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Test Cases for Combustion Chemistry in a Isobaric Reactor

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Extreme-Scale Data Science & Analytics (8739)

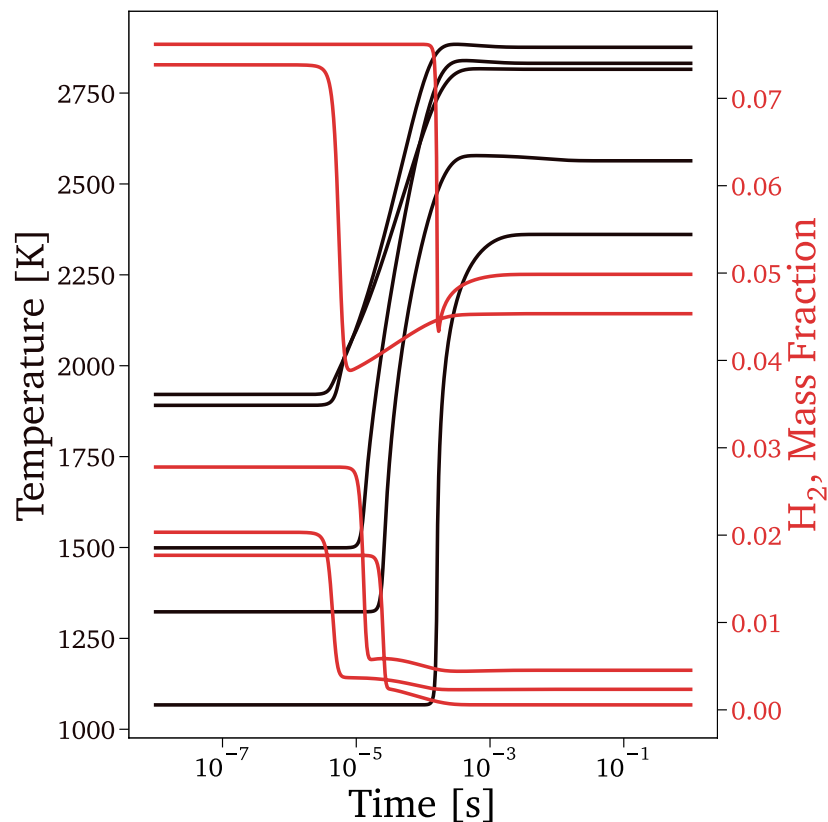


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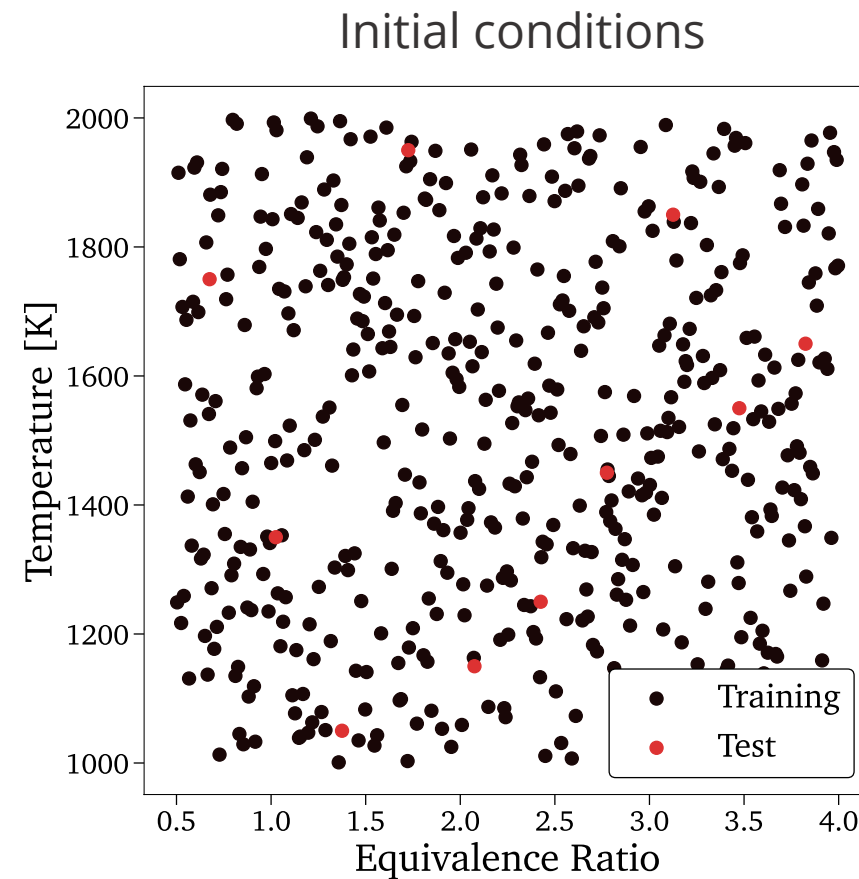
A Combustion Chemistry in Isobaric Reactor Test Case



Isobaric 0-D Reactor (Hydrogen-air), 20 state variables
(i.e., temperature and 19 species mass fractions)



Some training scenarios

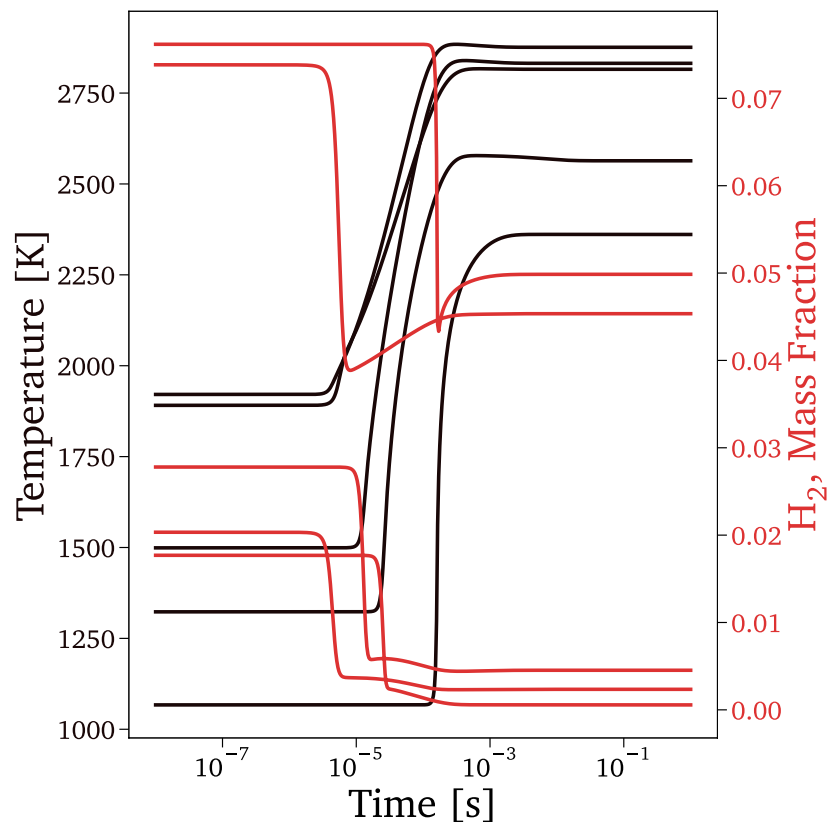


The physical system is implemented in
`$WORKSPACE_PATH/ROMNet/romnet/romnet/pinn/system/0DReact.py`

A Combustion Chemistry in Isobaric Reactor Test Case

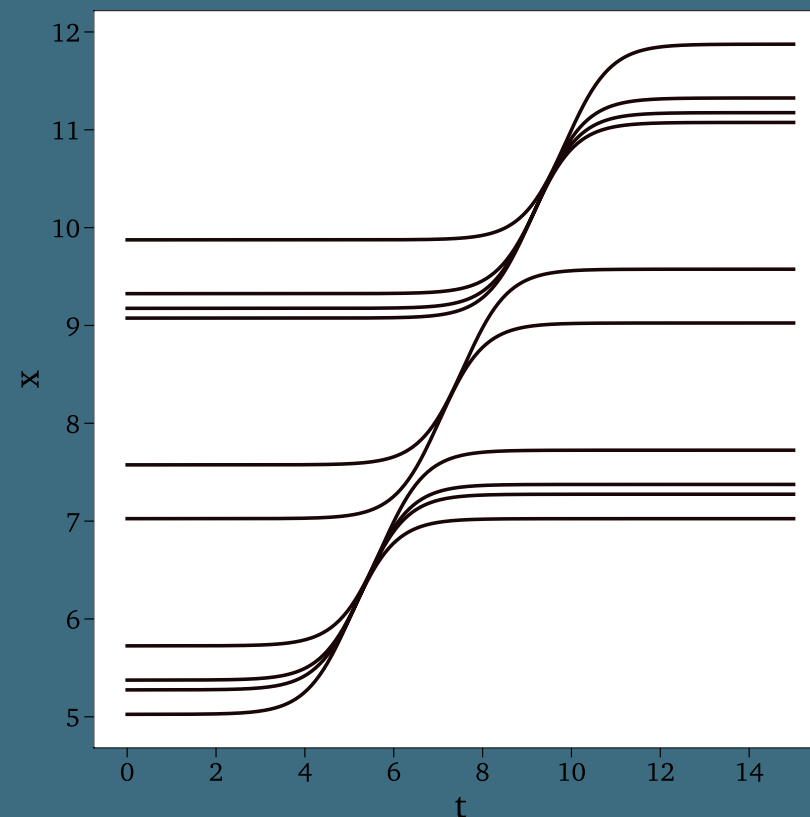


Isobaric 0-D Reactor (Hydrogen-air), 20 state variables
(i.e., temperature and 19 species mass fractions)



Some training scenarios

Note:
Similitudes with
translating hyperbolic tangent



The physical system is implemented in
\$WORKSPACE_PATH/ROMNet/romnet/romnet/pinn/system/0DReact.py

A Combustion Chemistry in Isobaric Reactor Test Case



Run python scrip:

`$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/0DReactor/Generate_Data_1_Isobaric.py`
for generating simulation data

