2023 UTSR & Advanced Turbines Program Review Meeting
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Development of a Neural ODE-based Scientific Machine Learning Framework Towards Acceleration of Combustion CFD Simulations

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Office of TECHNOLOGY TRANSITIONS

Technology Commercialization Fund (TCF) Program

CONVERGENT SCIENCE

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Argonne LCRC

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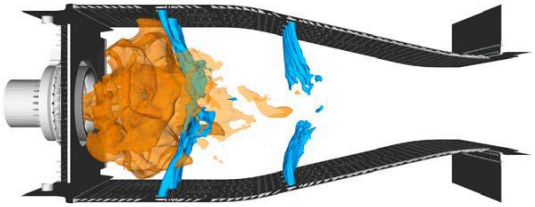
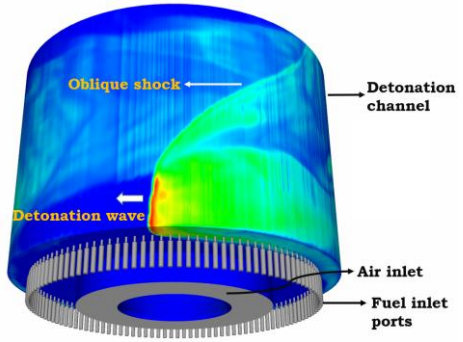
MOTIVATION

- 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 a 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 PROJECT GOALS

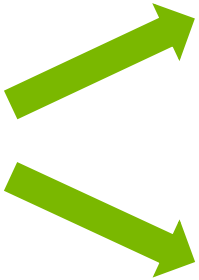
- Advance and demonstrate **ChemNODE**, a novel deep learning (DL) framework developed at Argonne to accelerate detailed chemistry computations, for reacting flow CFD simulations
  - ➢ Mature ChemNODE software technology by incorporating algorithmic enhancements to make the DL framework more efficient 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

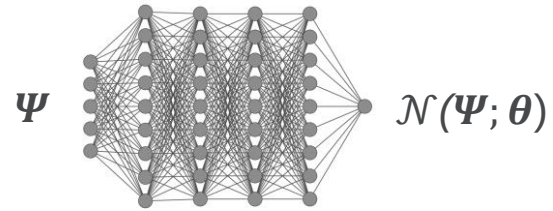
Accelerate Detailed Kinetics

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

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**

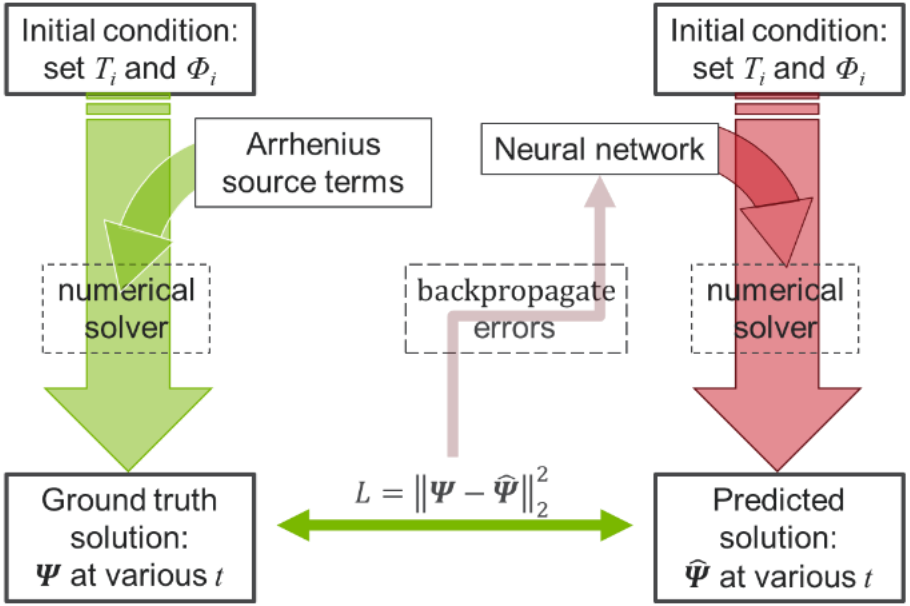
ChemNODE Approach

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

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

Owoyele & Pal, *Energy and AI*, 2021

ChemNODE: DEEP LEARNING FRAMEWORK



- First-of-its-kind application of neural ordinary differential equations (NODEs) to predict the evolution of chemical kinetics
- The deep learning framework is developed in Julia programming language widely used for scientific machine learning (SciML)
- Automatic differentiation techniques in Julia are used to compute the loss derivative terms, $\frac{\partial \hat{\Psi}}{\partial \theta}$, for backpropagation of errors

