Modeling Combustion Reaction ODEs with Neural Networks

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Rocky Mountain Fluid Mechanics Research Symposium

August 10, 2021
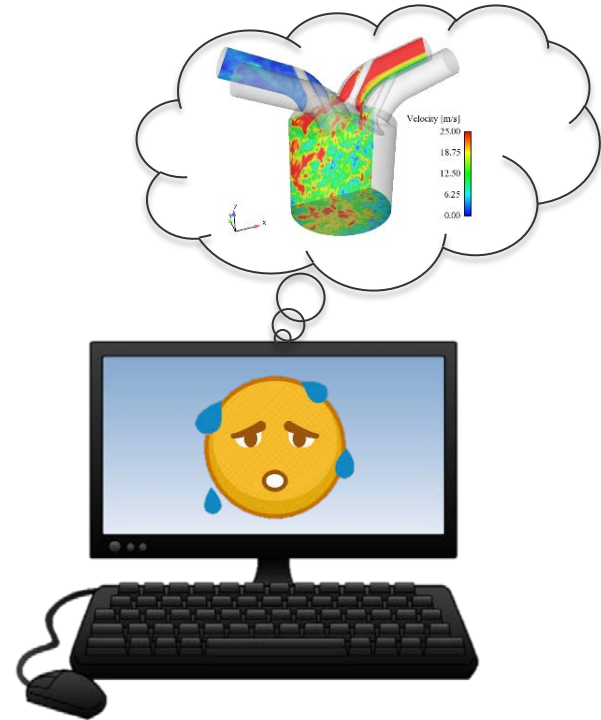
Motivation

Simulating combustion is expensive!

- Hundreds of reactions
- Non-linear kinetics models
- Stiff ODE solvers required for stability
- High fidelity, 3d simulations are expensive or intractable

Proposed solution

- Use machine learning (ML) to replace combustion kinetics ODE solvers

Velocity [m/s]
25.00
18.75
12.50
6.25
0.00

Methods

Supervised Machine learning

{Data: X,Y} → $Y = f(X)$

Neural Networks

- Structure inspired by the human brain
- Neuron transformation: $y = f(Wx+b)$
- Network of neurons in series and parallel
- Information passes from front to back
- At each learning iteration, the weights in each neuron are tuned
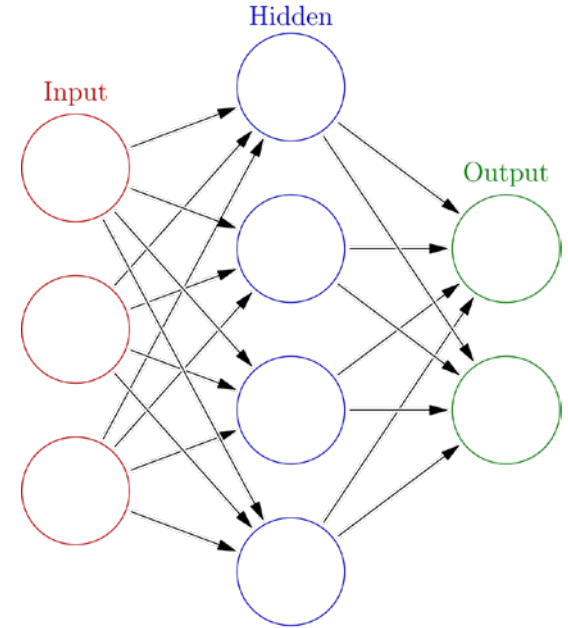

Simple 1-layer neural network

Background

Previous studies

— Common simplification: learn 0d combustion

— Focus on simple H_2 combustion mechanism (9 species, 19 reactions)

This study

— Much larger mechanism (methane combustion, 53 species, 325 reactions)

— Systematic study of prediction approaches, neural network architectures, and other ML-related details