Note: The script needs to be run twice, the second time for generating test data

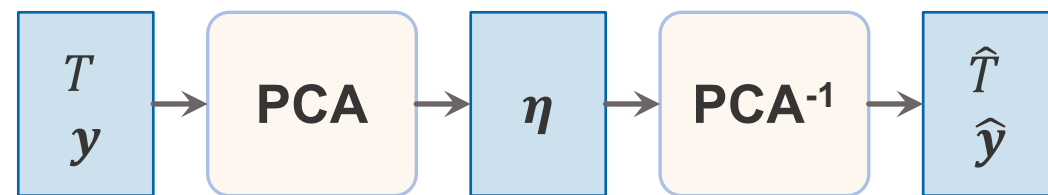
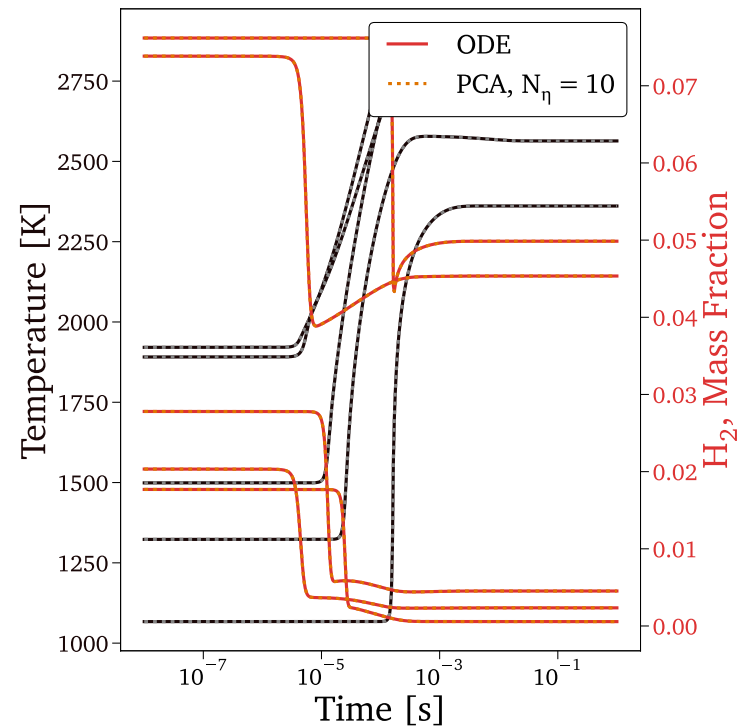
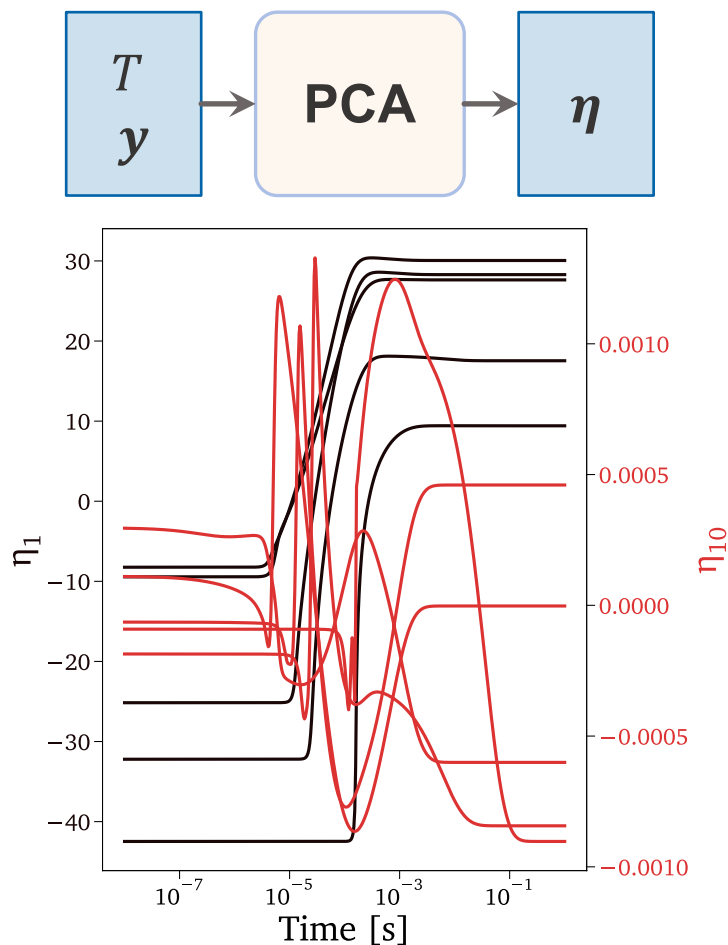
Run Jupyter Notebook:

`$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/0DReactor/Generate_Data_3_Isobaric.ipynb`
for generating training and test data

A Combustion Chemistry in Isobaric Reactor Test Case



Employed PCA for reducing the dimensionality of the state space



10 principal components (η) are sufficient for good accuracy

A Combustion Chemistry in Isobaric Reactor Test Case



Run python scrip:

`$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/0DReactor/Generate_Data_2_Isobaric.py`
for generating PCA simulation data

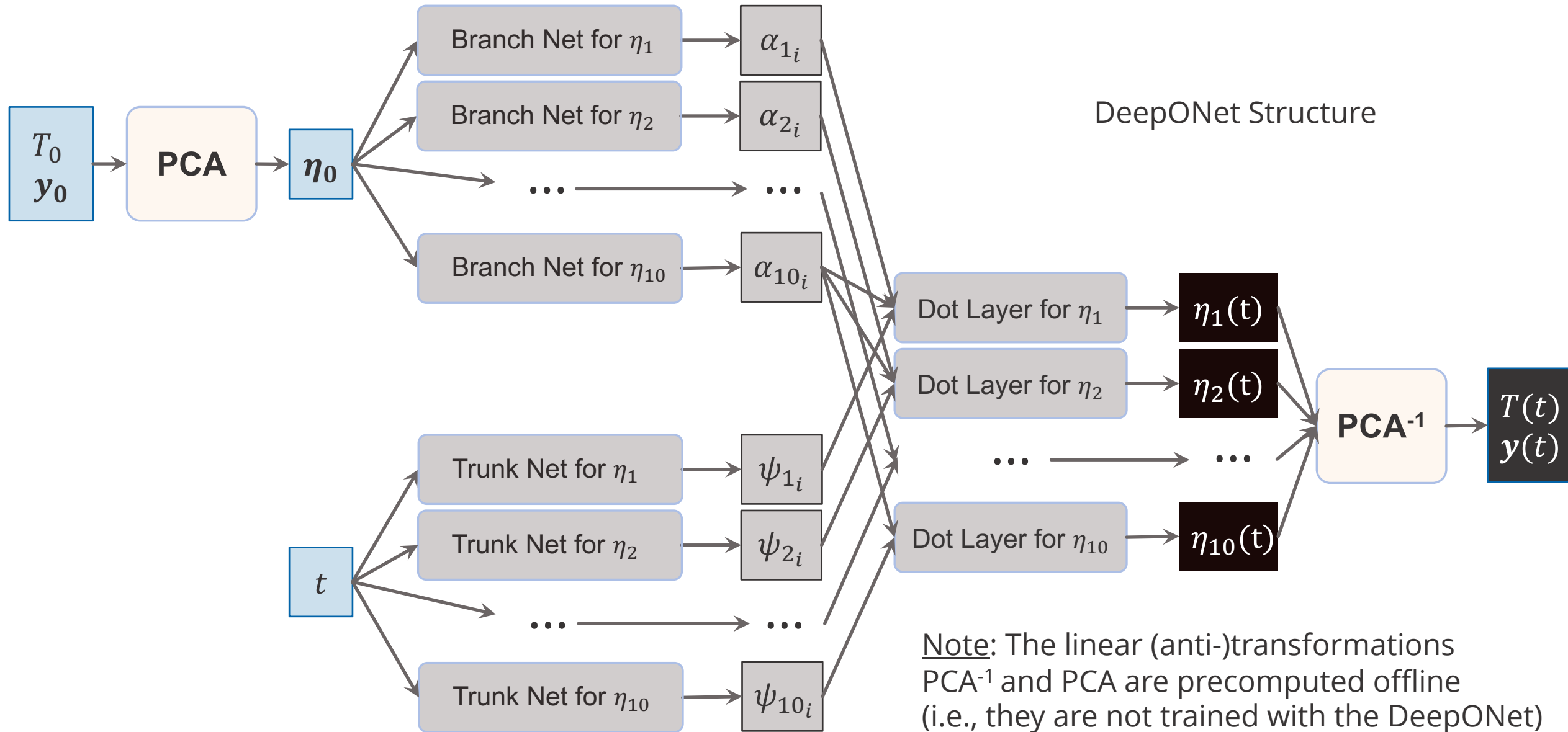
Note: The script needs to be run twice, the second time for generating test data

Run Jupyter Notebook:

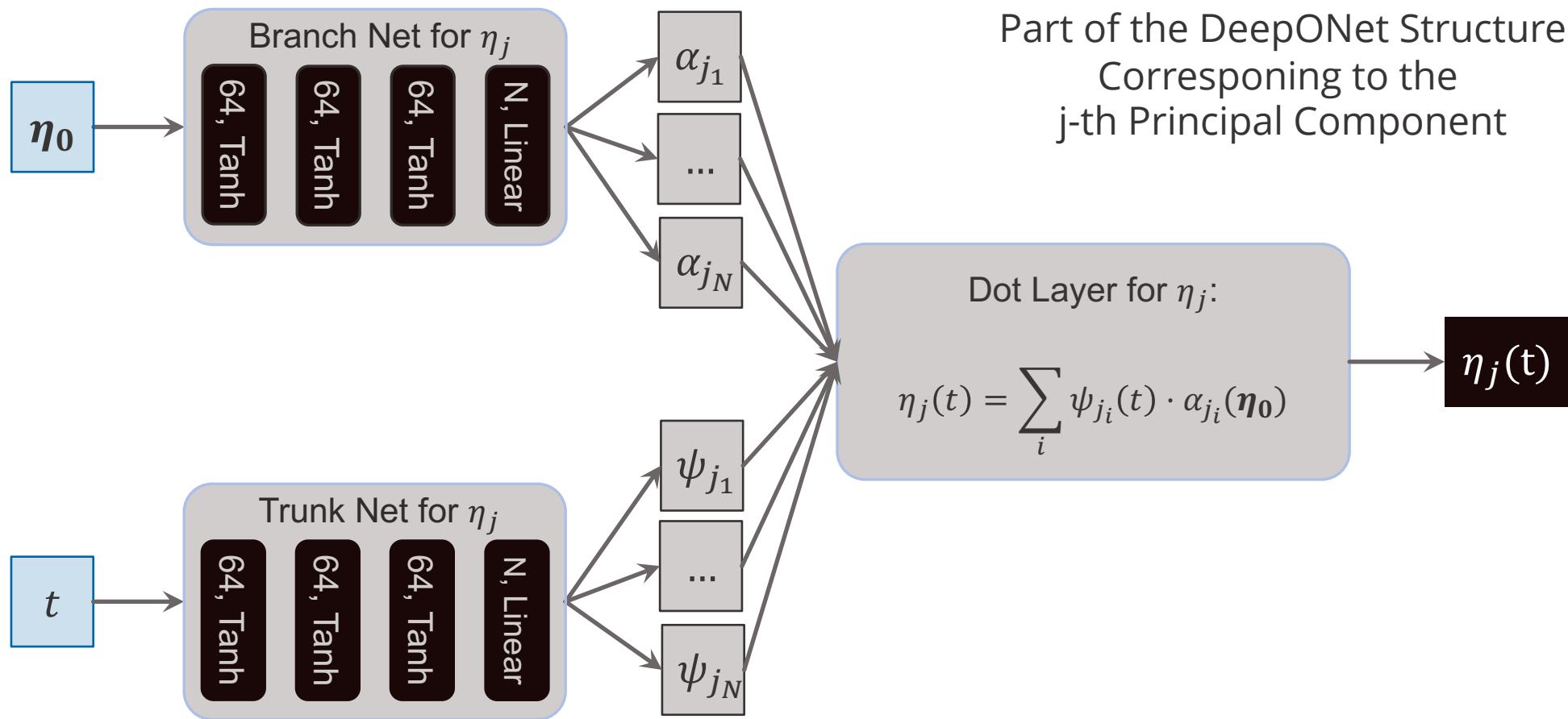
`$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/0DReactor/Generate_Data_4_Isobaric.ipynb`
for generating PCA training and test data

