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Constructing Surrogates for Combustion Chemistry: Operator Learning for Reduced Order Dynamics

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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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Motivation

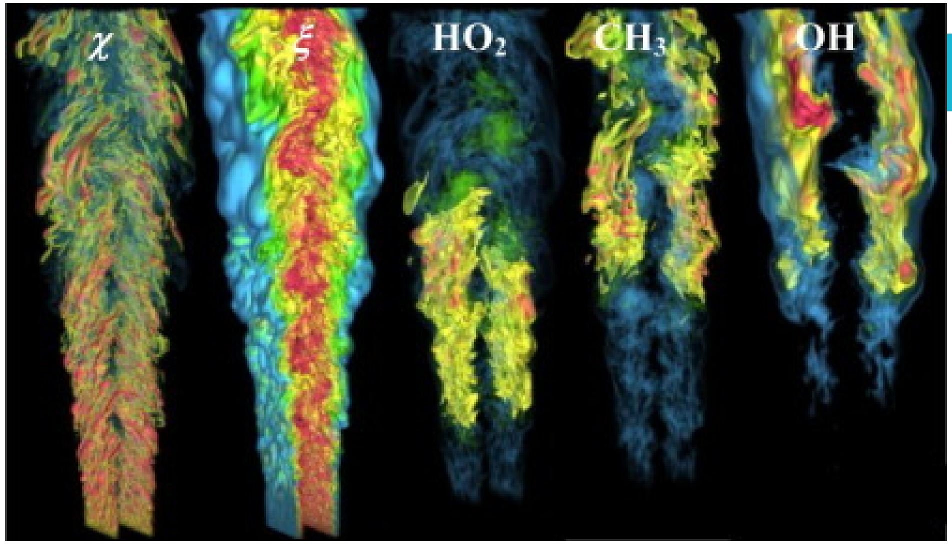
Discovery science

- Scale-resolved reacting flow simulations (e.g. turbulent combustion, fluid plasmas) are incredibly expensive
- Resolution of hydrodynamic scales alone is limiting, and drastically exacerbated by the dimension of the reaction model
- Typically use coarse grained chemical models relying on regime specific hypotheses, heuristics to reduce dimensionality

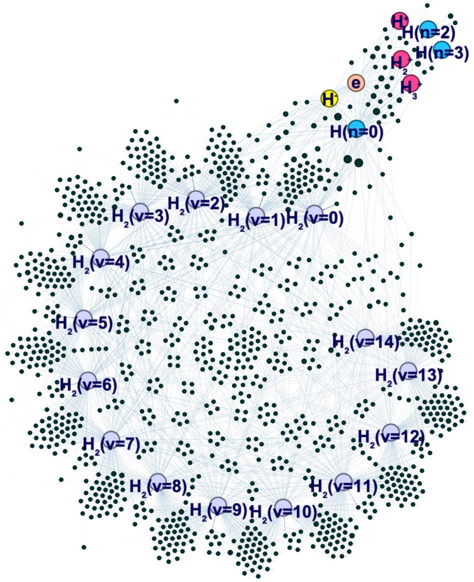
Predictive modeling

- Need accelerators to enable many-query studies
- Want to predict under uncertainty

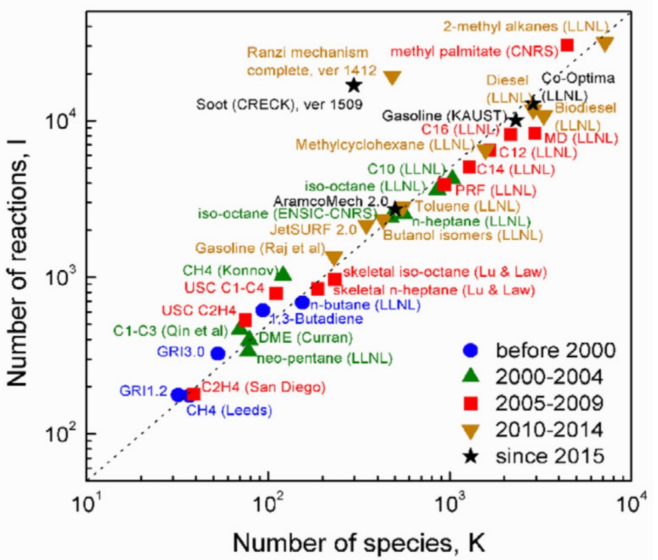
Pursue a data driven reduction for the chemical component, and retain the hydrodynamic model discretization



Chen, Proc. Comb. Inst. [2011]

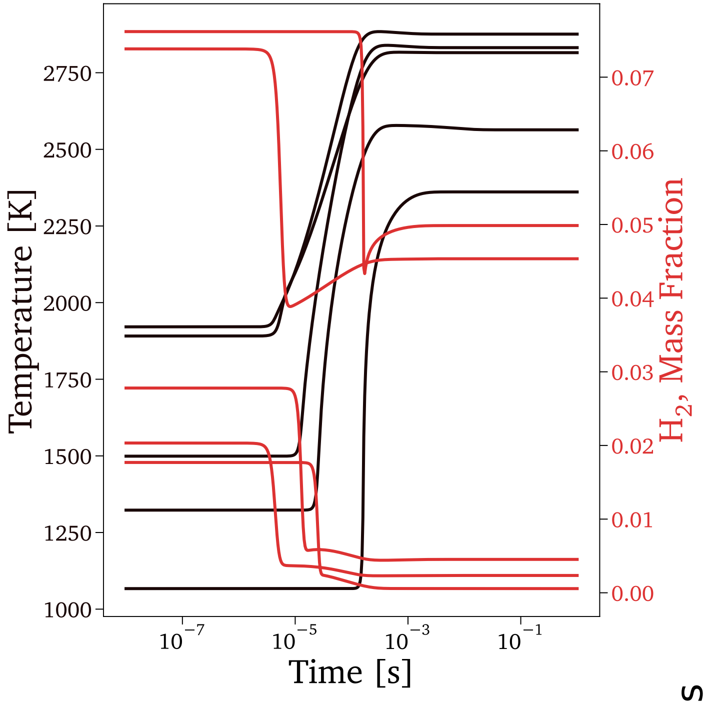


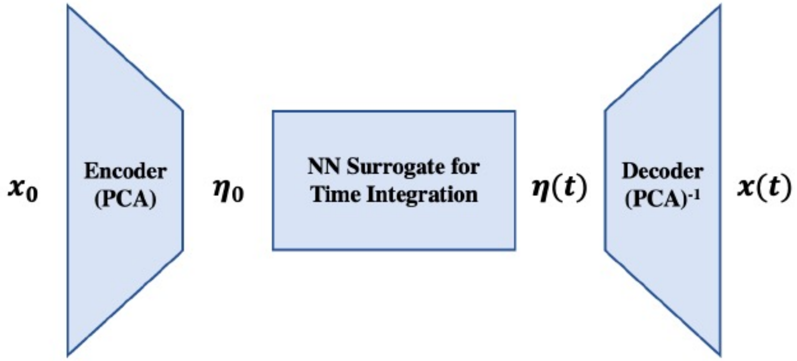
H_2 plasma/excited state chemical reaction network



