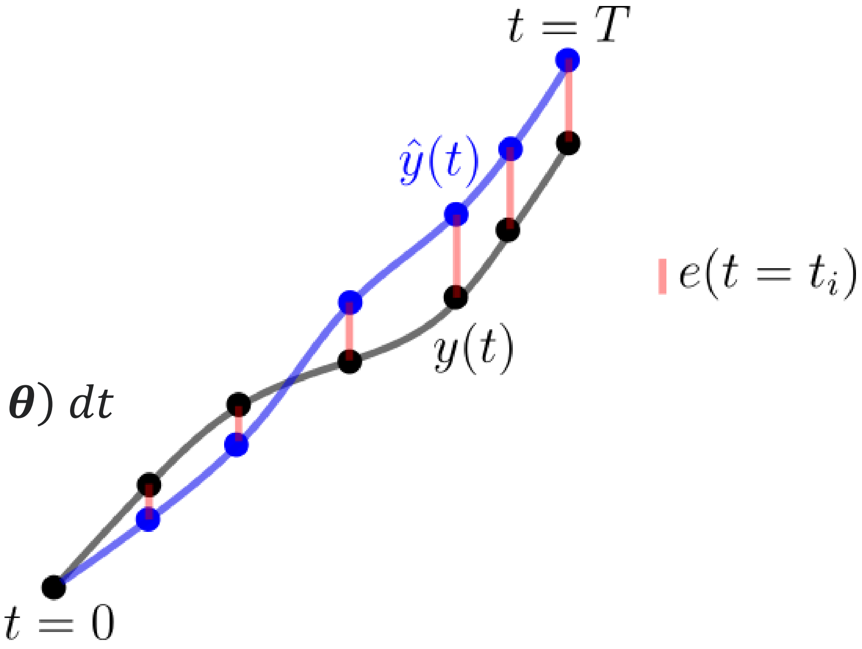
$$\frac{d\boldsymbol{y}}{dt} = \frac{\dot{\omega}}{\rho} \longrightarrow$$

Ground truth, $\boldsymbol{y}$

Model

$$\frac{d\widehat{\boldsymbol{y}}}{dt} = \mathrm{g}(\hat{y};\theta) \longrightarrow \widehat{\boldsymbol{y}}(\boldsymbol{t}) = \boldsymbol{y_o} + \int \boldsymbol{g}(\hat{y};\boldsymbol{\theta})\, dt$$

The deep learning framework is developed in Julia programming language widely used for scientific machine learning (SciML)



Forward pass constitutes solving the ODEs using NN-predicted source terms

Owoyele & Pal, *Energy and AI*, 2021

ChemNODE: BASIC APPROACH

Governing equations

$$\frac{d\boldsymbol{y}}{dt} = \frac{\dot{\omega}}{\rho}$$

→ Ground truth, $\boldsymbol{y}$

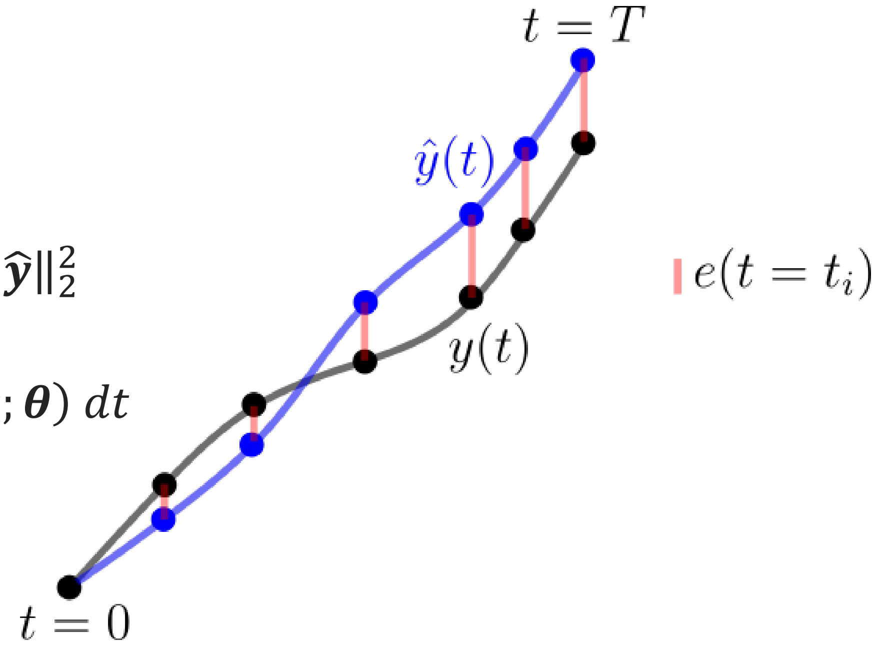
$$\mathcal{L} = \|\boldsymbol{y} - \widehat{\boldsymbol{y}}\|_2^2$$