Test Case 9

A Combustion Chemistry in Isobaric Reactor Test Case



A Combustion Chemistry in Isobaric Reactor Test Case



After being trained (even with large number of data and large number of neurons, N),
the DeepONet generates highly oscillatory predictions

A Combustion Chemistry in Isobaric Reactor Test Case



Test Case 9: Data-driven deep operator network (DeepONet) for predicting Principal Components

- 9.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/ODReact/DeepONet/TestCase9/ROMNet_Input.py to \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py
- 9.2. In \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py, change:
 - 9.2.1. "self.WORKSPACE_PATH = ..."
- 9.3. Move to \$WORKSPACE_PATH/ROMNet/romnet/app/
- 9.4. Run: "python3 ROMNet.py ../input/"
- 9.5. Postprocess results via: \$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/ODReact/DeepONet/Predict_DeepONet.ipynb

A Combustion Chemistry in Isobaric Reactor Test Case



Investigating the issue: a principal component analysis

Aggregation of training scenarios for $\eta_j(t)$, where i represents the scenario index:

$$\mathbf{H}_j = \begin{bmatrix} | & | & \cdots & | & | \\ \eta_{j1} & \eta_{j2} & \cdots & \eta_{j499} & \eta_{j500} \\ | & | & & | & | \end{bmatrix}$$

$$\dim(\mathbf{H}_j) = N_t \times N_s$$

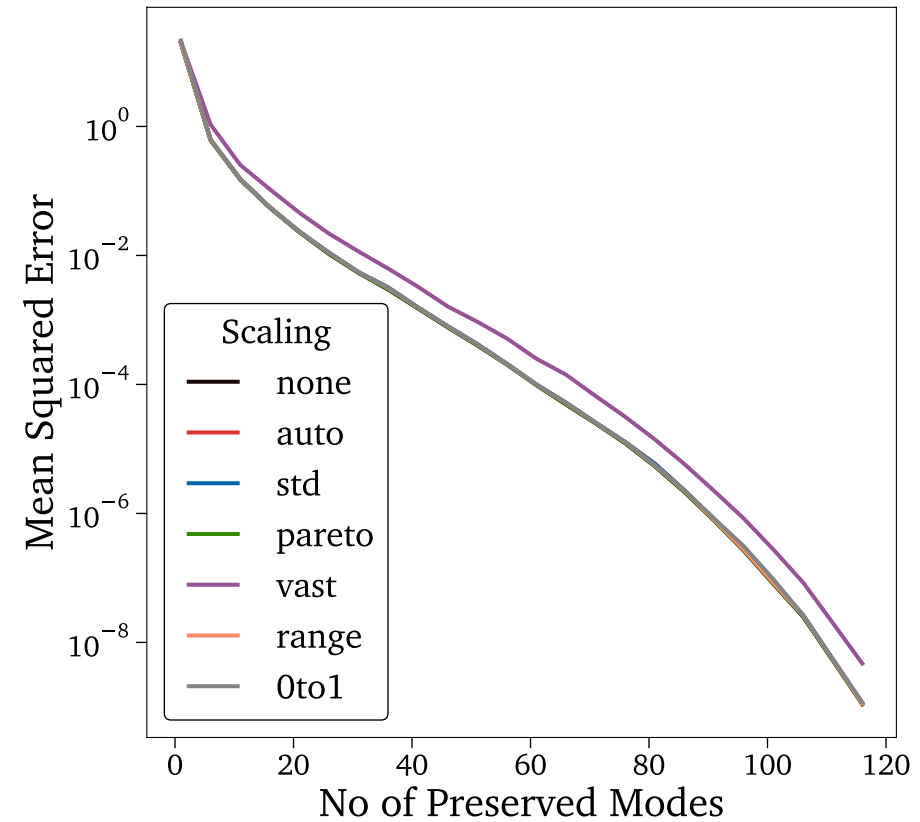
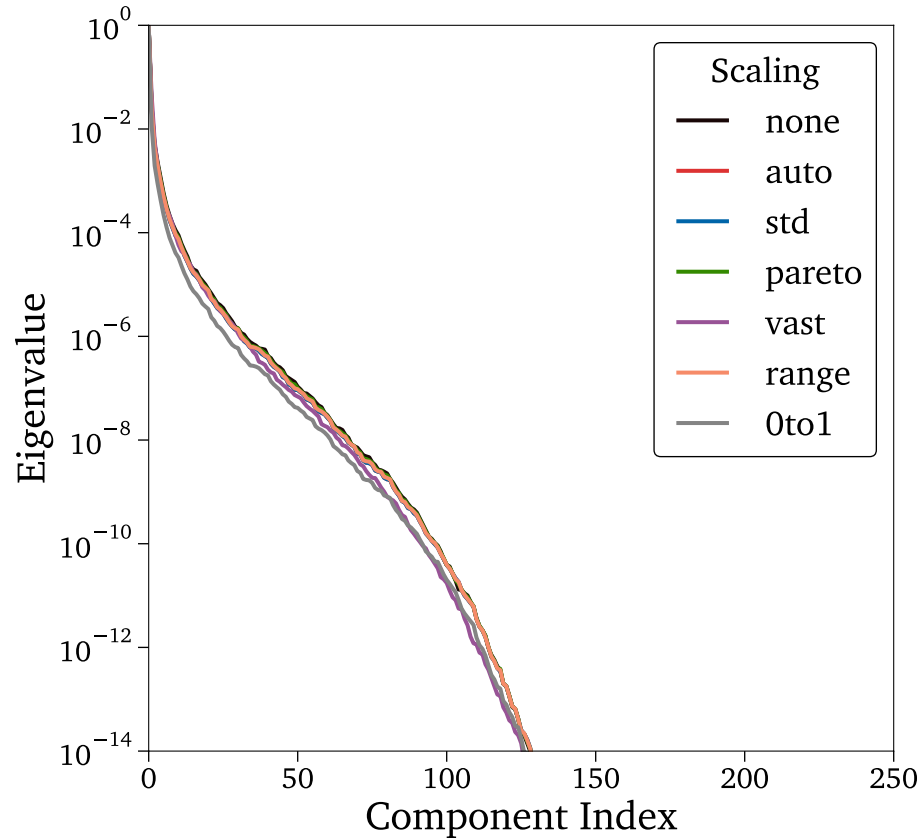
No. time
instants

No. of
scenarios

A Combustion Chemistry in Isobaric Reactor Test Case



Eigendecomposition of R_{H_j} : $\Psi_j = \frac{H_j - C_j}{D_j} A_j$ (Note: results are shown for $j = 1$ (i.e., for η_1))

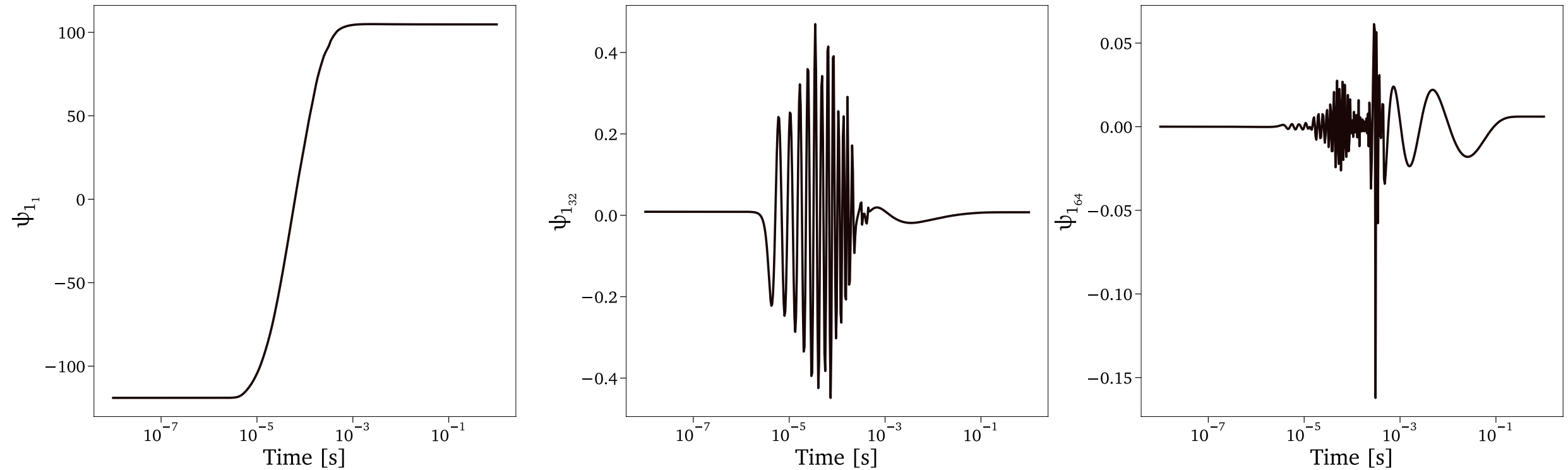


A relatively large number of modes needs to be preserved in order to predict η_j with good accuracy

A Combustion Chemistry in Isobaric Reactor Test Case



Low energy modes are highly oscillatory and hard to be learnt by the DeepONet's trunk nets