Mechanism complexity for combustion fuels, Curran et. al. [2019]

H_2-air combustion chemistry: retaining N_η PCs





NN-based surrogate that maps

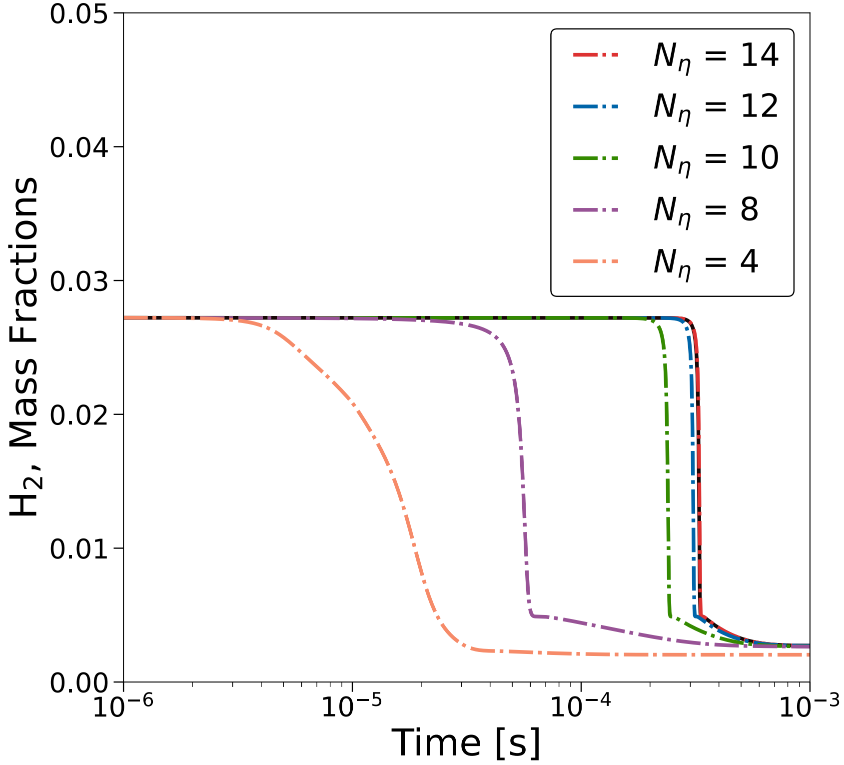
$$\frac{d\boldsymbol{\eta}}{dt} \rightarrow \boldsymbol{\eta}$$

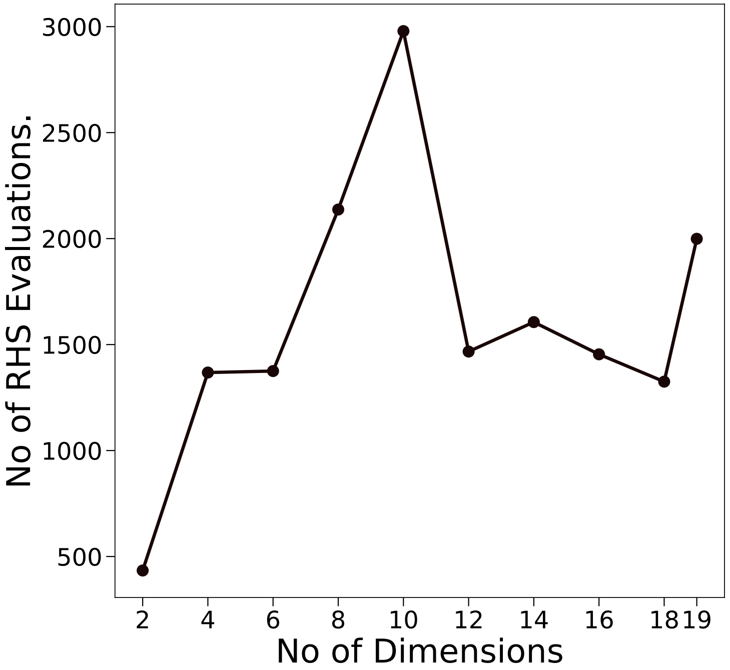
$$\frac{d\eta_1}{dt} = f_{NN}\left(\eta_1, \eta_2, \ldots, \eta_{N_\eta}\right)$$

$$\frac{d\eta_2}{dt} = f_{NN}\left(\eta_1, \eta_2, \ldots, \eta_{N_\eta}\right)$$

$$\ldots$$

$$\frac{d\eta_{N_\eta}}{dt} = f_{NN}\left(\eta_1, \eta_2, \ldots, \eta_{N_\eta}\right)$$





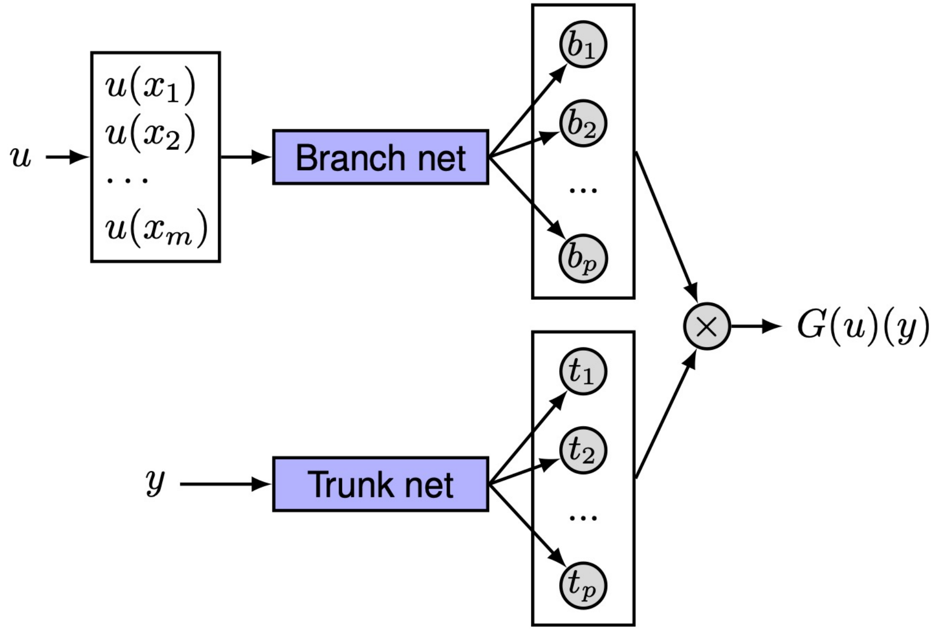
Operator Learning: DeepOnet

- We are interested in advancing the chemical state in time, not necessarily by surrogating source terms