Owoyele & Pal, *Energy and AI*, 2021

CASE STUDY: H_2-AIR AUTOIGNITION

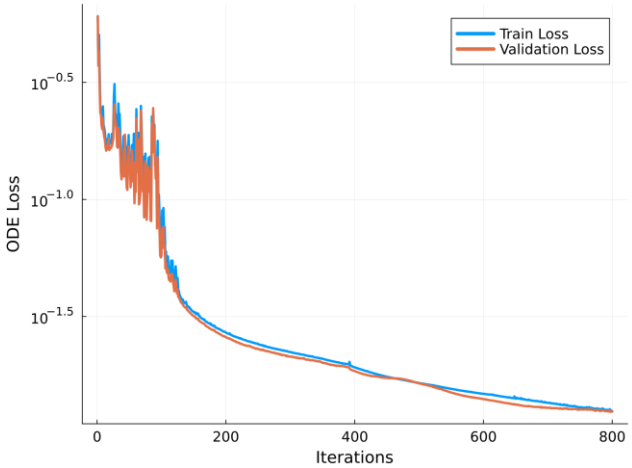
- Ground truth data is generated from 0D simulations in Cantera
- 0D homogenous constant pressure hydrogen-air reactor at 1 atm
- Baseline detailed kinetic mechanism with 9 species and 19 reactions [O'Conaire *et al*. 2004]; NO_x chemistry not included in the mechanism
- Ground truth data is generated from 0D simulations in Cantera
- Initial temperature (T_i) range of 1000-1200K and initial equivalence ratio (Φ_i) range of 0.5-1.5 considered
- Time series data is generated for 30 initial conditions; 50 points are sampled from each time series
- Data is sampled from each time series such that there is a 50%-25%-25% data distribution split between pre-ignition, ignition, and post-ignition phases

ChemNODE TRAINING APPROACH

- Single NN with two hidden layers (48 neurons each); 9 inputs/outputs; *tanh* activation function for each hidden layer; NN outputs are scaled by the maximum source term values from the dataset
- An implicit–explicit solver available in Julia was used for ODE integration during training
- 2nd order Levenberg-Marquardt optimizer used to minimize loss function based on Mean Squared Error (MSE):

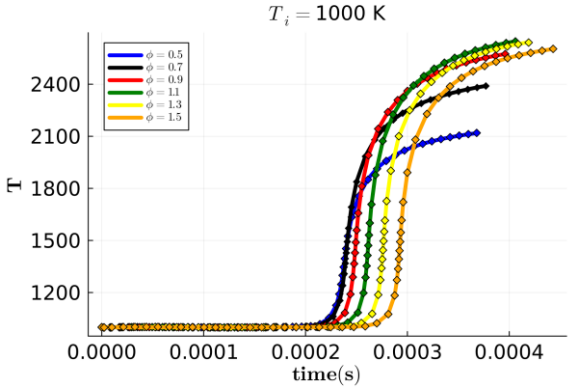
$$L_{MSE} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\boldsymbol{\Psi} - \hat{\boldsymbol{\Psi}}}{\boldsymbol{\Psi_{max}} - \boldsymbol{\Psi_{min}}}\right)^2$$

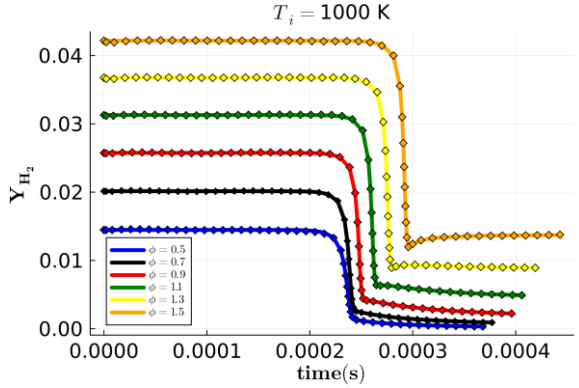
$$\boldsymbol{\Psi} = \left[\log(T), \log(Y_{H_2}), \log(Y_{O_2}) \ldots, \log(Y_{H_2O_2})\right]^{\boldsymbol{T}}$$