A Combustion Chemistry in Isobaric Reactor Test Case

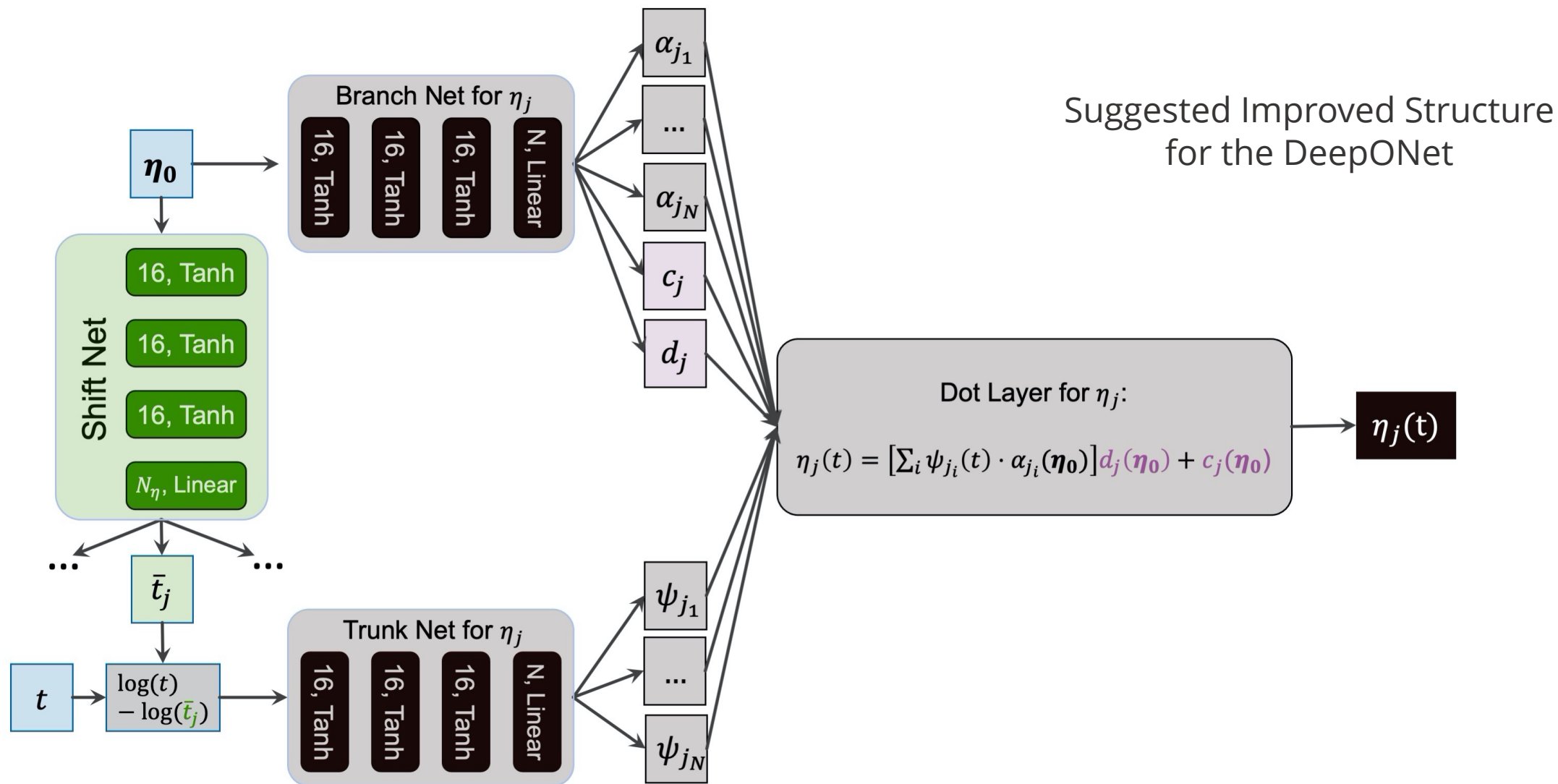


Run Jupyter Notebook:
\$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/0DReactor/Generate_Data_6.ipynb
for generating PCA data



Test Case 10

A Combustion Chemistry in Isobaric Reactor Test Case

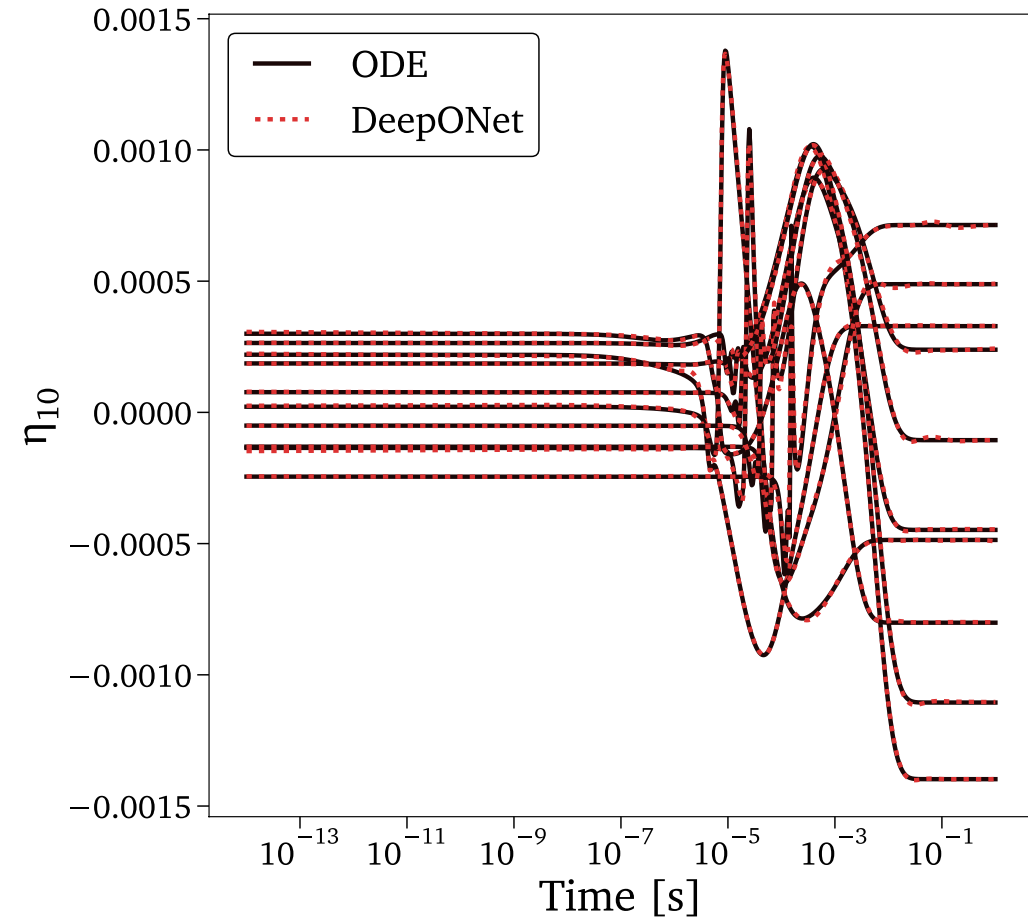
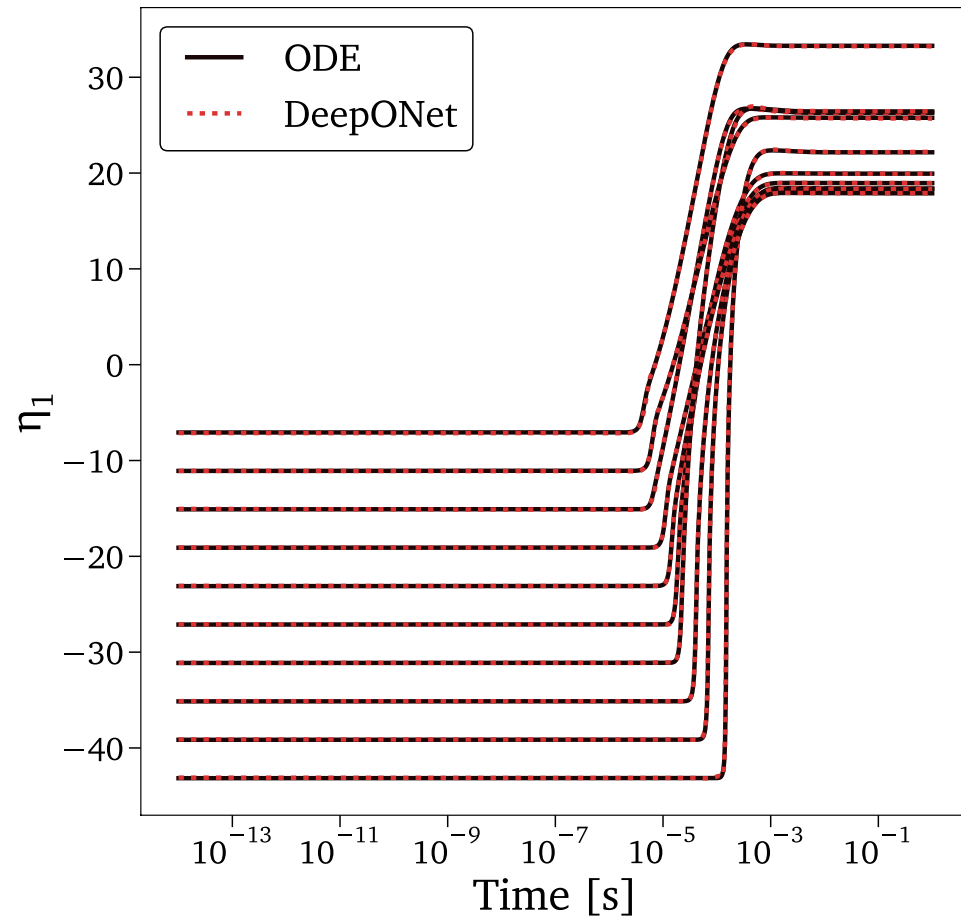


A Combustion Chemistry in Isobaric Reactor Test Case



Results from the improved structure

Predicted time-dependent principal components for test scenarios

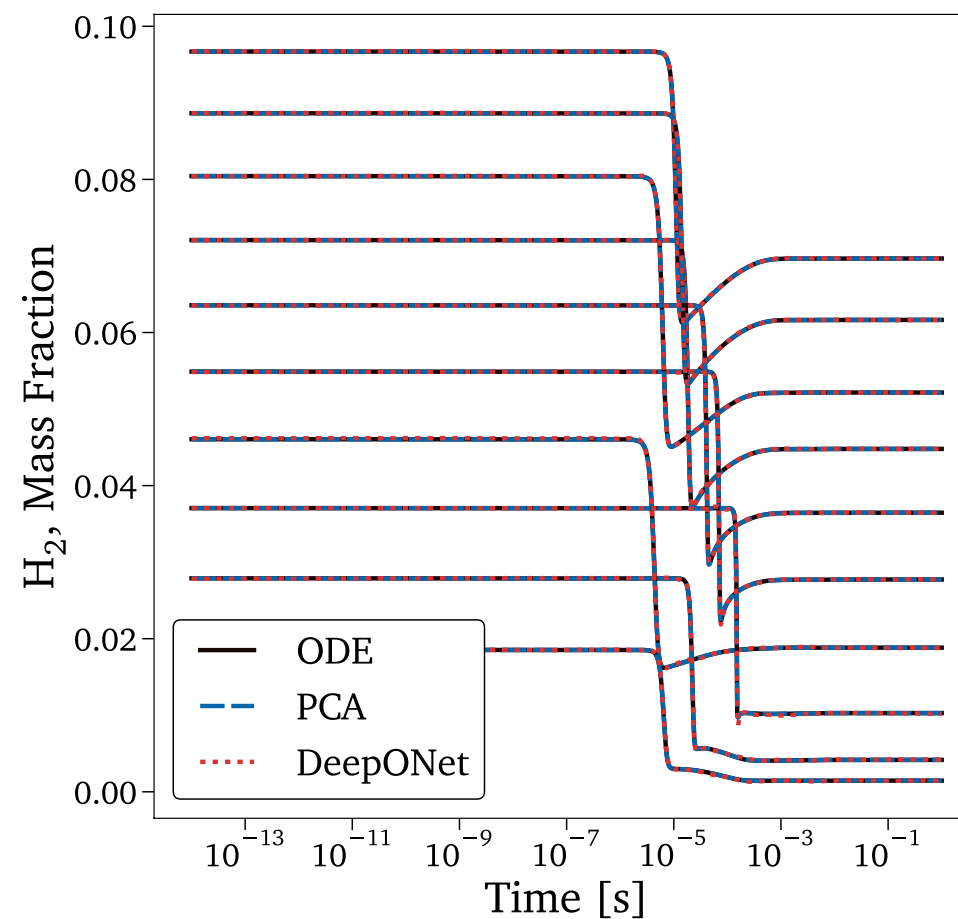
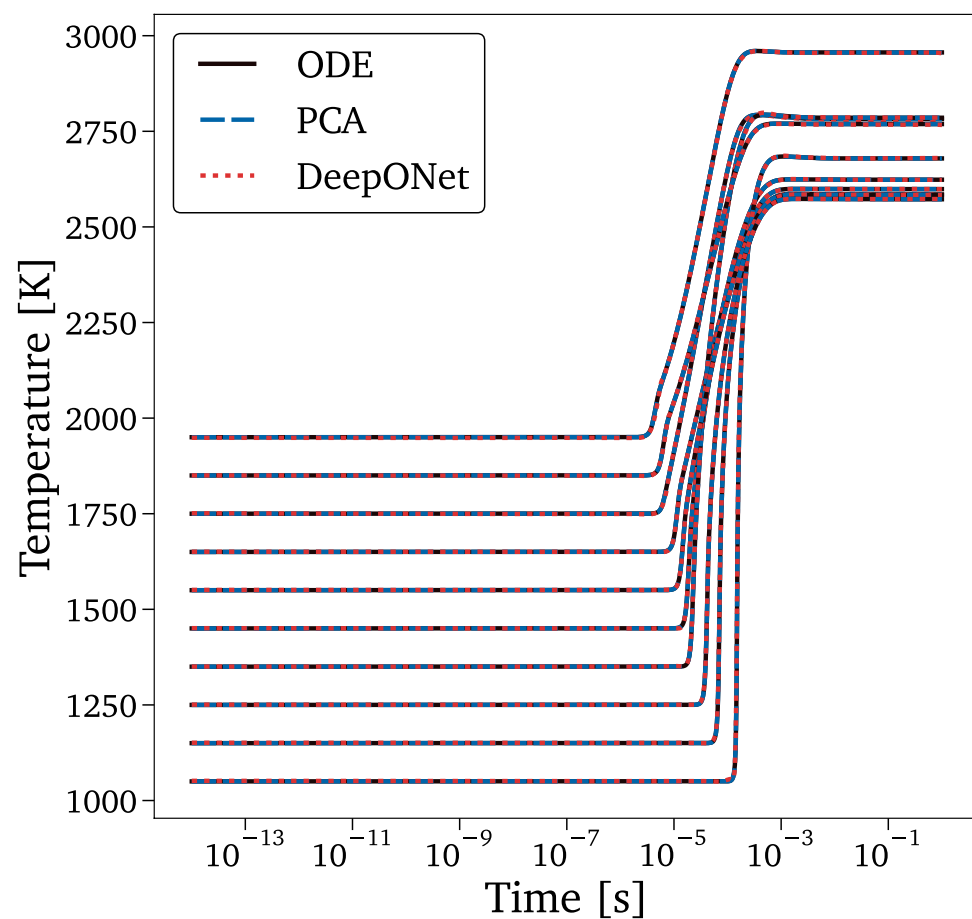