Universal approximation theorem of operators [1]

$$\left| G(u)(y) - \sum_{k=1}^{p}\underbrace{\sum_{i=1}^{n} c_i^k \sigma\left(\sum_{j=1}^{m}\xi_{ij}^k u(x_j)+\theta_i^k\right)}_{\text{branch}} \underbrace{\sigma(w_k\cdot y+\zeta_k)}_{\text{trunk}}\right| < \epsilon$$

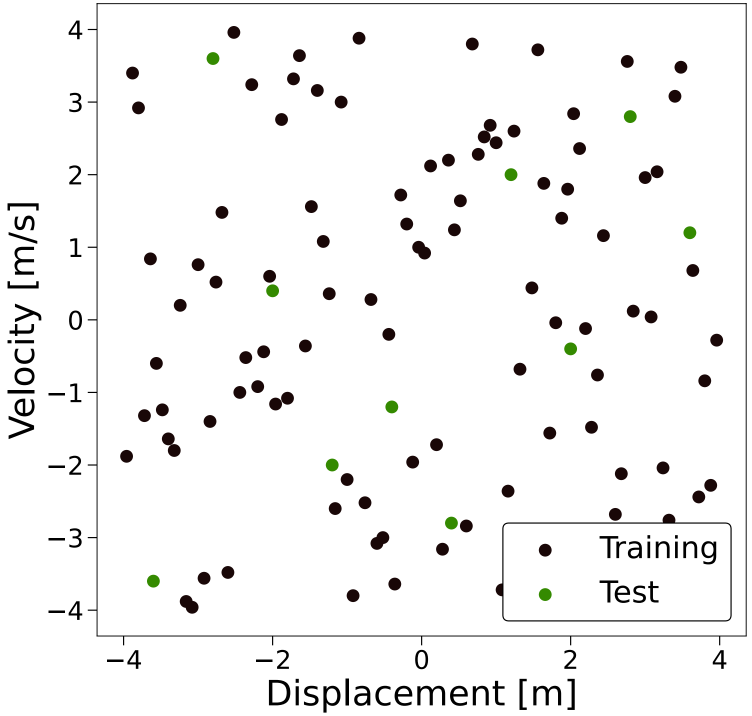
(Unstacked) DeepONet [2]

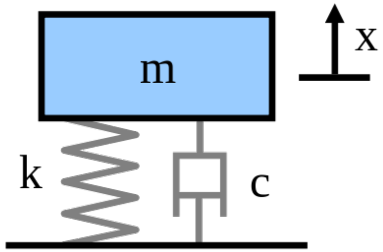


[1] T. Chen and H. Chen - *Universal approximation to nonlinear operators by neural networks with arbitrary activation functions and ...* - 1995
[2] L. Lu et al. - *Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators* - 2021

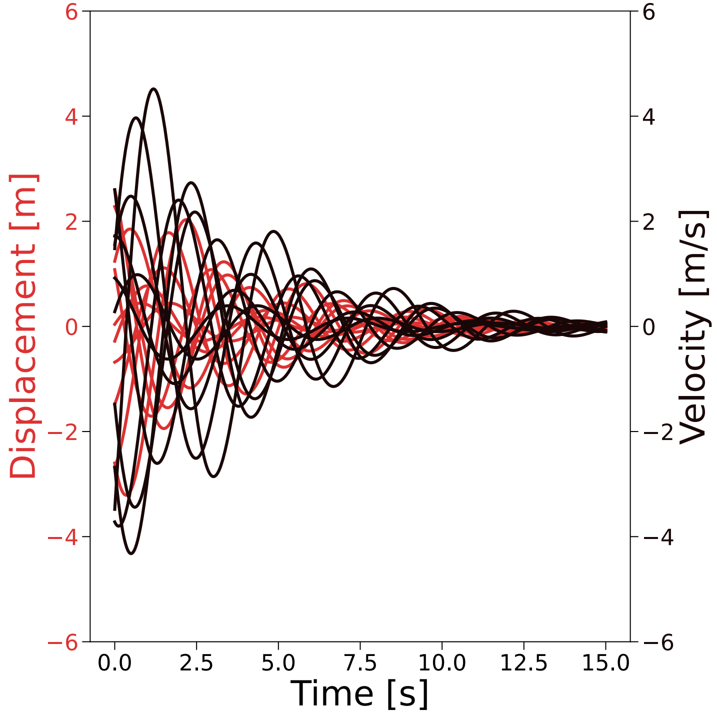
Example: Mass-Spring-Damper Test Case

100 independent I.C.s





100 scenarios



Equations of motion:

$$\begin{cases} \begin{bmatrix} \dot{x} \\ \ddot{x} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{c}{m} \end{bmatrix} \begin{bmatrix} x \\ \dot{x} \end{bmatrix} \\ x(t=0) = x_0, \\ \dot{x}(t=0) = v_0. \end{cases}$$

GOAL: To construct an accurate surrogate for the dynamics

[1] S. Venturi and T. Casey - *SVD Perspectives for Augmenting DeepONet Flexibility and Interpretability* – April 2022

Example: Mass-Spring-Damper Test Case

Scenario-Aggregated Snapshot Matrix

$$X = \begin{bmatrix} | & | & & | & | \\ x_1 & x_2 & \cdots & x_{99} & x_{100} \\ | & | & & | & | \end{bmatrix}$$

$$\dim(X) = N_t \times N_s$$

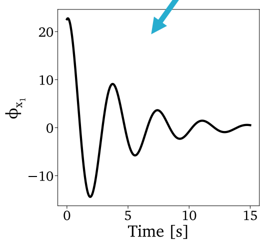
SVD/PCA →

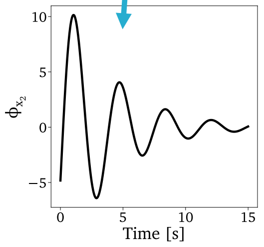
$$\boxed{X = \Phi_x A_x^T}$$

$$A_x = \begin{bmatrix} | & | \\ \alpha_{x_1} & \alpha_{x_2} \\ | & | \end{bmatrix} \qquad \Phi_x = \begin{bmatrix} | & | \\ \phi_{x_1} & \phi_{x_2} \\ | & | \end{bmatrix}$$