Model

$$\frac{d\widehat{\boldsymbol{y}}}{dt} = \mathrm{g}(\hat{y};\theta)$$

→ $\widehat{\boldsymbol{y}}(\boldsymbol{t}) = \boldsymbol{y_o} + \int \boldsymbol{g}(\hat{y};\boldsymbol{\theta})\,dt$

The deep learning framework is developed in Julia programming language widely used for scientific machine learning (SciML)



Backprop to optimize NN weights

Owoyele & Pal, *Energy and AI*, 2021

CASE STUDY: H_2-AIR AUTOIGNITION

- Ground truth data was generated from 0D homogenous constant pressure hydrogen-air reactor 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:

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

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

PHYSICS-ENHANCED LOSS FUNCTION

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

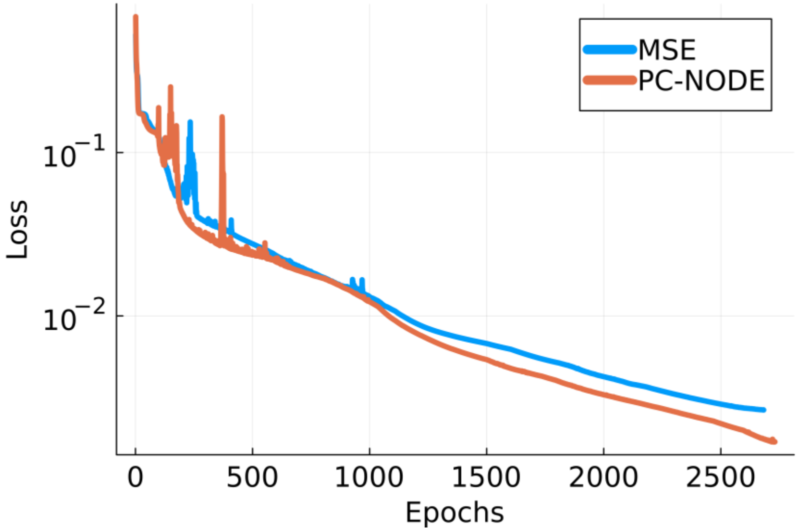
$$L_{Phy-ChemNODE} = L_{ODE} + \lambda_1 L_{ele-H} + \lambda_2 L_{ele-O}$$

$$L_{ODE} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\boldsymbol{\Psi}_{\mathbf{i}} - \widehat{\boldsymbol{\Psi}_{\mathbf{i}}}}{\boldsymbol{\Psi}_{\boldsymbol{max}} - \boldsymbol{\Psi}_{\boldsymbol{min}}}\right)^2$$

