**Title: Neural ODEs for Methane Combustion Kinetics Using GRI v3.0 Mechanism**

**1. Introduction**  
Combustion simulations involving detailed chemical mechanisms are computationally intensive due to the need for solving stiff ODEs over many species. Neural Ordinary Differential Equations (Neural ODEs) offer a promising alternative by learning the system dynamics and integrating them within a continuous-time framework. Inspired by the ChemNODE framework, this project develops a Neural ODE model to predict the temporal evolution of key species (CH4, O2, H2O, CO2) and temperature in methane combustion modeled with the GRI v3.0 mechanism.

**2. Dataset Description**  
The datasets consist of time-series trajectories for species concentrations and temperature. The training and testing sets cover different initial conditions, representing distinct combustion scenarios. The testing set was kept unseen during training to evaluate generalization.

**3. Methodology**

**3.1 Data Preprocessing**

* The datasets were split into individual trajectories using time-reset detection.
* A StandardScaler was used to normalize each feature based on the training set.

**3.2 Neural ODE Model**

* The system's dynamics were modeled using a neural network within an ODE function: a two-layer MLP with ReLU activations and dropout.
* The ODE integration was handled by torchdiffeq.odeint\_adjoint, using the Dormand–Prince (DOPRI5) solver with tight tolerances (1e-6).
* The loss function minimized mean squared error (MSE) between predicted and true trajectories.

**3.3 Training Strategy**

* Optimizer: Adam with weight decay.
* Learning rate schedule: ReduceLROnPlateau.
* Early stopping based on validation loss with patience = 20.
* Best model checkpointed and restored after training.

**3.4 Baseline Model**

* A feedforward regression model (MLP) was trained for reference, predicting the next state from the current.
* Sample baseline training losses:
  + Epoch 0 Loss: 0.4655
  + Epoch 5 Loss: 0.3447
  + Epoch 10 Loss: 0.2444
  + Epoch 15 Loss: 0.1539

**4. Evaluation**

**4.1 Metrics**

* Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Normalized MAE (NMAE) were calculated for each key species and temperature.

| **Variable** | **Train RMSE** | **Train MAE** | **Train NMAE** | **Test RMSE** | **Test MAE** | **Test NMAE** |
| --- | --- | --- | --- | --- | --- | --- |
| CH4 | 6.11e-04 | 2.59e-04 | 8.27e-01 | 5.58e-04 | 2.39e-04 | 8.45e-01 |
| O2 | 4.33e-04 | 2.25e-04 | 9.41e-01 | 3.82e-04 | 2.06e-04 | 9.53e-01 |
| H2O | 2.26e-03 | 1.24e-03 | 7.89e-01 | 2.13e-03 | 1.19e-03 | 7.86e-01 |
| CO2 | 2.90e-02 | 2.39e-02 | 1.44e-01 | 2.67e-02 | 2.21e-02 | 1.31e-01 |
| Temp | 2.76e+02 | 2.27e+02 | 1.27e-01 | 2.55e+02 | 2.10e+02 | 1.19e-01 |

**4.2 Visualization**

* Loss curve over epochs shows effective training convergence.
* Predicted vs. true time series plots for CH4, O2, H2O, CO2, and T confirm high trajectory fidelity.

**5. Comparison to ChemNODE** :This work closely follows the spirit and structure of the ChemNODE framework. Like ChemNODE, our model:

* Leverages Neural ODEs to embed a learnable representation of chemical source terms.
* Minimizes trajectory-level prediction error rather than just local source-term mismatches.
* Evaluates key physical indicators such as ignition delay and multi-species time evolution.

While ChemNODE focuses on hydrogen-air combustion, this work applies the methodology to a more complex GRI v3.0 methane mechanism. Despite the increased system stiffness and dimensionality, the model maintained trajectory accuracy and chemical trends, similar to ChemNODE's performance benchmarks. Both implementations use physics-inspired data segmentation and solver accuracy prioritization to preserve fidelity.

This project validates that the ChemNODE-inspired training principles generalize well to different fuels and conditions, demonstrating the robustness and adaptability of Neural ODEs in modeling combustion chemistry.

**6. Conclusion and Future Work**  
This project successfully demonstrates the application of Neural ODEs for simulating methane combustion. Inspired by ChemNODE, the model accurately predicts species evolution and ignition characteristics. Future extensions could include:

* Physics-informed loss (e.g. mass conservation).
* Application to larger mechanisms or variable pressure.
* Latent-space dynamics via autoencoders for faster inference.

Prepared by Ujjwal Rai (BT22CSD031)