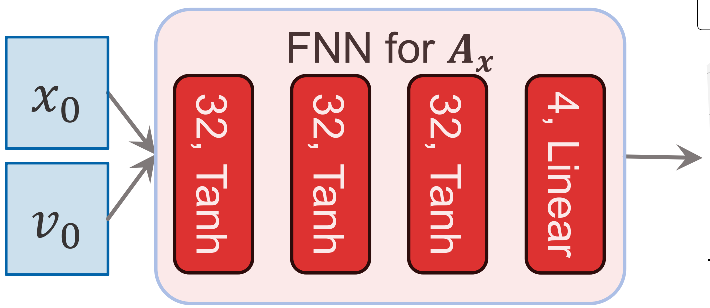
$$\dim(\Phi_x) = N_t \times 2$$

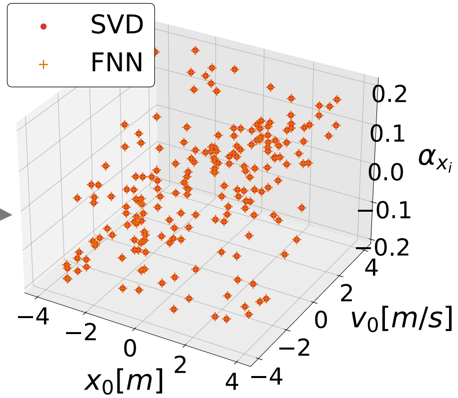
$$\dim(A_x) = N_s \times 2$$

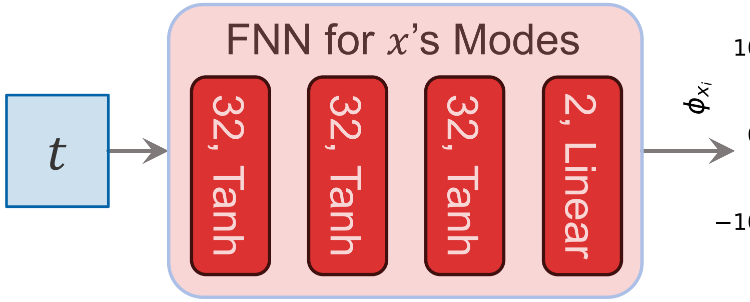


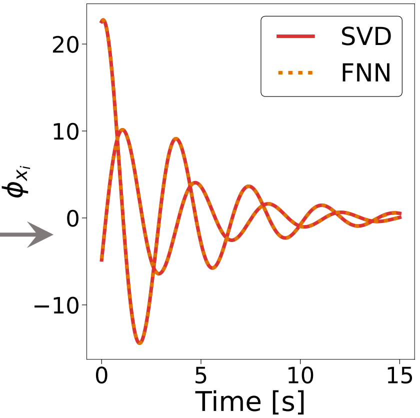


We can map $A_x \rightarrow (x_0, v_0)$ and $\Phi_x \rightarrow t$



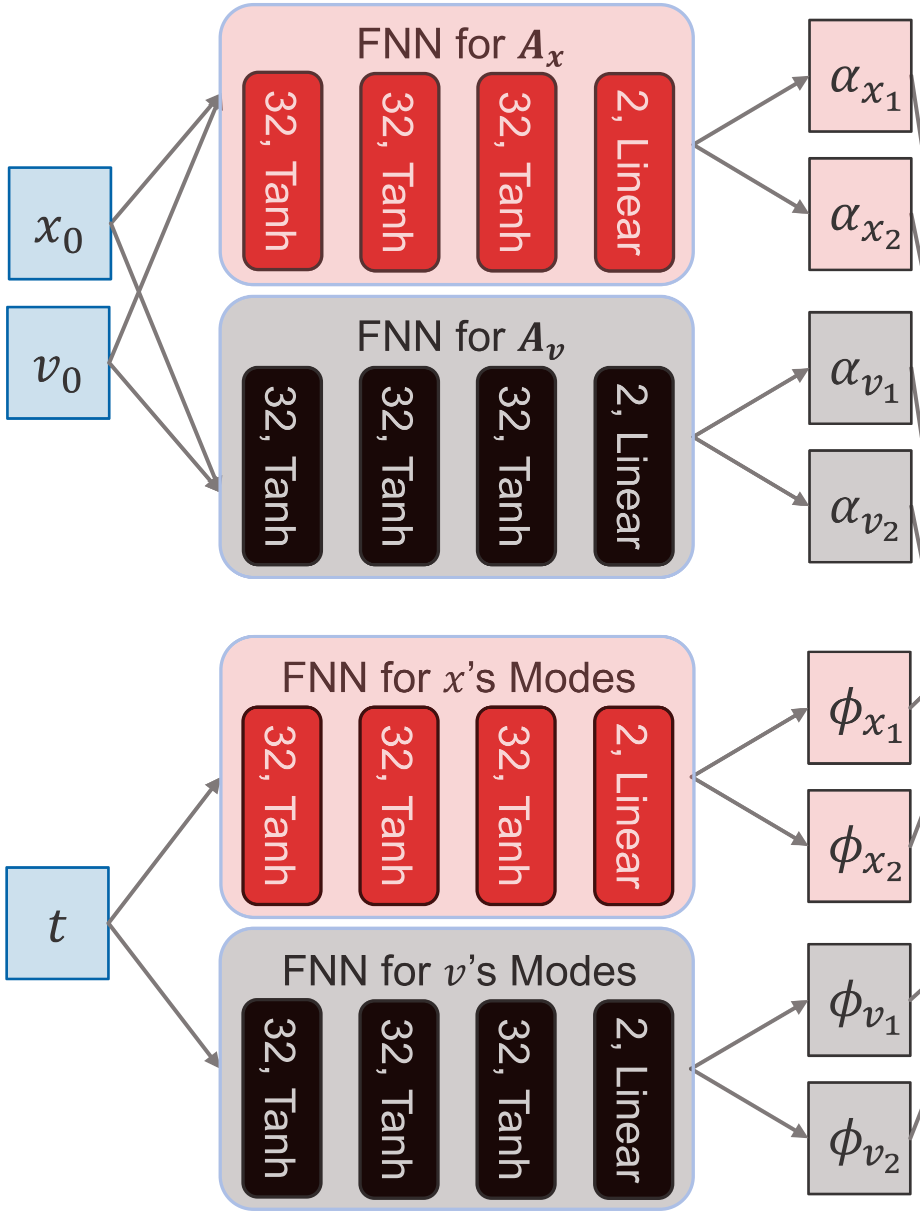