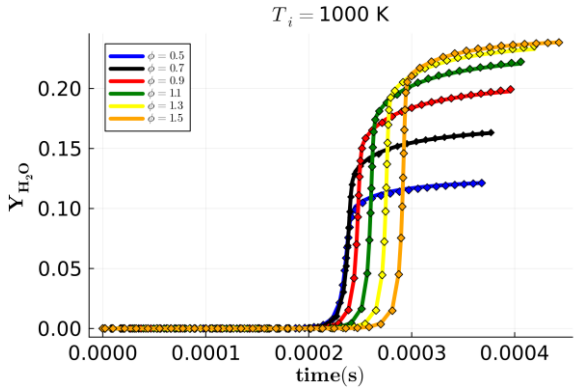


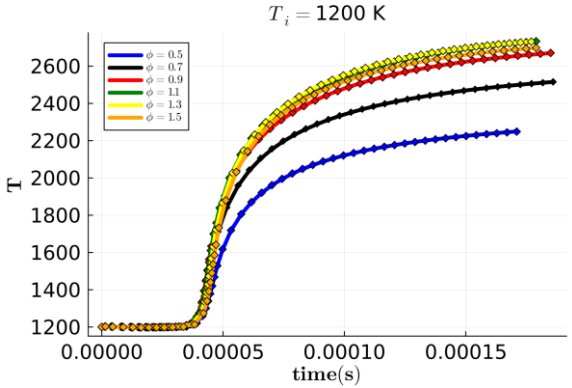
A POSTERIORI ChemNODE-CANTERA TESTS

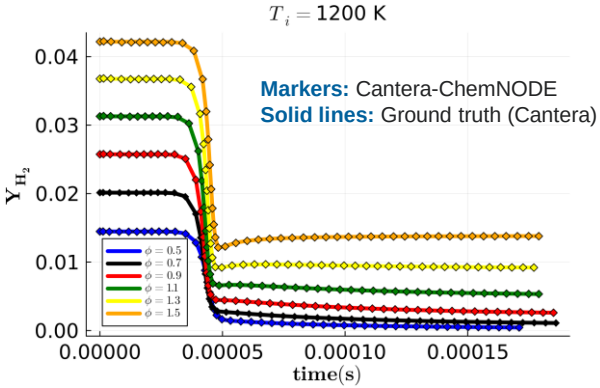
In-sample initial conditions



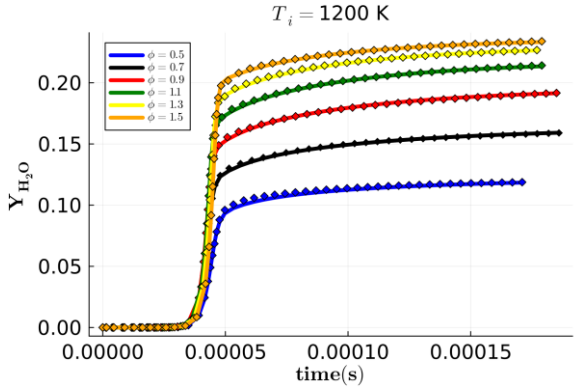








Markers: Cantera-ChemNODE
Solid lines: Ground truth (Cantera)



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

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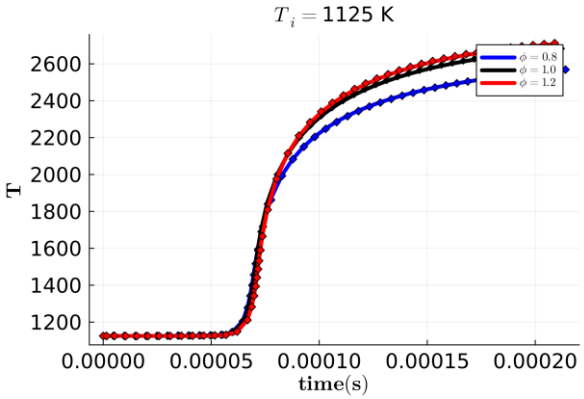
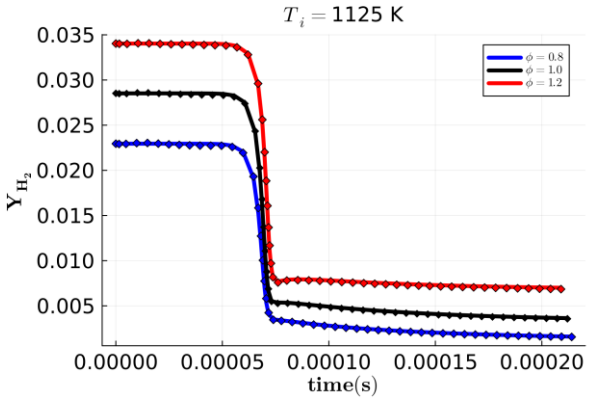
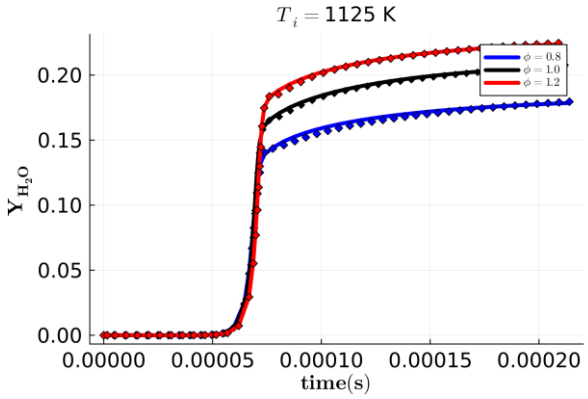
A POSTERIORI ChemNODE-CANTERA TESTS