— Search for network that generalizes well
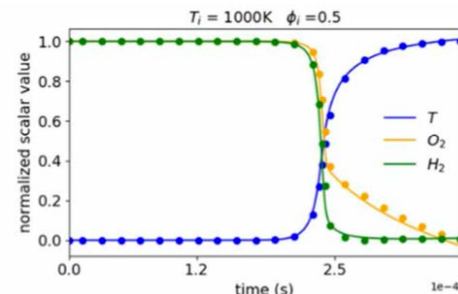
Owoyele and Pal's neural ODE predicted combustion trajectories with high training accuracy.[1]
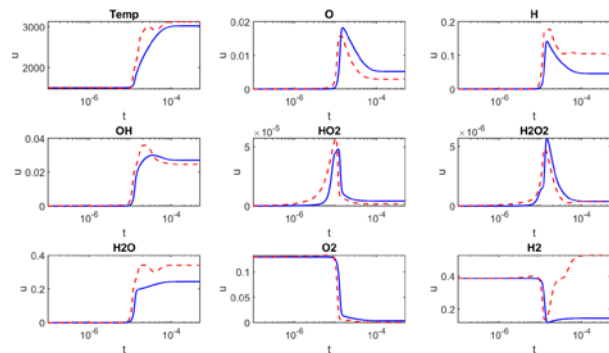
Brown et al.'s ResNet generalized well with temperature, but not as well with equivalence ratio.[2]

[1] Opeoluwa Owoyele and Pinaki Pal. Chemnode: A neural ordinary differential equations approach for chemical kinetics solvers, 2021.
[2] Thomas S. Brown, Harbir Antil, Rainald L̈ohner, Fumiya Togashi, and Deepanshu Verma. Novel dnns for stiff odes with applications to chemically reacting flows, 2021.
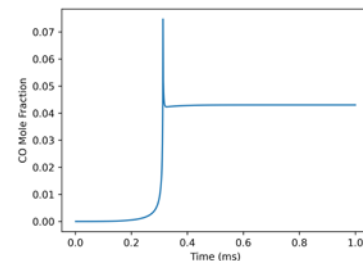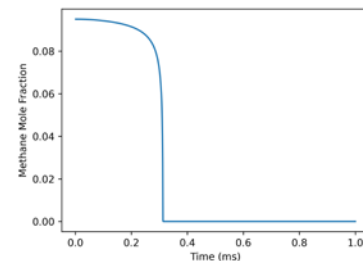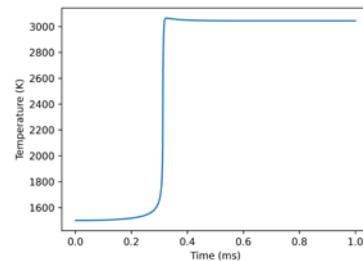
Model Screening

Systematically compare models:

- Prediction strategy: state, derivative, or trajectory
- Architectures: artificial neural network, ResNet[1], Neural ODE[2]
- Hyperparameters: width, depth, activation function, dropout rate

Training Data

- Methane combustion runs using Cantera[3]
- Based on GRI-Mech 3.0[4] reaction mechanism
- 125 combustion runs

Methane combustion at 1500 K, 5 atm, ϕ = 1 using Cantera.

[1] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition, 2015.
[2] Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. Neural ordinary differential equations, 2018.
[3] David G. Goodwin, Raymond L. Speth, Harry K. Moffat, and Bryan W. Weber. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. https://www.cantera.org, 2021.Version 2.5.1.
[4] Gregory P. Smith, David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, C. Thomas Bowman, Ronald K. Hanson, Soonho Song, William C. Gardiner, Jr., Vitali V. Lissianski, and Zhiwei Qin http://www.me.berkeley.edu/gri_mech/

Predictive Approaches

Predict state
- At each timestep, predict next thermodynamic state
- $X_{i+1} = NN(X_i, dt)$

Predict derivative
- Predict time derivative of thermodynamic state and integrate using Euler's method
- $X_{i+1} = X_i + NN(X_i)*dt$

Predict trajectory
- Wrap architecture of choice in a recurrent neural network (RNN)
- Define hidden state to be the thermodynamic state
- $X(t) = RNN(X_0, dt)$
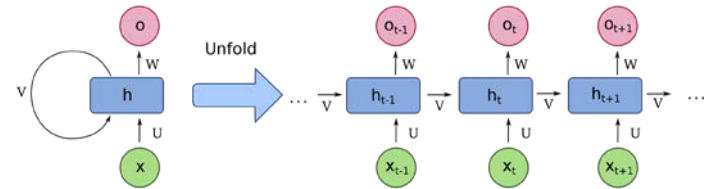
An RNN can time evolve a hidden state (i.e., the thermodynamic state) over many timesteps, yielding a full prediction of the thermodynamic trajectory.