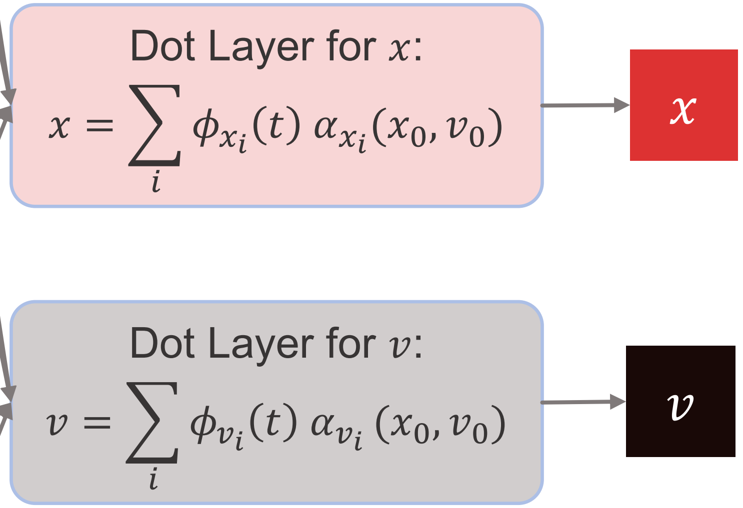


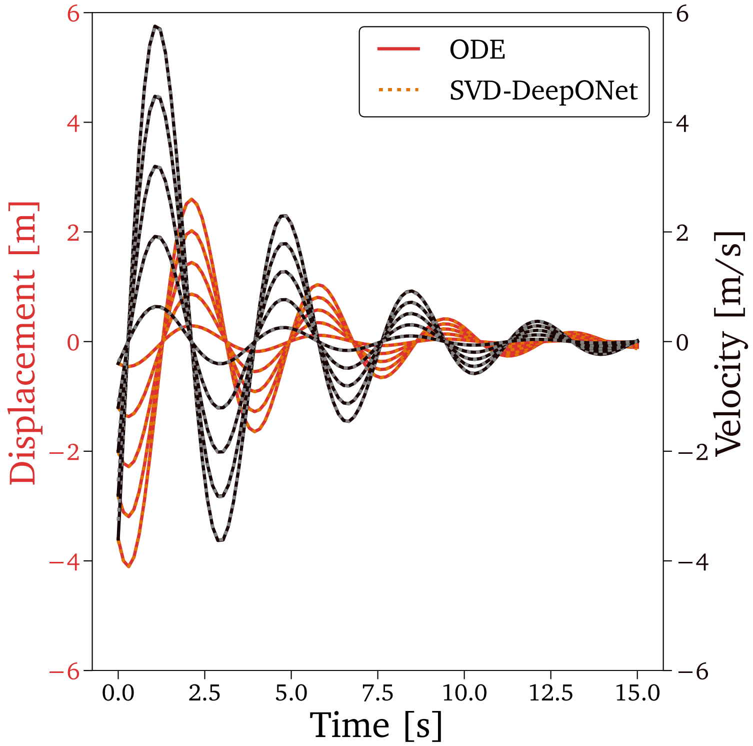


Example: Mass-Spring-Damper Test Case

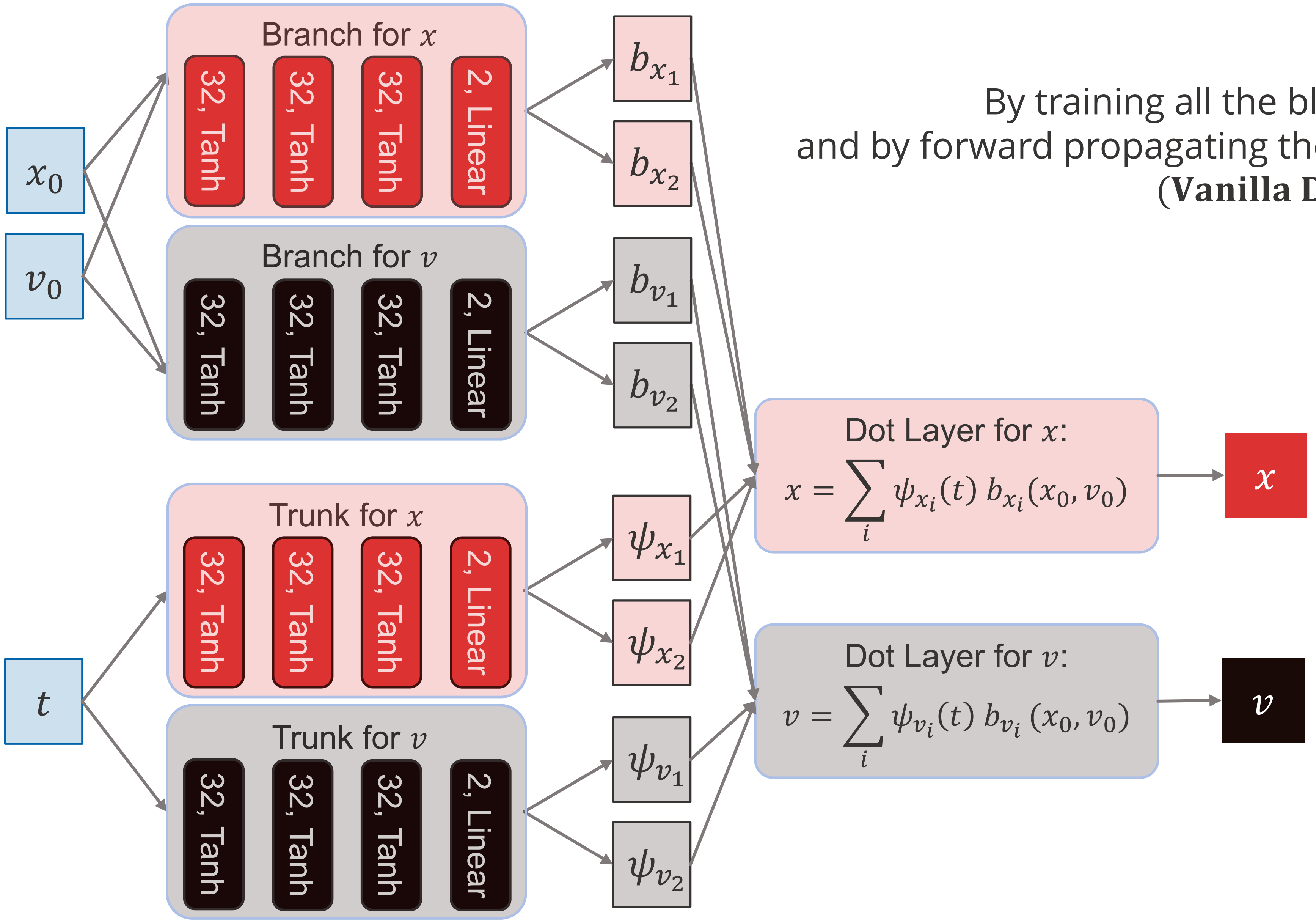
By assembling the **pre-trained blocks** for x and v
and by forward propagating the input inside the architecture…
$(\mathbf{SVD-DeepONet})$