Out-of-sample initial conditions

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







- Initial conditions $T_i = 1125$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

PHYSICS-CONSTRAINED LOSS FUNCTION

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

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

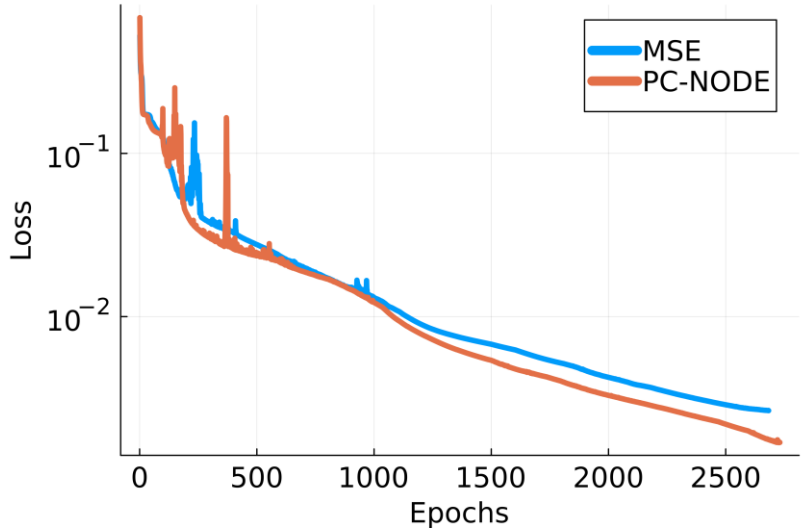
where

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

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

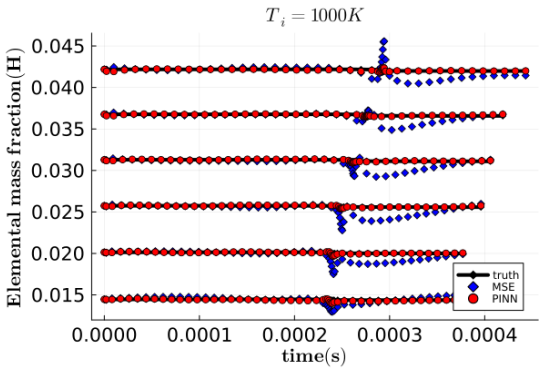
$$L_{ele-O} = \sum_{i=1}^{N}\left(\log\left(1 + \left|\sum_{k}^{N_s}\frac{N_O^k MW_O}{MW_k}\left(Y_{k,i} - \widehat{Y_{k,i}}\right)\right|\right)\right)^2$$

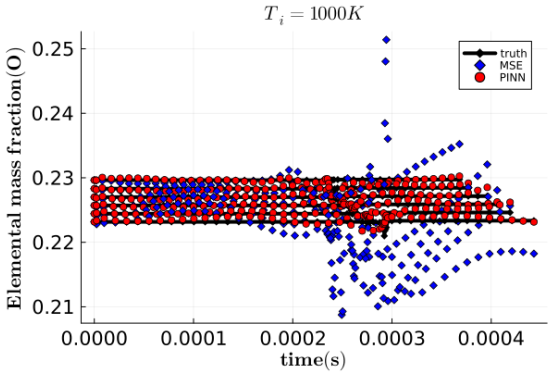
$$\lambda_1 = 3, \quad \lambda_2 = 3$$

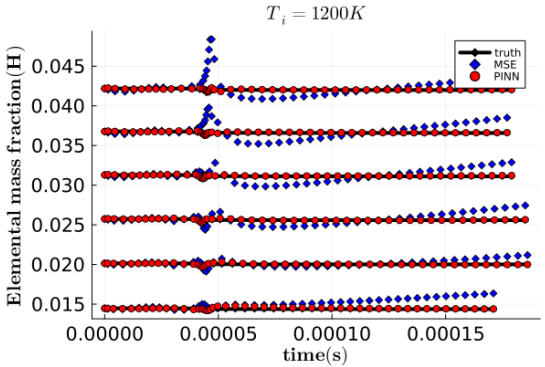


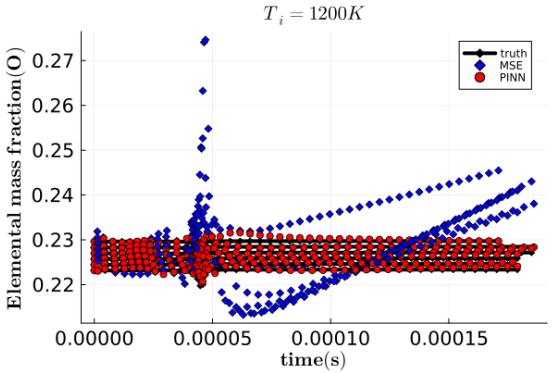
Kumar et al., *NeurIPS*, 2023 (in press)