A Combustion Chemistry in Isobaric Reactor Test Case



Results from the improved structure

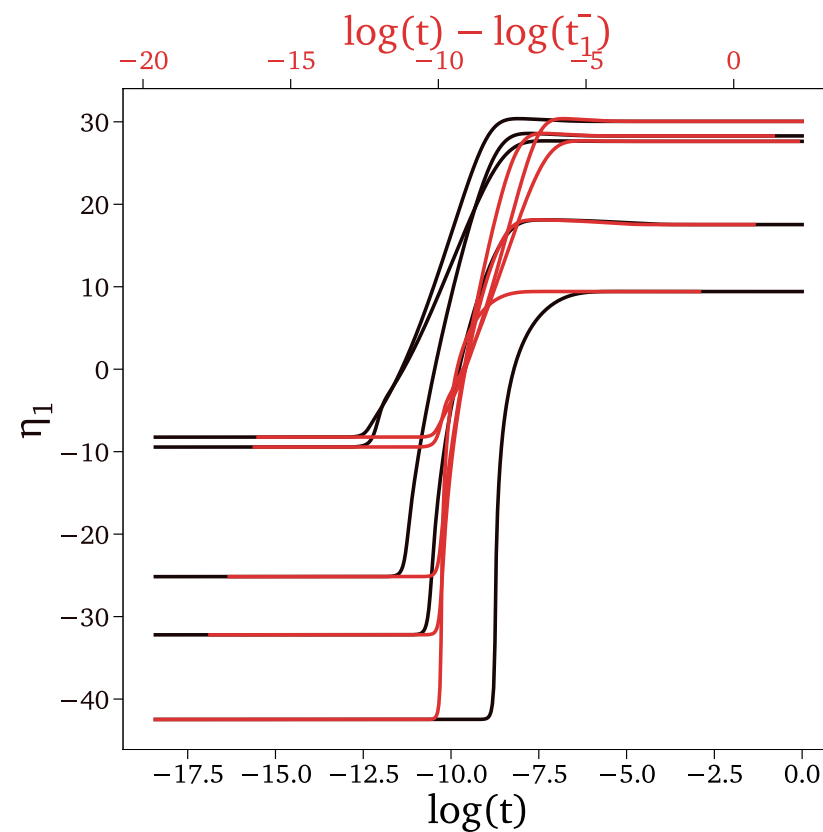
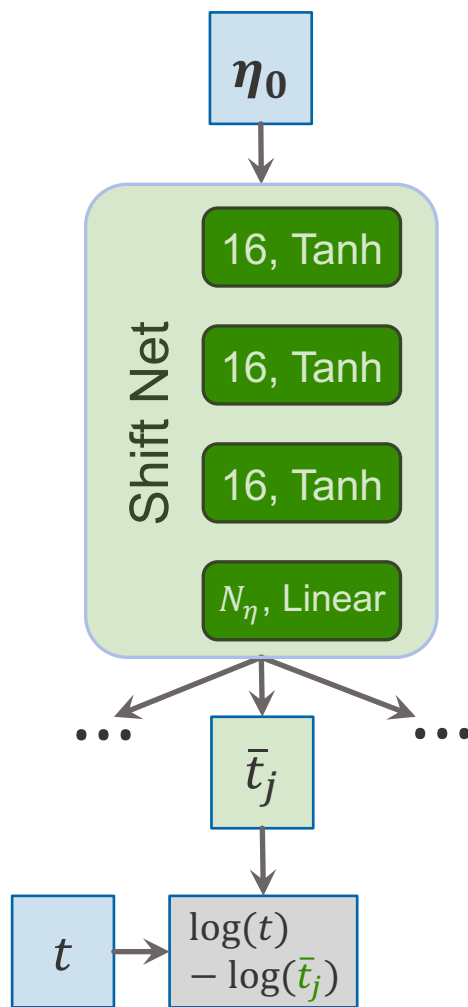
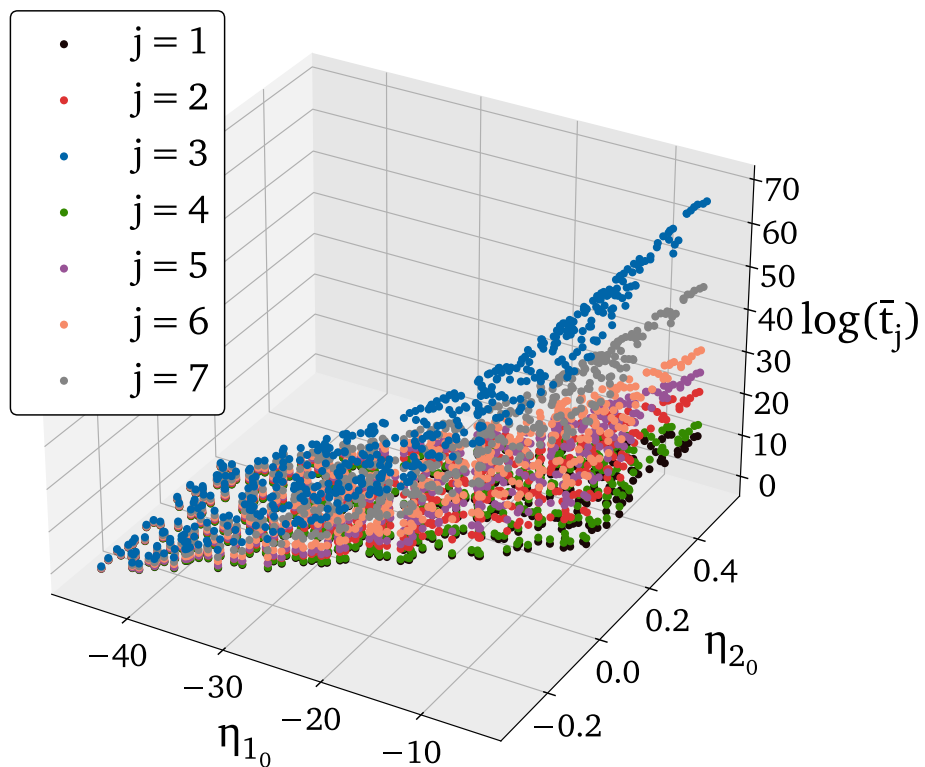
Reconstructed time-dependent temperature and species for test scenarios



A Combustion Chemistry in Isobaric Reactor Test Case



Results from the improved structure





Test Case 10: Data-driven improved deep operator network (DeepONet) for predicting Principal Components

10.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/0DReact/DeepONet/TestCase10/ROMNet_Input.py
to \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py

10.2. In \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py, change:
10.2.1. "self.WORKSPACE_PATH = ..."

10.3. Move to \$WORKSPACE_PATH/ROMNet/romnet/app/

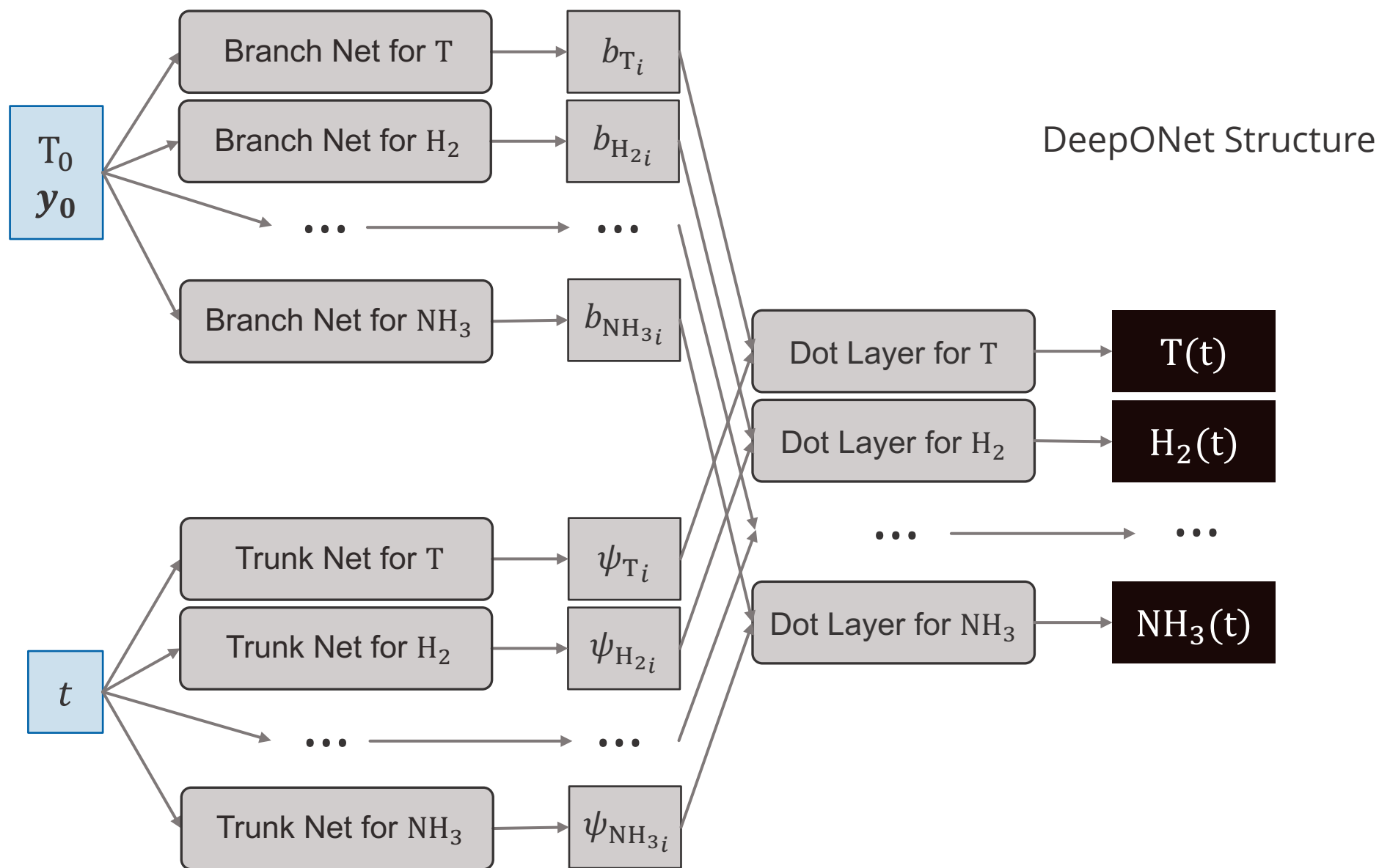
10.4. Run: "python3 ROMNet.py ../input/"