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

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

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

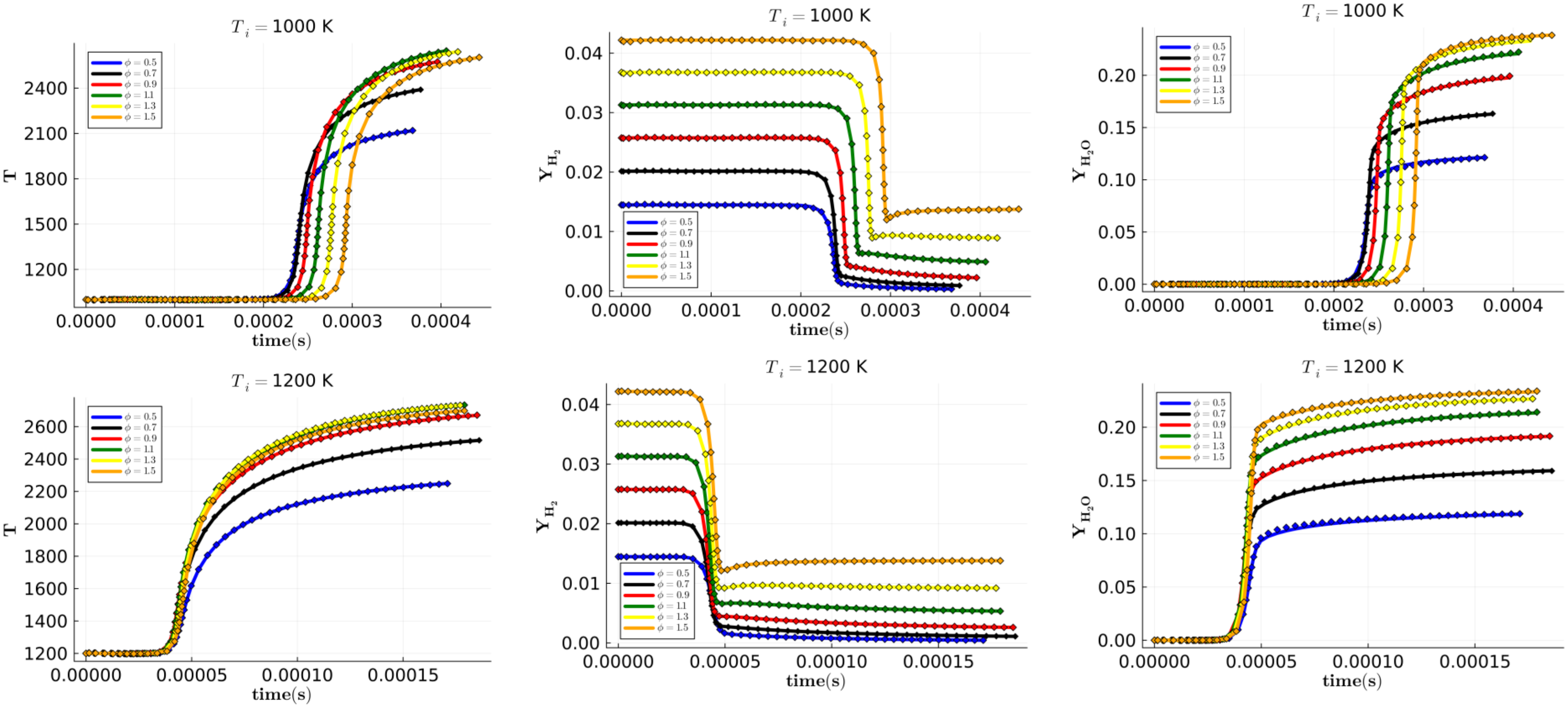


Kumar et al., *NeurIPS ML for Physical Sciences*, 2023

Phy-ChemNODE: H_2-AIR AUTOIGNITION

A-posteriori studies

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

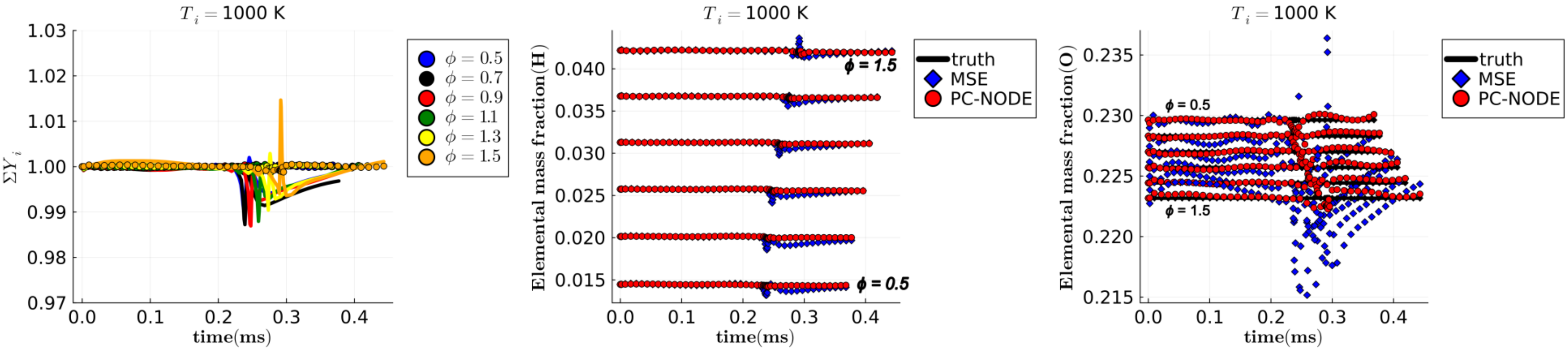


Inference speedup : ~3X over H_2/air detailed chemical mechanism

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

Phy-ChemNODE: H_2-AIR AUTOIGNITION

A-posteriori studies



- Better total and elemental mass conservation for PC-NODE