ELEMENTAL MASS CONSERVATION



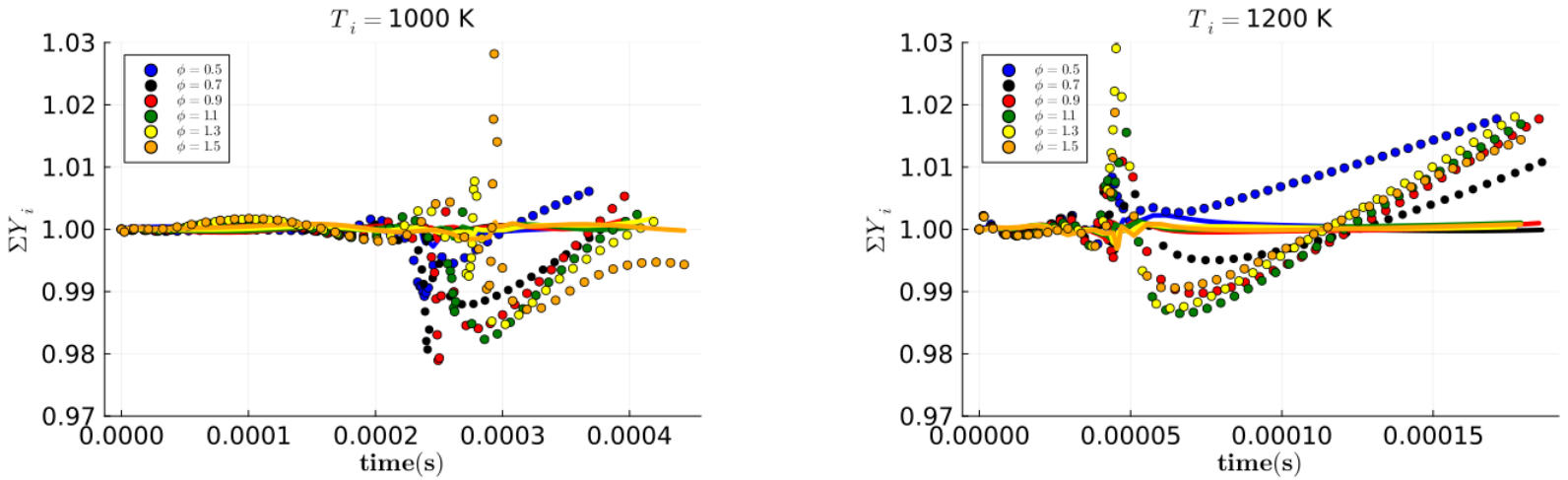






Kumar et al., *NeurIPS*, 2023 (in press)