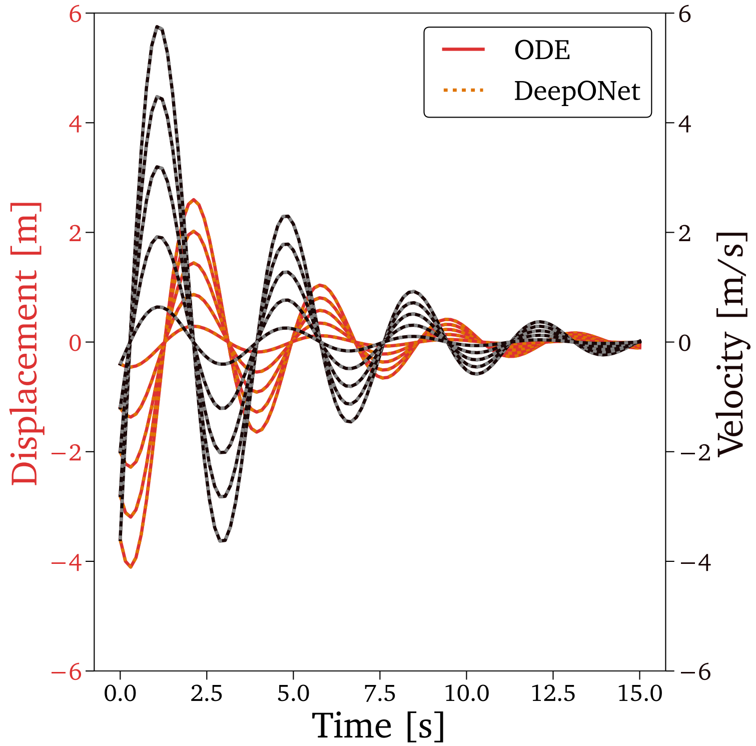




Example: Mass-Spring-Damper Test Case



By training all the blocks simultaneously
and by forward propagating the input inside the architecture…
(**Vanilla DeepONet**)



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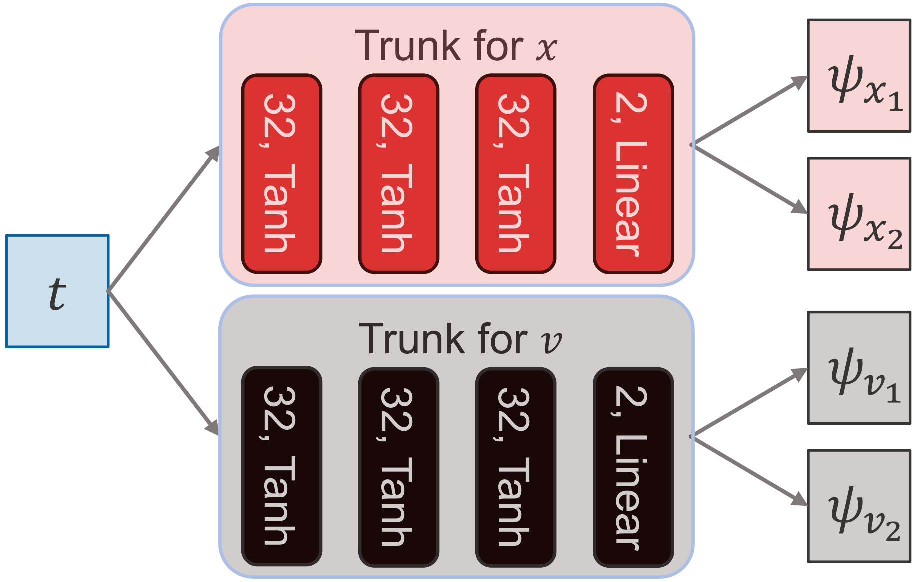
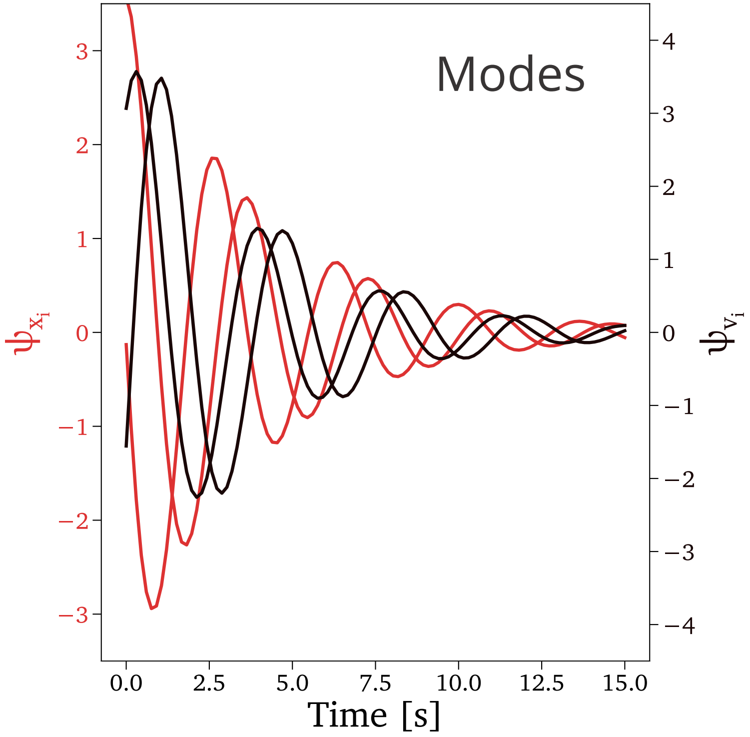
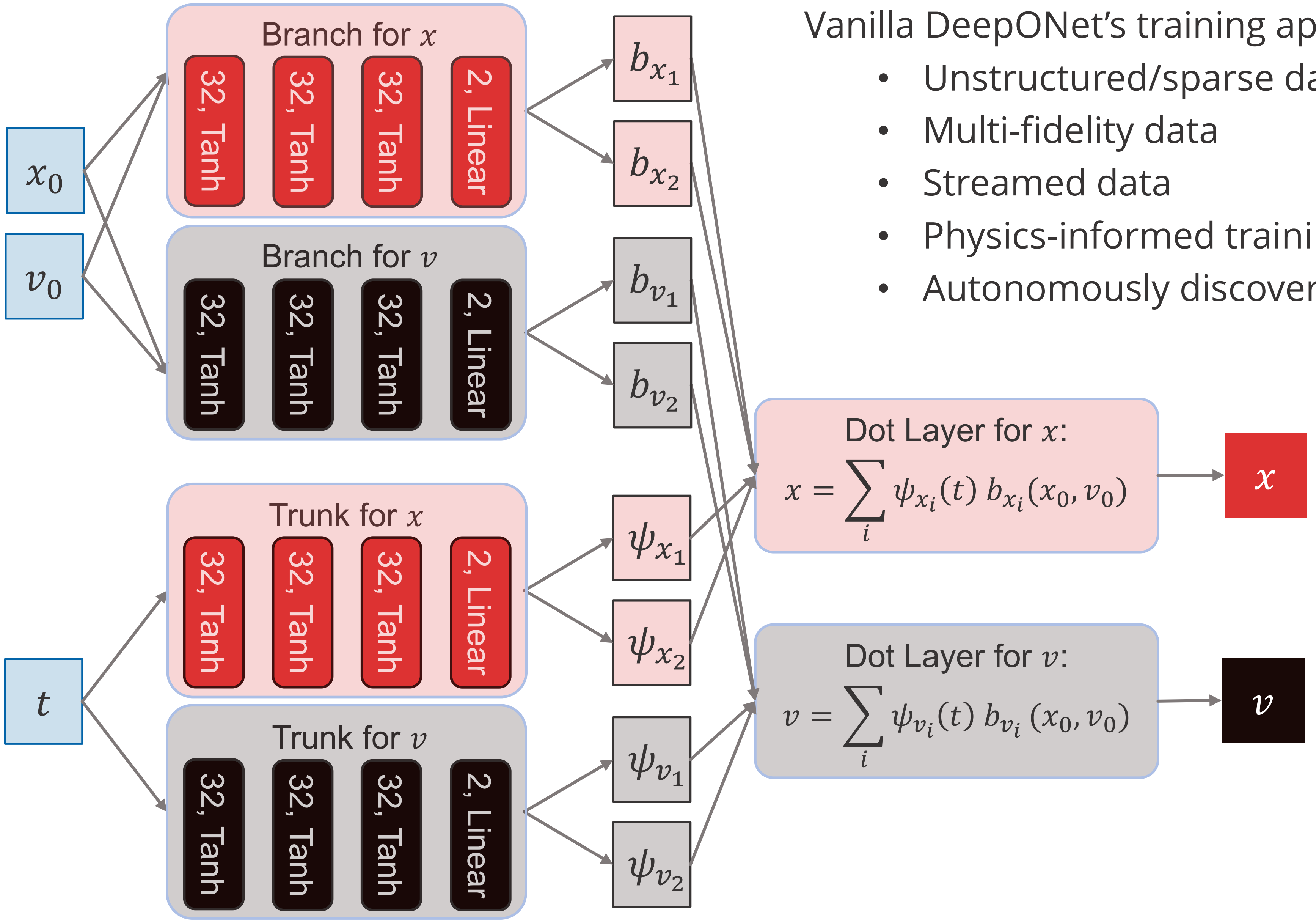