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

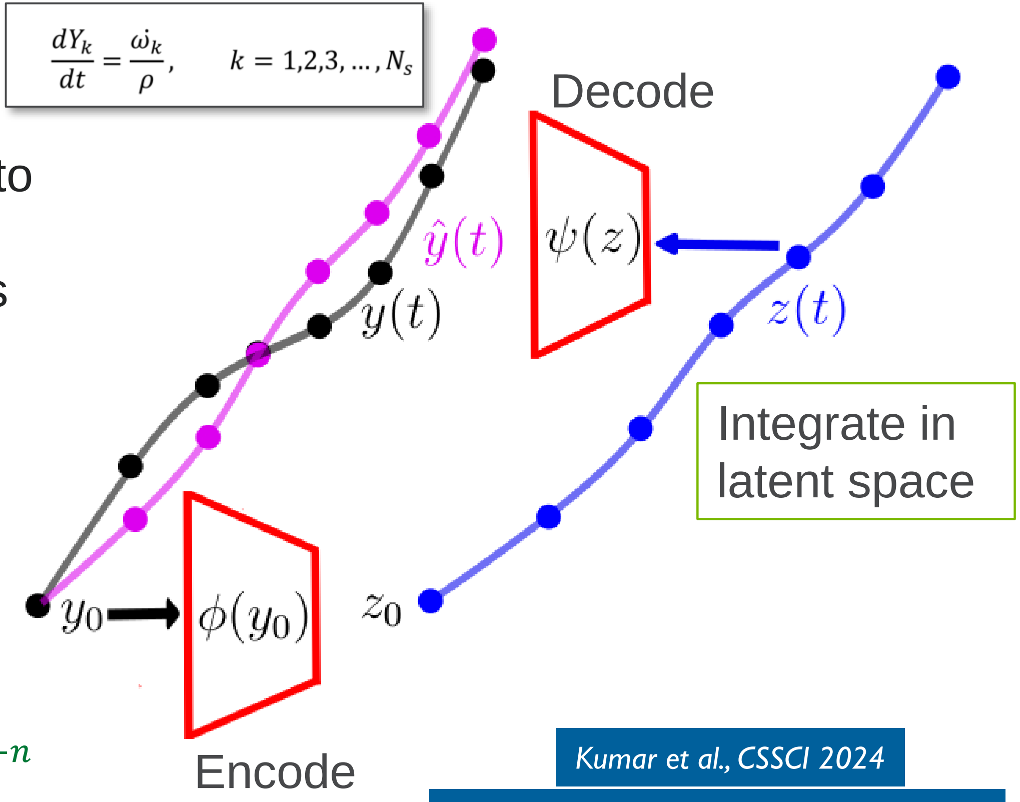
EXTENSION TO HYDROCARBON CHEMISTRY

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

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

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



$$\frac{dY_k}{dt} = \frac{\dot{\omega}_k}{\rho}, \qquad k = 1,2,3,\ldots,N_s$$

Kumar et al., CSSCI 2024

Kumar et al., AIAA SciTech 2025 (submitted)

EXTENSION TO HYDROCARBON CHEMISTRY

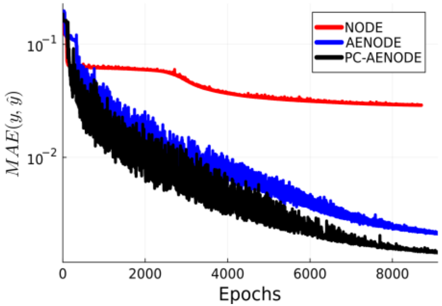
Phy-ChemNODE demonstration for methane combustion kinetics

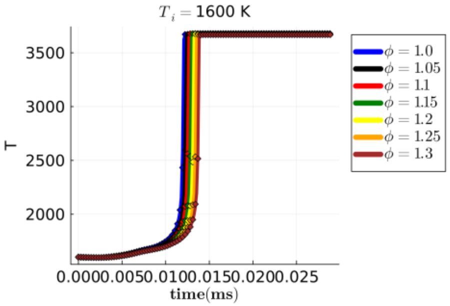