10.5. Postprocess results via: \$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/0DReact/DeepONet/Predict_DeepONet.ipynb

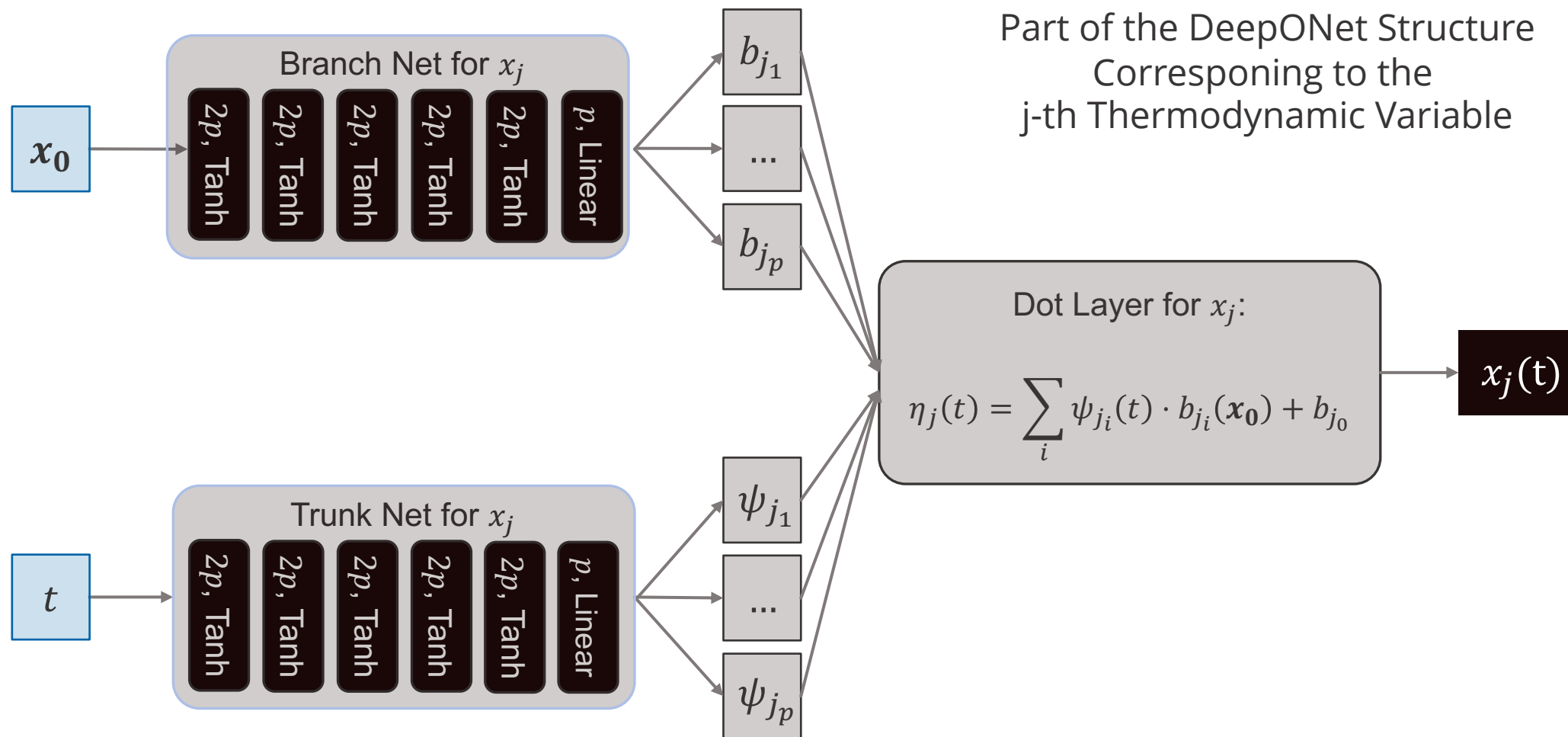


Test Case 11

A Combustion Chemistry in Isobaric Reactor Test Case



A Combustion Chemistry in Isobaric Reactor Test Case



After being trained (even with large number of data and large number of neurons, N),
the DeepONet generates highly oscillatory predictions

A Combustion Chemistry in Isobaric Reactor Test Case



Test Case 11: Data-driven deep operator network (DeepONet) for predicting Thermodynamic Variables

11.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/0DReact/DeepONet/TestCase11/ROMNet_Input.py
to \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py

11.2. In \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py, change:
11.2.1. "self.WORKSPACE_PATH = ..."

11.3. Move to \$WORKSPACE_PATH/ROMNet/romnet/app/

11.4. Run: "python3 ROMNet.py ../input/"

11.5. Postprocess results via: \$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/0DReact/DeepONet/Predict_DeepONet_Orig.ipynb

Relevant Input Variables:

self.data_preproc_type: if `self.norm_input_flg/self.norm_output_flg == True`, then then input/data is center and/or scaled based on the technique specified by **data_preproc_type**.
(Note: auto-scaling is the preset centering and scaling)

self.rectify_flg: If set to True in order to guarantee the positivity of the outputs, a ReLu postprocessing layer is applied at the end of DeepONet.

A Combustion Chemistry in Isobaric Reactor Test Case



Investigating the issue: a principal component analysis

Aggregation of training scenarios for $\mathbf{H}_2(t)$, where i represents the scenario index:

$$\mathbf{H}_2 = \begin{bmatrix} | & | & \dots & | & | \\ \mathbf{H}_{21} & \mathbf{H}_{22} & \dots & \mathbf{H}_{2499} & \mathbf{H}_{2500} \\ | & | & & | & | \end{bmatrix}$$

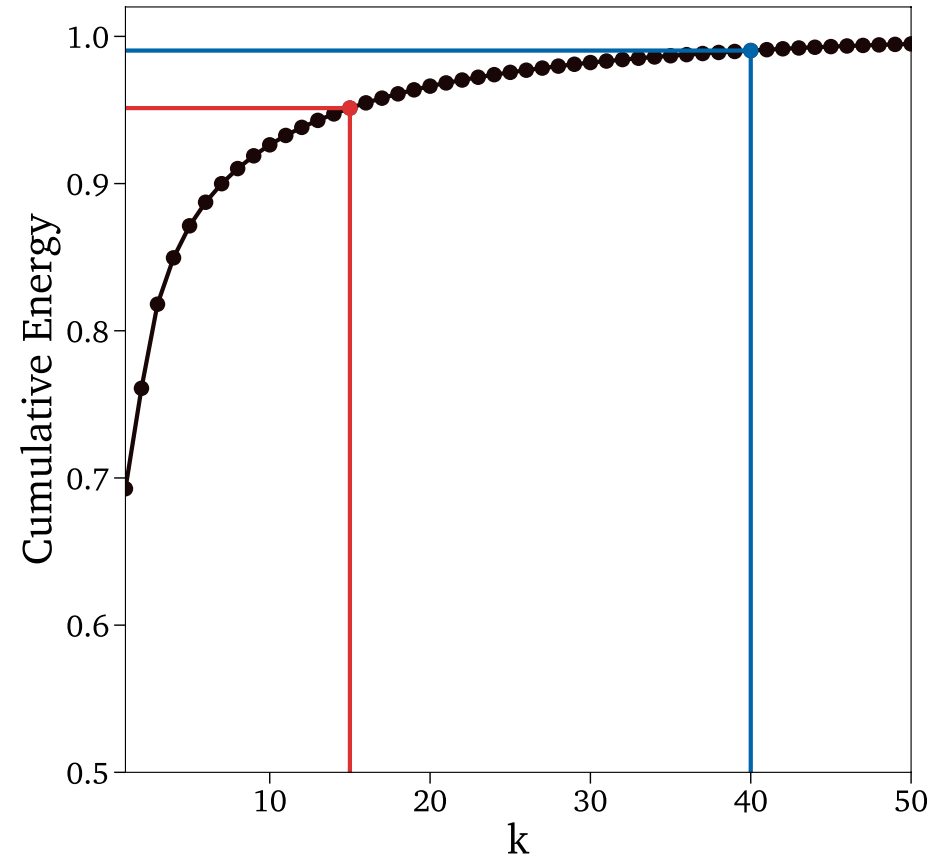
$$\dim(\mathbf{H}_2) = N_t \times N_s$$

No. time
instants No. of
scenarios

A Combustion Chemistry in Isobaric Reactor Test Case



Eigendecomposition of R_{H_2} :
$$\Psi_{H_2} = \frac{H_2 - C_{H_2}}{D_{H_2}} A_{H_2}$$