Neural Network Architectures

Artificial Neural Network (ANN)

– Limitations with training deep networks
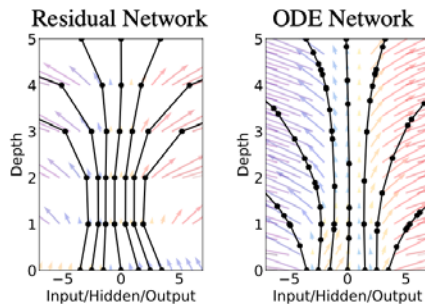
Residual Neural Network (ResNet)[1]

– Skip connections increase the efficiency of training deep networks

Neural ODE[2]

– Structured as an ANN wrapped in an ODE solver
– Functions like a "smart" ResNet with adaptable number of layers
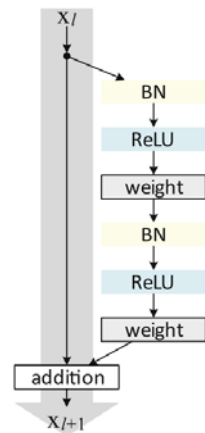
Skip connection in a ResNet.[1]

A neural ODE is a continuous analog to ResNets.[2]

[1] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Identity mappings in deep residual networks, 2016.
[2] Ricky T. Q. Chen, Yulia Rubanova, Jesse Bettencourt, and David Duvenaud. Neural ordinary differential equations, 2018.

Optimal Model Identified From Screening

Approach

– Predicting trajectories performed best

– Predicting next step yielded reasonable results

– Predicting derivative was unstable
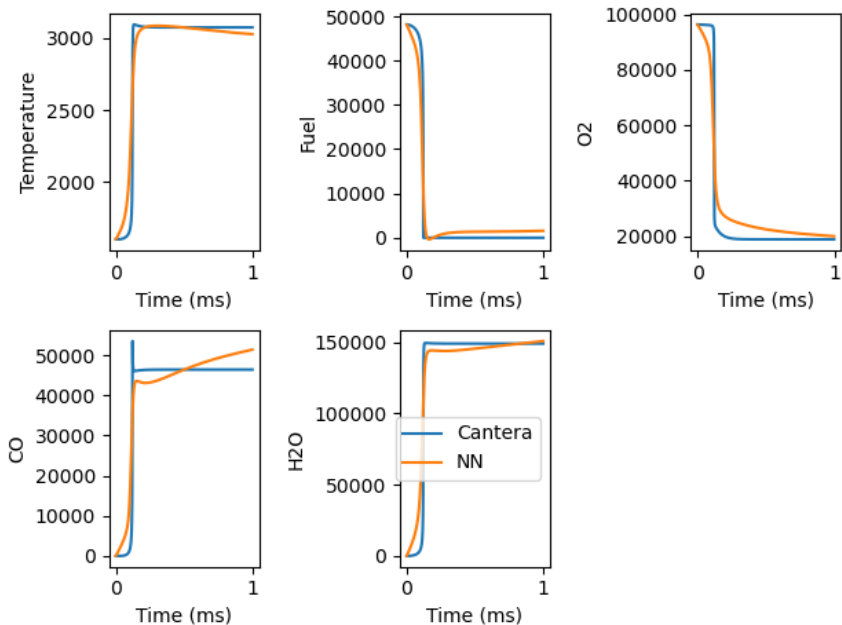
Optimal Model

– ResNet predicting trajectories

– Width 400, Depth 2, tanh activation
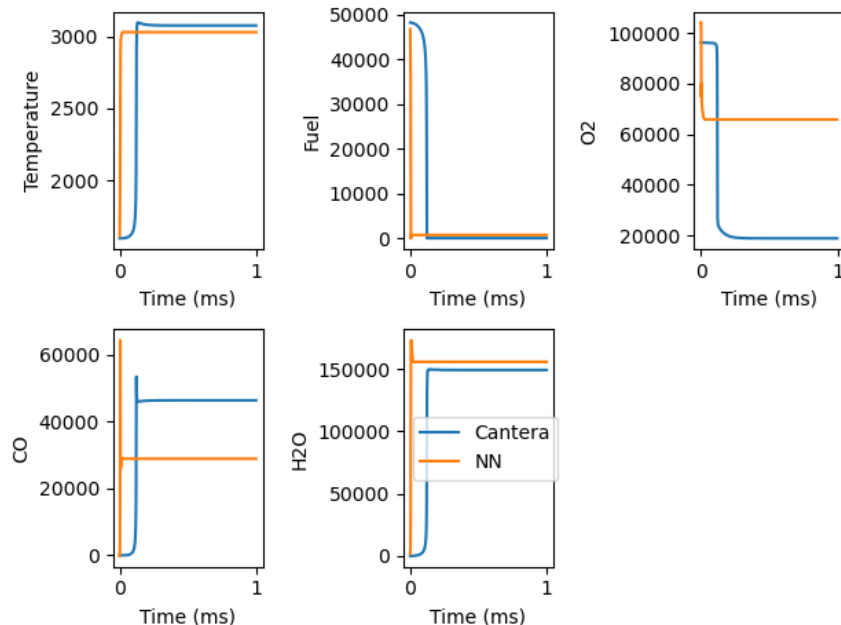
– Demonstrated generalized learning
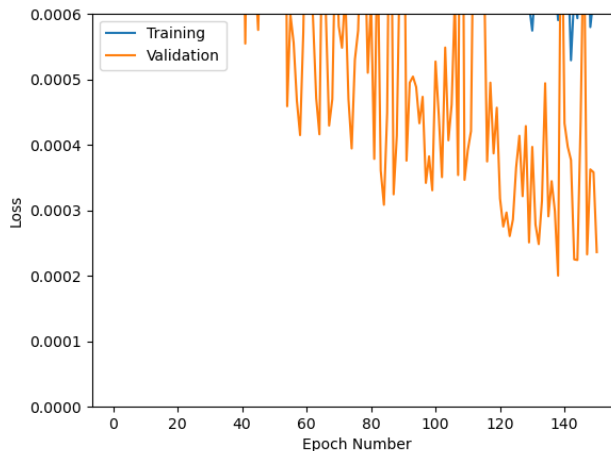
Decreasing validation loss over training.