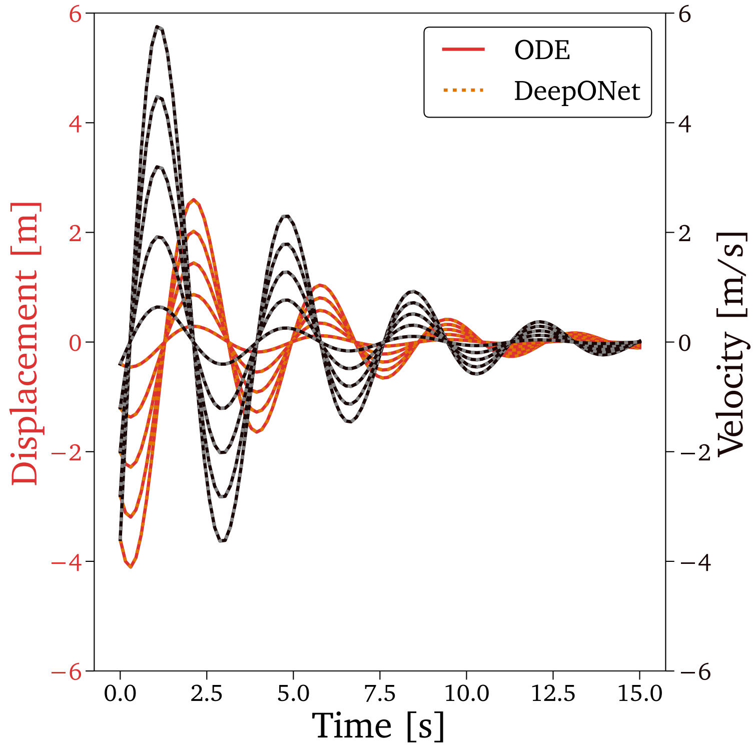


Example: Mass-Spring-Damper Test Case



Vanilla DeepONet's training approach enables flexibility:

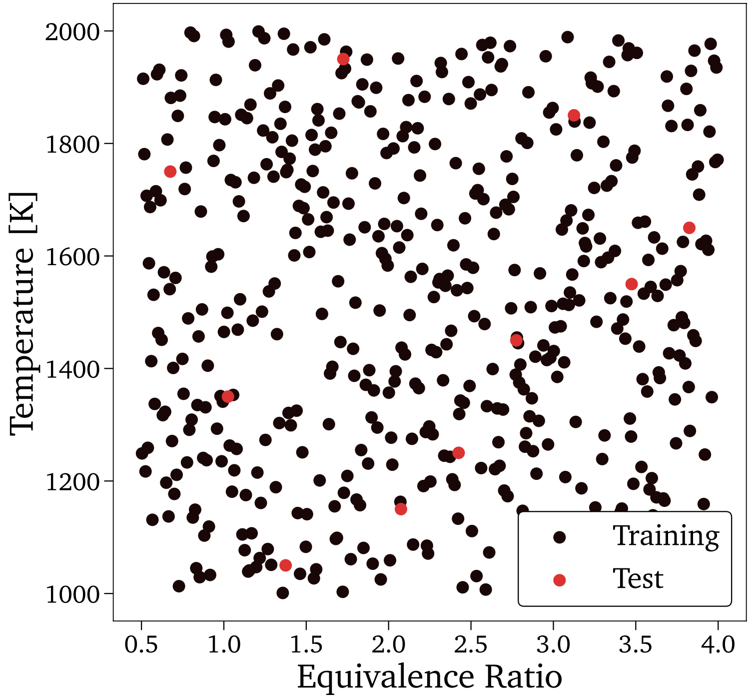
- Unstructured/sparse data
- Multi-fidelity data
- Streamed data
- Physics-informed training
- Autonomously discovered pre-transformations