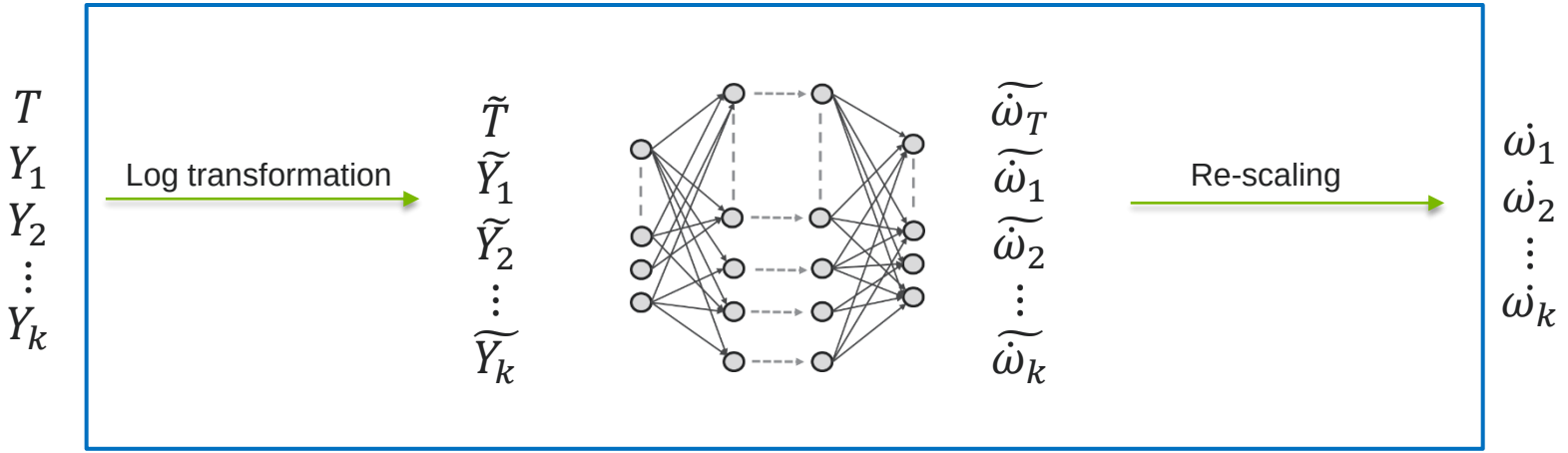
TOTAL MASS CONSERVATION



Markers: MSE
Solid lines: PC-NODE

Kumar et al., *NeurIPS*, 2023 (in press)

CFD SOLVER INTEGRATION



`sage_molefrac`

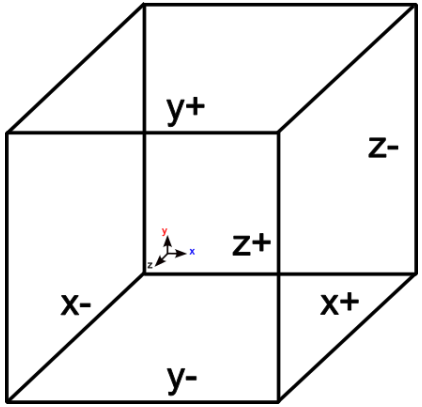
CONVERGE UDF

`sage_molefrac_dot`

A POSTERIORI ChemNODE-CFD TESTS

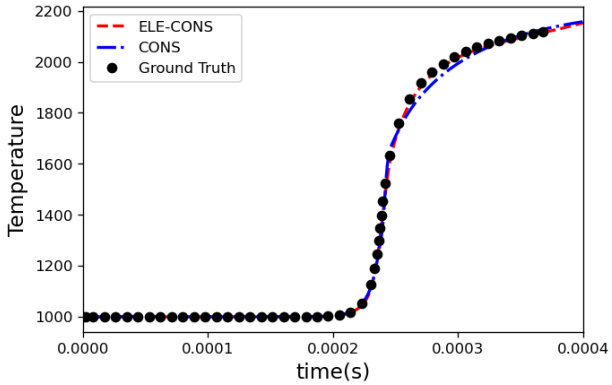
Simulation setup

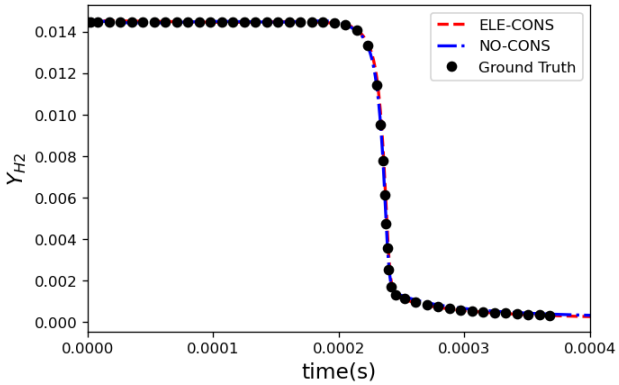
- 0D constant pressure autoignition mimicked in CONVERGE as a 3D single cell problem with edge length $l = 100\ \mu m$
- Homogeneous temperature and species mass fractions are specified as initial conditions in the box
- Boundary conditions:
  - $\boldsymbol{x}^{+}$: Dirichlet for pressure, zero gradient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