Prediction on Validation Set
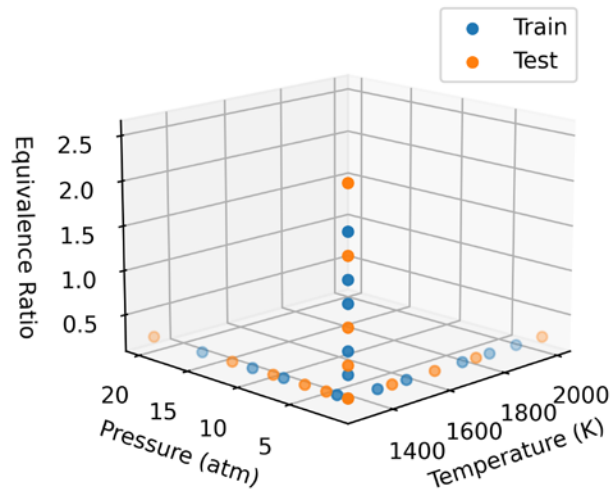
Optimal Model

Best Step-Predicting Model

Optimal Model Study

Evaluate optimal model

– Rigorous training (5 repetitions per model)

– Rigorous testing (125 combustion runs)

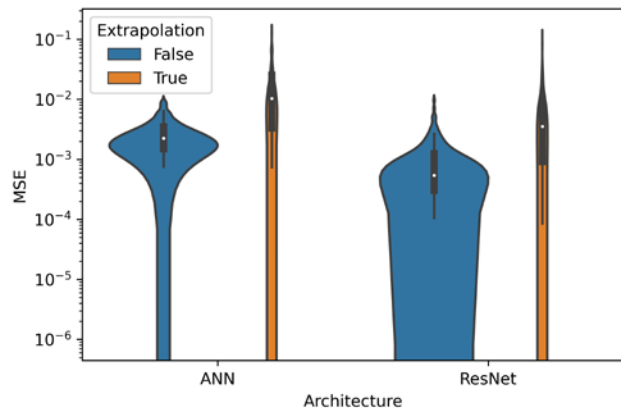**Parameter Sensitivity Analysis**

– Architecture (e.g., width, depth)

– Data (e.g., scaling, species representation)

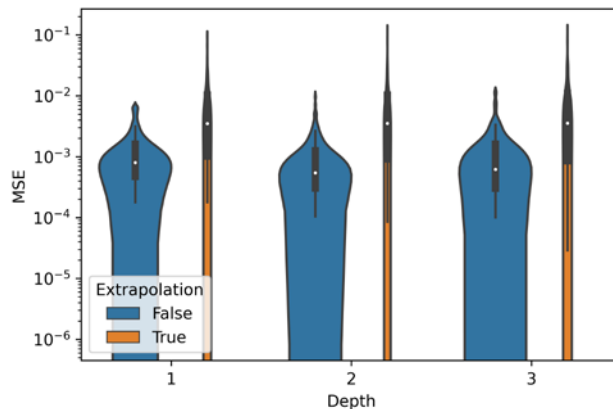– Loss terms (e.g., conservation of mass)