- **32-species, 266-rxns** FFCM-1 mechanism
- Training data based on 0D constant pressure homogeneous autoignition of methane-oxygen mixture at 20 bar for φ = 1-1.3 and T_i = 1600-2000 K
- Ground truth data generated for 63 initial conditions
- **Explicit Solver** used to integrate the NeuralODE, **BackwardAdjoint** 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

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

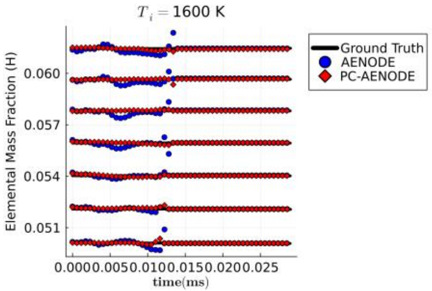
$$L_{total} = L + \lambda_1 L_{ele-H} + \lambda_2 L_{ele-O} + \lambda_3 L_{ele-C}$$

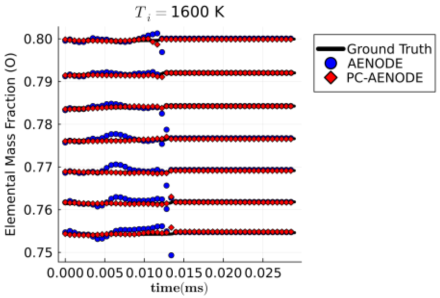
Markers: PC-AENODE
Solid lines: Ground truth (Cantera)