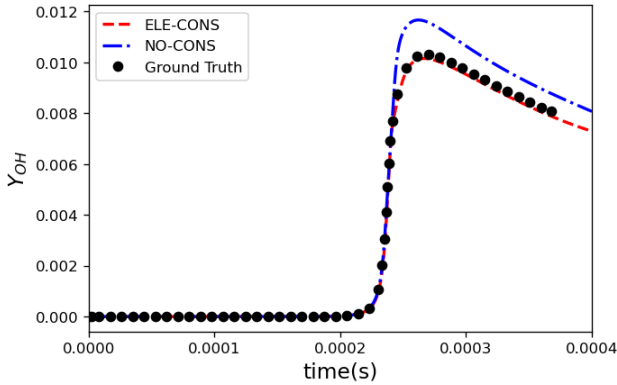


A POSTERIORI ChemNODE-CFD TESTS

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



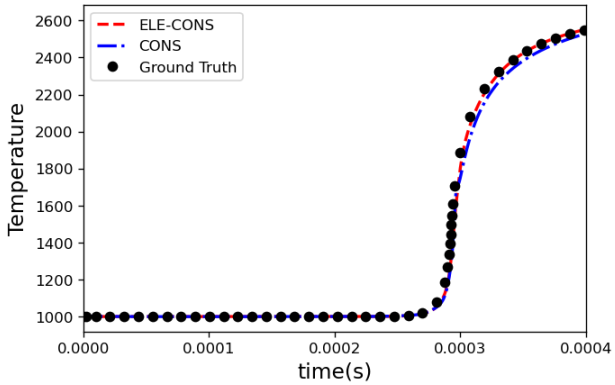


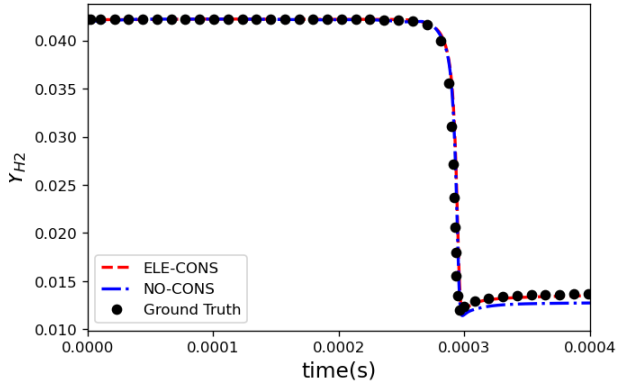


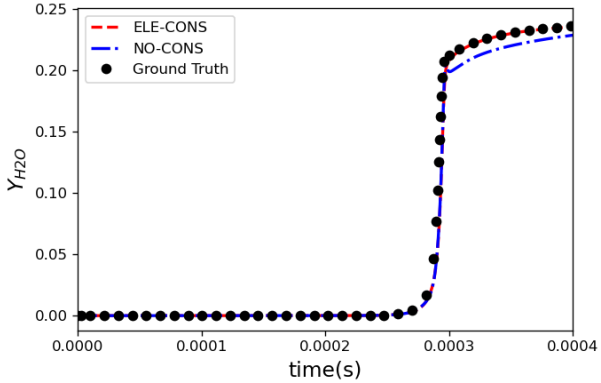
- Predictions are more accurate for physics-constrained ChemNODE

A POSTERIORI ChemNODE-CFD TESTS

$$T_i = 1000\ \boldsymbol{K}, \boldsymbol{\phi} = 1.5$$





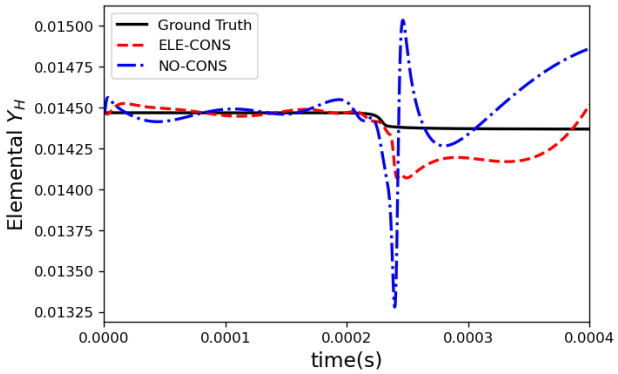


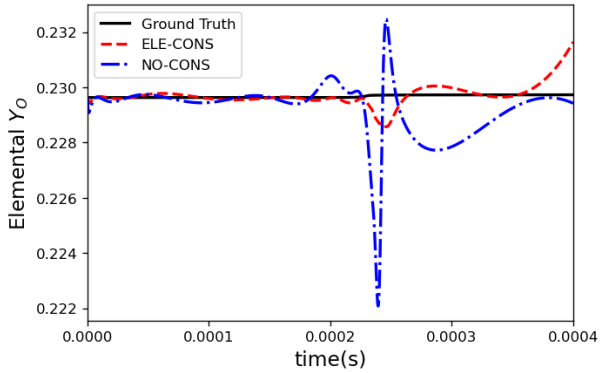
- Predictions are more accurate for physics-constrained ChemNODE