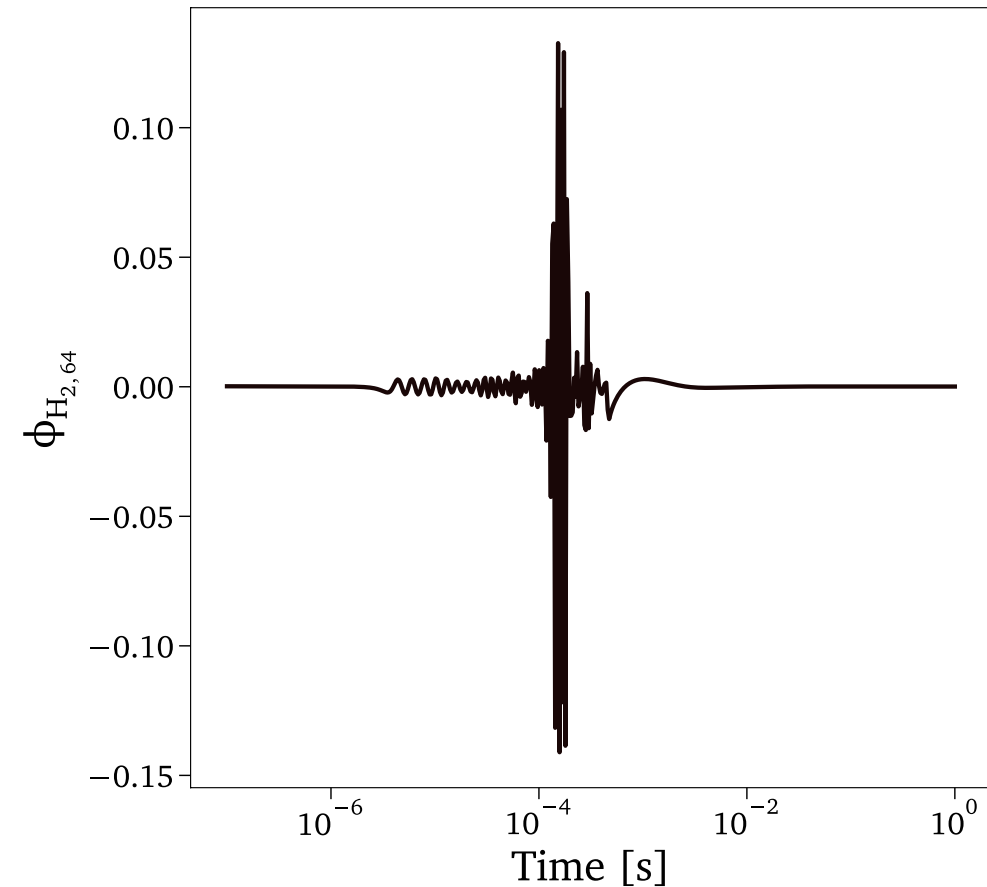
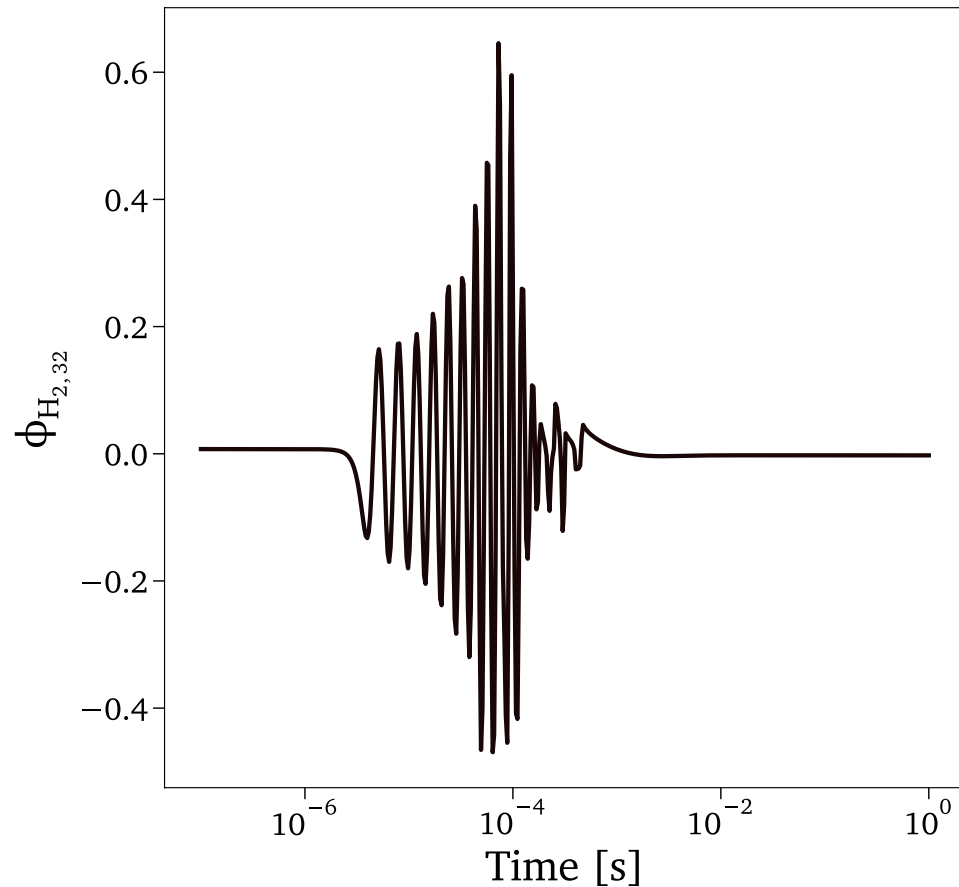


A relatively large number of modes needs to be preserved in order to predict T with good accuracy

A Combustion Chemistry in Isobaric Reactor Test Case



Low energy modes are highly oscillatory and hard to be learnt by the DeepONet's trunk nets



A Combustion Chemistry in Isobaric Reactor Test Case

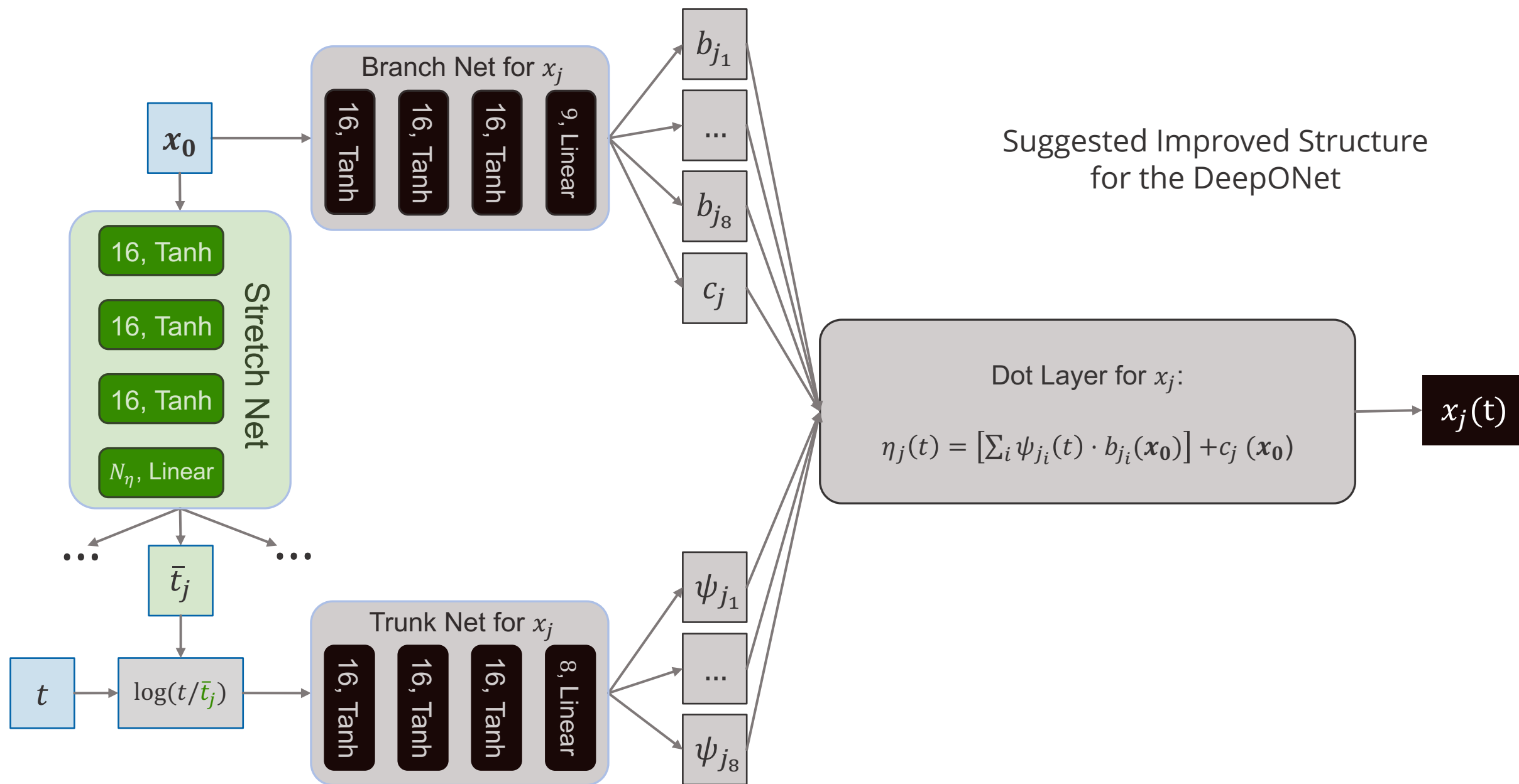


Run Jupyter Notebook:
\$WORKSPACE_PATH/ROMNet/romnet/scripts/generating_data/0DReactor/Generate_Data_5.ipynb
for generating PCA data



Test Case 12

A Combustion Chemistry in Isobaric Reactor Test Case

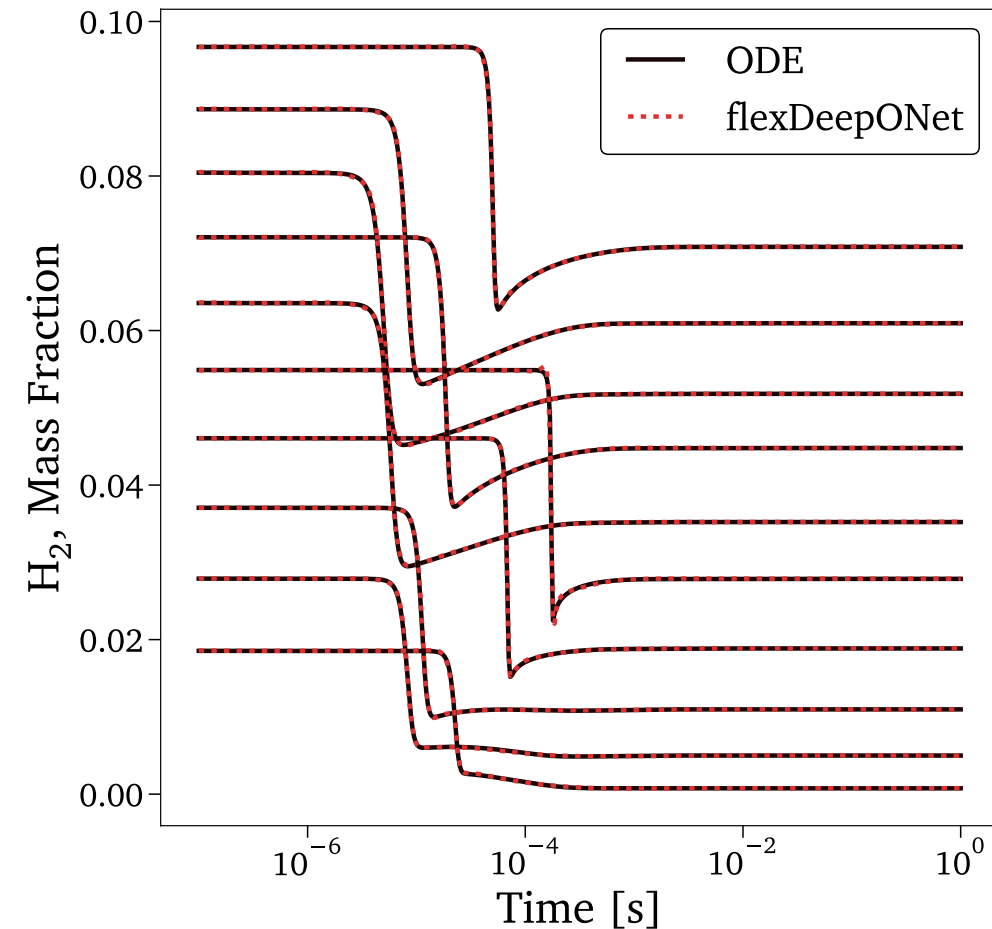
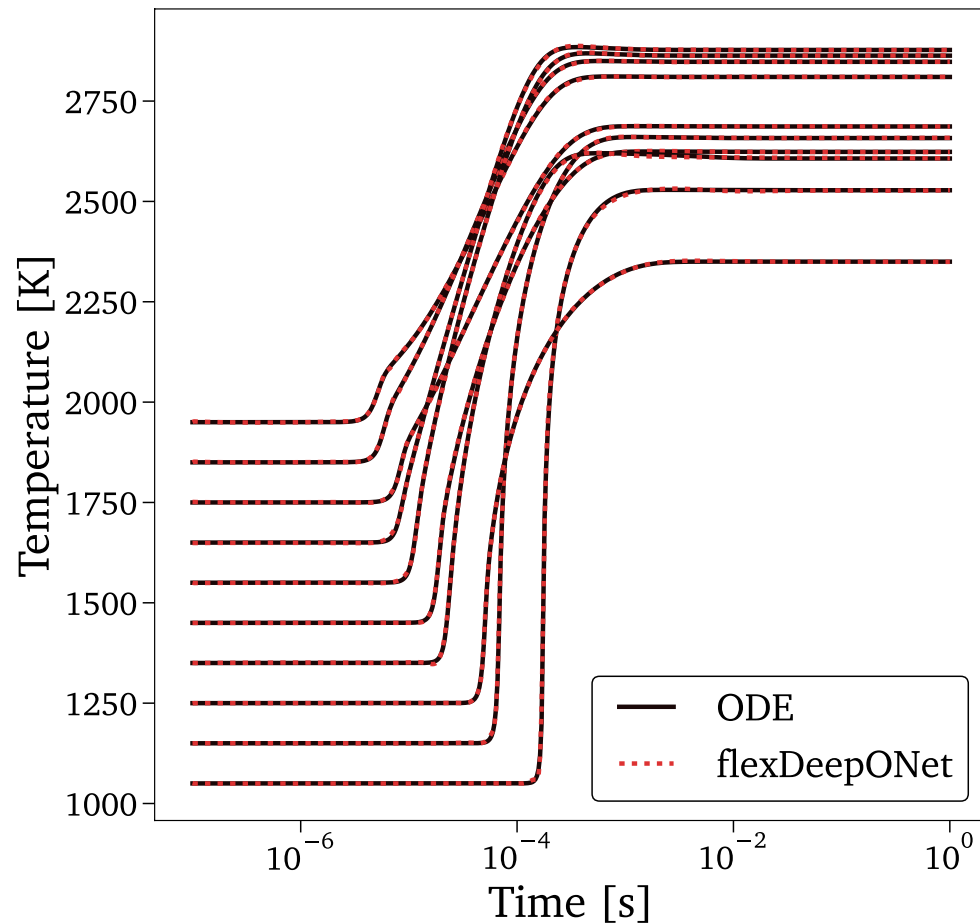