~10X over full chemical mechanism



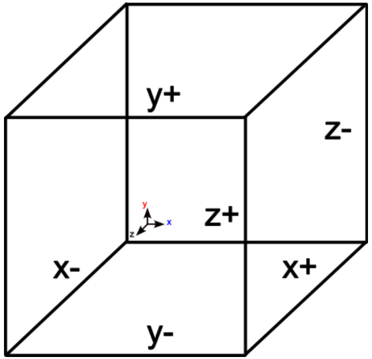


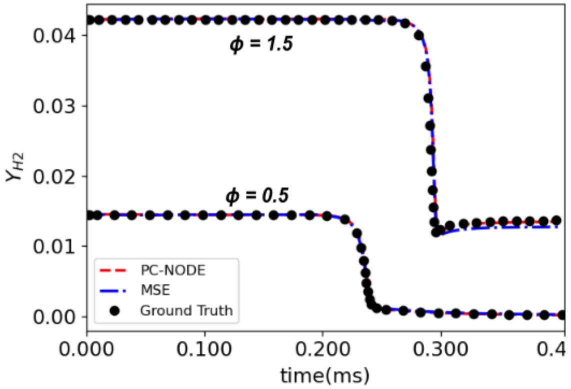
Kumar et al., CSSCI 2024

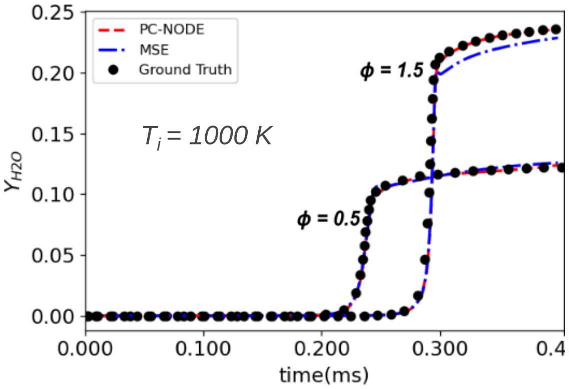
Kumar et al., AIAA SciTech 2025 (submitted)

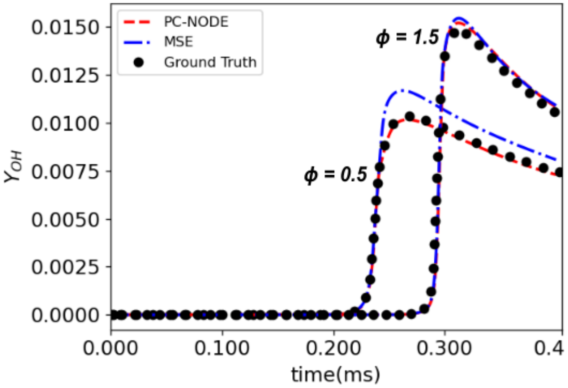
A-POSTERIORI Phy-ChemNODE+CFD TESTS

Hydrogen-air case









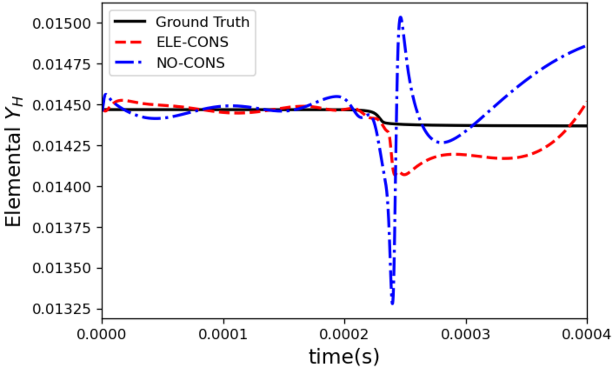
- 0D constant pressure autoignition mimicked in CONVERGE CFD solver as a 3D single cell problem with edge length $l = 100\ \mu m$
- Homogeneous temperature and species mass fractions are specified as initial conditions in the box
- Boundary conditions:
  - $\boldsymbol{x^+}$: Dirichlet for pressure,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