Each dot shows a parameter value used for systematic study.
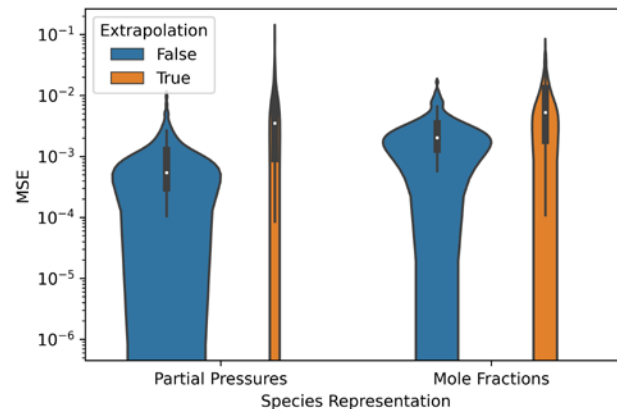
Critical Aspects of Model Design

Our model was shown to be optimal with respect to all tested parameters.
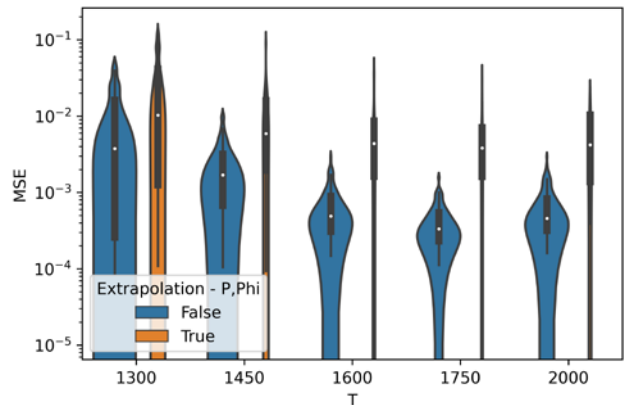

The ResNet is a superior architecture.

Depth of 2 yields good balance between accuracy and speed (42% faster training than depth of 3).
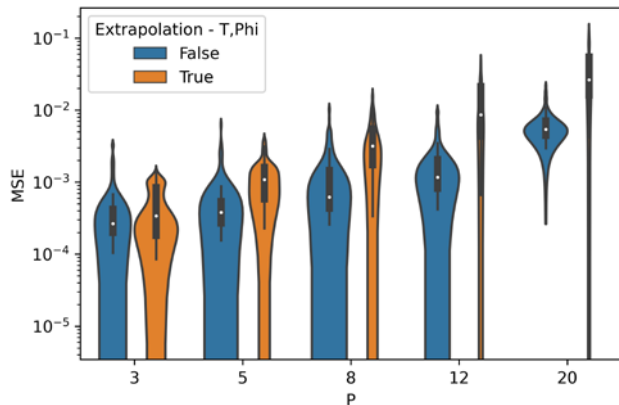
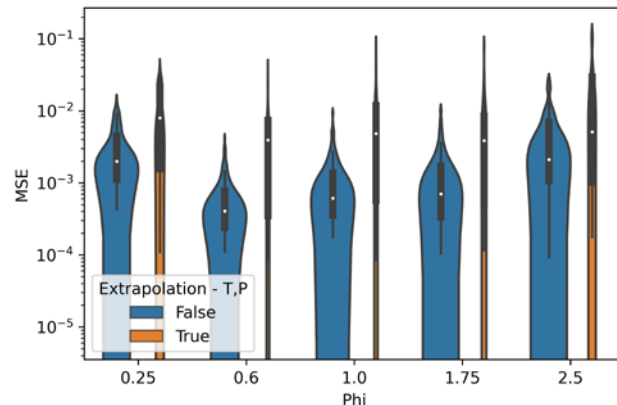*Representing species by their partial pressure is simpler and more accurate.*

Local Accuracy of Model

The model performs better at higher temperatures.

The model performs better at lower pressures.

The model performs better for fuel lean combustion within training data range.

Conclusions and Next Steps

Conclusions

- A neural network was trained to predict the chemical kinetics of methane combustion
- Several predictive strategies were attempted, but the best was predicting the thermodynamic trajectory using a ResNet wrapped in an RNN
- A loss was constructed to help the model to learn conservation of mass

Next steps

- The model will be adapted to handle discontinuities, such as fuel injection or changing volume
- Longer training runs with more data (especially from T,P,ϕ regions with lower accuracy) will be performed in order to increase accuracy

Thank you!

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