A POSTERIORI ChemNODE-CFD TESTS

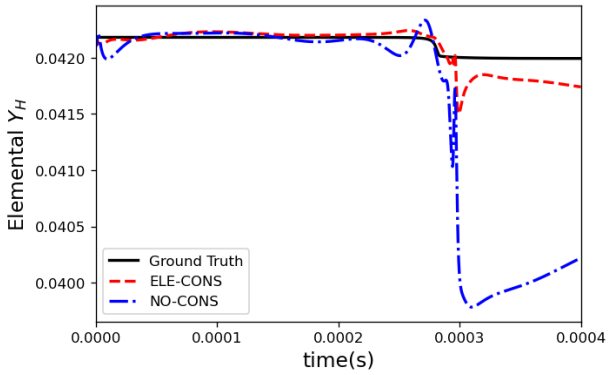
Comparison of elemental mass fractions

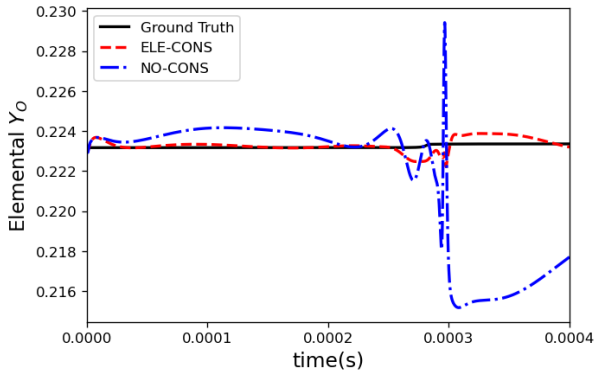
$\phi = 0.5$
T_i = 1000 K





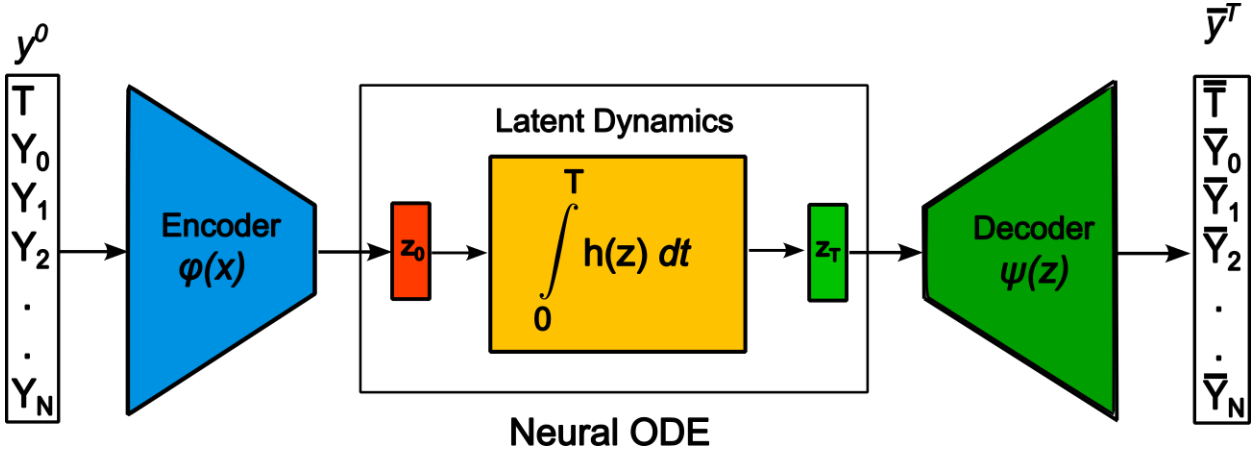
$\phi = 1.5$
$T_i = 1000$ K





ChemNODE EXTENSION FOR LARGE MECHANISMS

Learning the dynamics in a lower-dimensional latent space



- **Coupling ChemNODE with autoencoders**
  - Encoder generates the latent space representation of thermochemical state
  - NeuralODE captures the dynamics of the chemical system in the latent space
  - Decoder maps the latent space variable back to original thermochemical state space
  - Demonstration studies are underway for larger kinetic mechanisms of fuels of interest (methane, ammonia) to power generation applications

SUMMARY

- Proof-of-concept studies were performed with ChemNODE for H_2/air 0D homogeneous autoignition
- Elemental mass conservation was incorporated within the ML training framework
- ChemNODE accurately captured the temporal evolution of thermochemical scalars for different initial temperatures and equivalence ratios, while achieving 3X speedup over the H_2/air detailed mechanism
- ChemNODE was coupled with CONVERGE CFD solver via UDFs and *a posteriori* demonstration studies were performed

ONGOING & FUTURE WORK

- Extension of ChemNODE for larger kinetic mechanisms → coupling with autoencoders, high-P conditions, constant volume autoignition
- Demonstration studies currently underway for methane and ammonia combustion
- Future studies will focus on application of ChemNODE to 2D/3D combustion CFD

PUBLICATIONS

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

THANK YOU

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