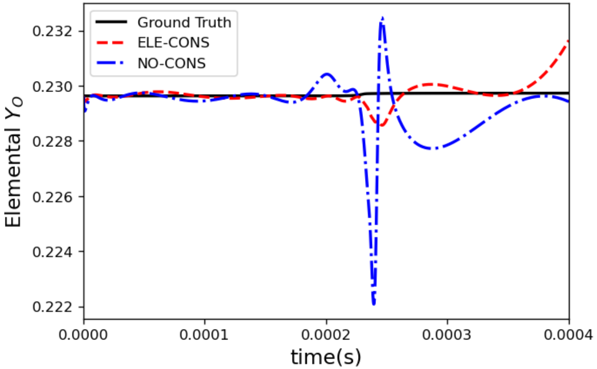
Kumar et al., arXiv:2312.00038, 2023

A-POSTERIORI Phy-ChemNODE+CFD TESTS

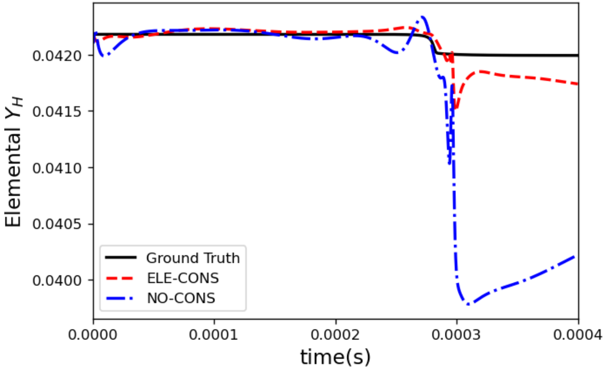
Comparison of elemental mass fractions (hydrogen-air case)