A Combustion Chemistry in Isobaric Reactor Test Case



Results from the improved structure

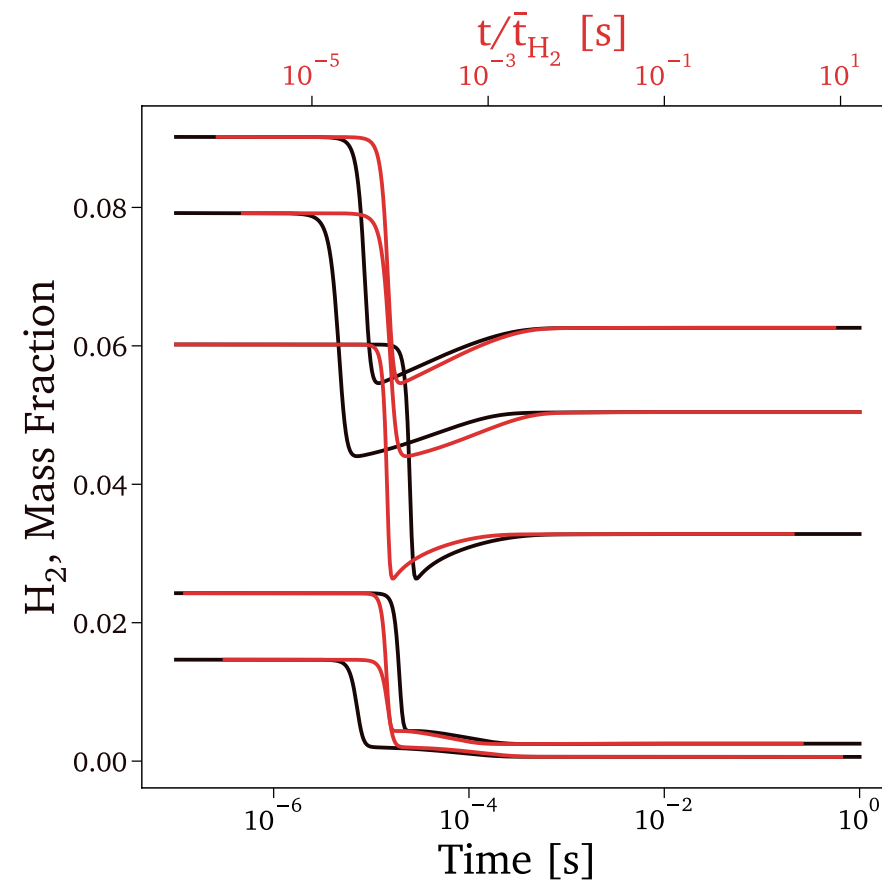
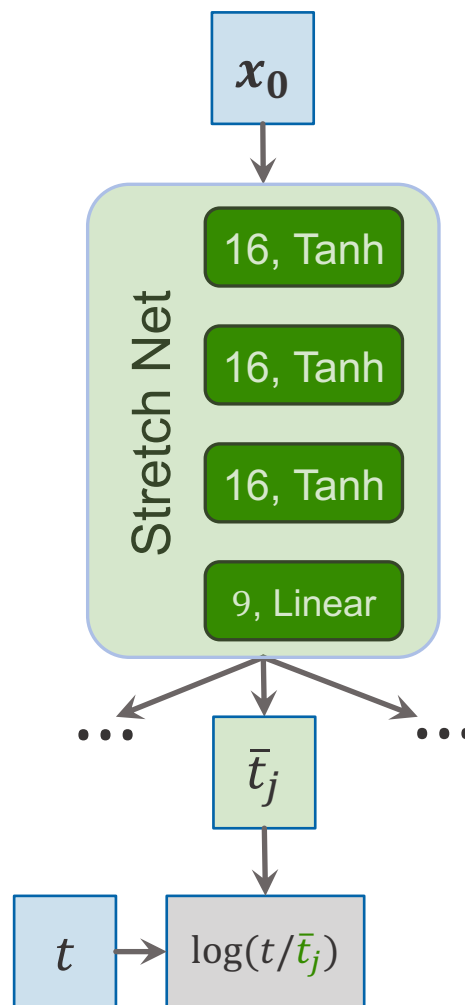
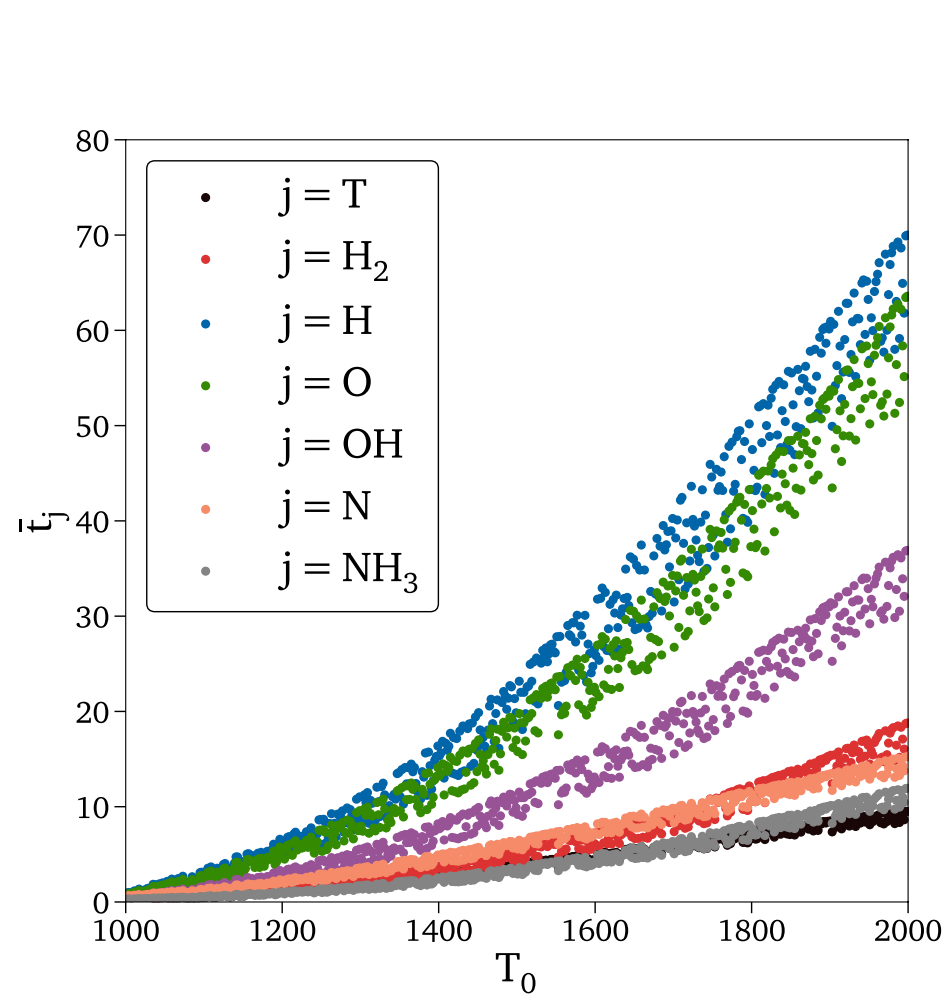
Predicted time-dependent temperature and species for test scenarios



A Combustion Chemistry in Isobaric Reactor Test Case



Results from the improved structure





Test Case 12: Data-driven improved deep operator network (DeepONet) for predicting Thermodynamic Variables

12.1. Copy \$WORKSPACE_PATH/ROMNet/romnet/input/0DReact/DeepONet/TestCase12/ROMNet_Input.py
to \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py

12.2. In \$WORKSPACE_PATH/ROMNet/romnet/input/ROMNet_Input.py, change:
12.2.1. "self.WORKSPACE_PATH = ..."

12.3. Move to \$WORKSPACE_PATH/ROMNet/romnet/app/

12.4. Run: "python3 ROMNet.py ../input/"

12.5. Postprocess results via: \$WORKSPACE_PATH/ROMNet/romnet/scripts/postprocessing/0DReact/DeepONet/Predict_DeepONet_Orig.ipynb

Relevant Input Variables:

self.data_preproc_type: if `self.norm_input_flg/self.norm_output_flg == True`, then then input/data is center and/or scaled based on the technique specified by **data_preproc_type**.
(Note: auto-scaling is the preset centering and scaling)

self.rectify_flg: If set to True in order to guarantee the positivity of the outputs, a ReLu postprocessing layer is applied at the end of DeepONet.