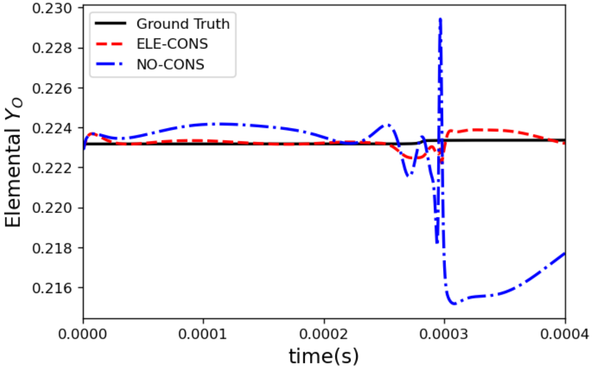
$\phi = 0.5$
$T_i = 1000$ K





$\phi = 1.5$
$T_i = 1000$ K

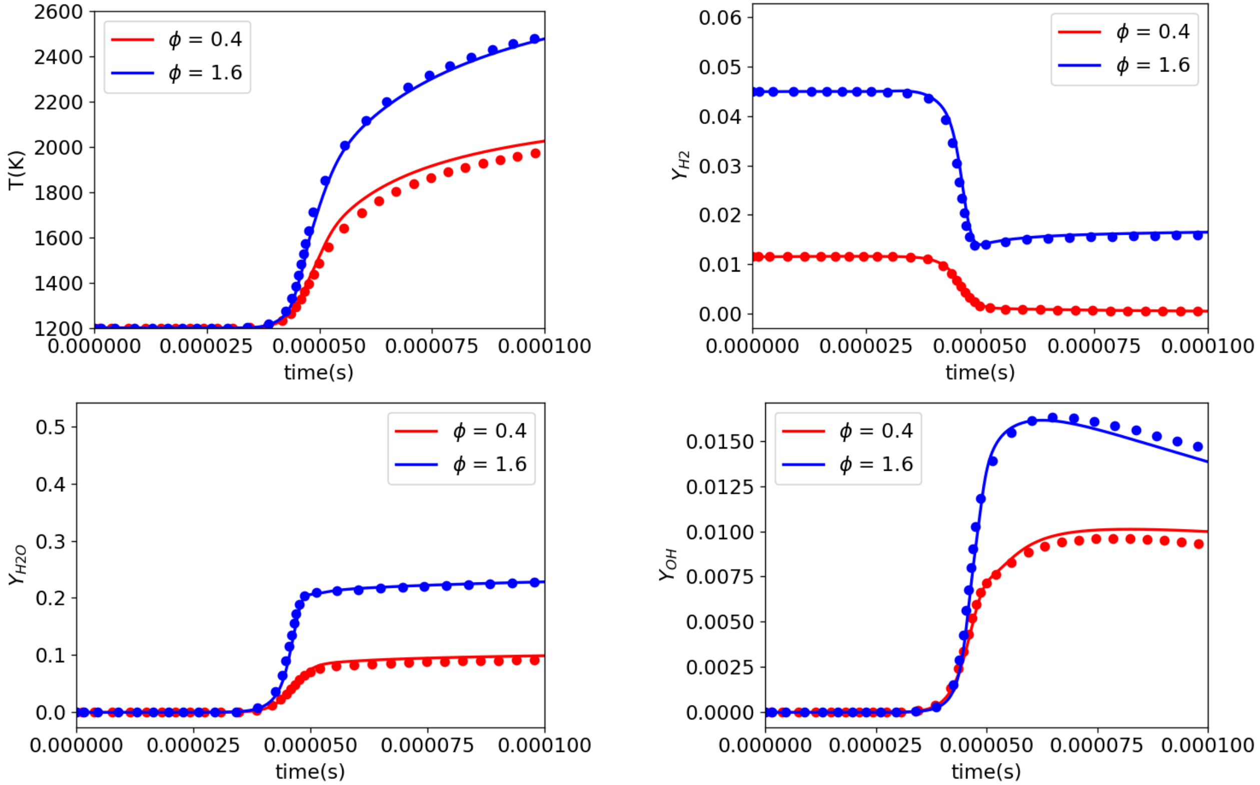




Kumar et al., arXiv:2312.00038, 2023

*A-POSTERIORI Phy-*ChemNODE+CFD TESTS

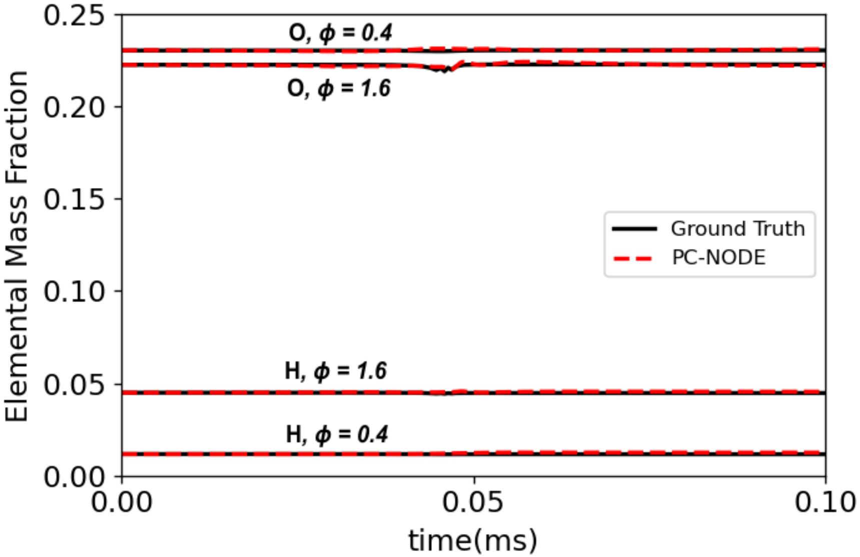
Extrapolation tests (hydrogen-air case)



Kumar et al., arXiv:2312.00038, 2023

A-POSTERIORI Phy-ChemNODE+CFD TESTS

Extrapolation tests: Elemental mass conservation (hydrogen-air case)



Kumar et al., arXiv:2312.00038, 2023

ONGOING WORK

- Scaling of Phy-ChemNODE training to wider range of initial conditions and larger gas-phase kinetic mechanisms (~*O*(100) species))

- Demonstration studies for 3D CFD simulations of full-scale gas turbine combustors

- Coupling of Phy-ChemNODE with Argonne's GPU-capable CFD solver NekRS

Phy-ChemNODE framework is general: (1) can be applied to other types of chemistry (e.g., biomass pyrolysis kinetics); (2) can be coupled with different CFD solvers

PUBLICATIONS

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

- 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.

THANK YOU

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