Application: Isobaric 0D Reactor, H_2 Ignition

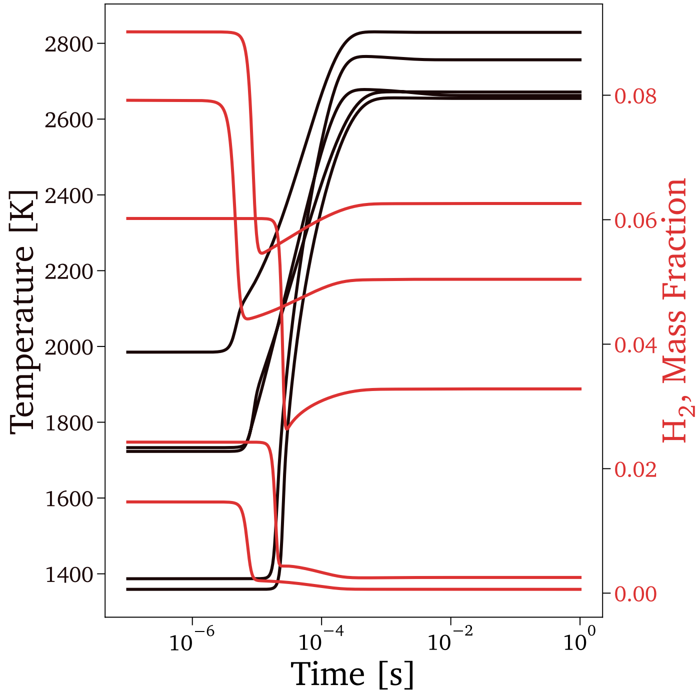
Hydrogen-air gas mixture, 19 state variables (i.e., temperature and 18 species mass fractions)

500 I.C.s



Isobaric 0-D Reactor

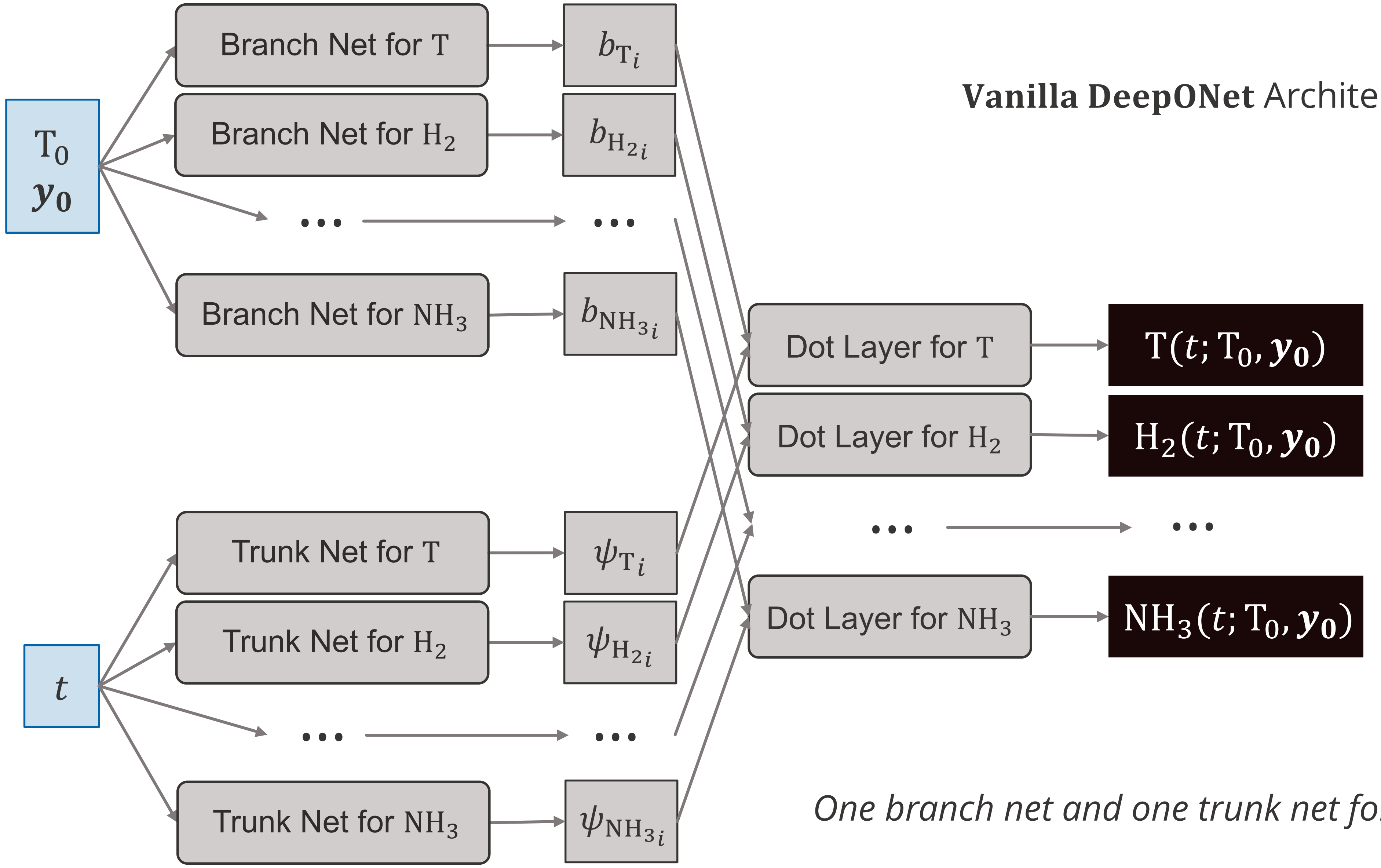
Some training scenarios



<u>GOAL</u>: To construct an accurate surrogate for the dynamics

Application: Isobaric 0D Reactor, H_2 Ignition

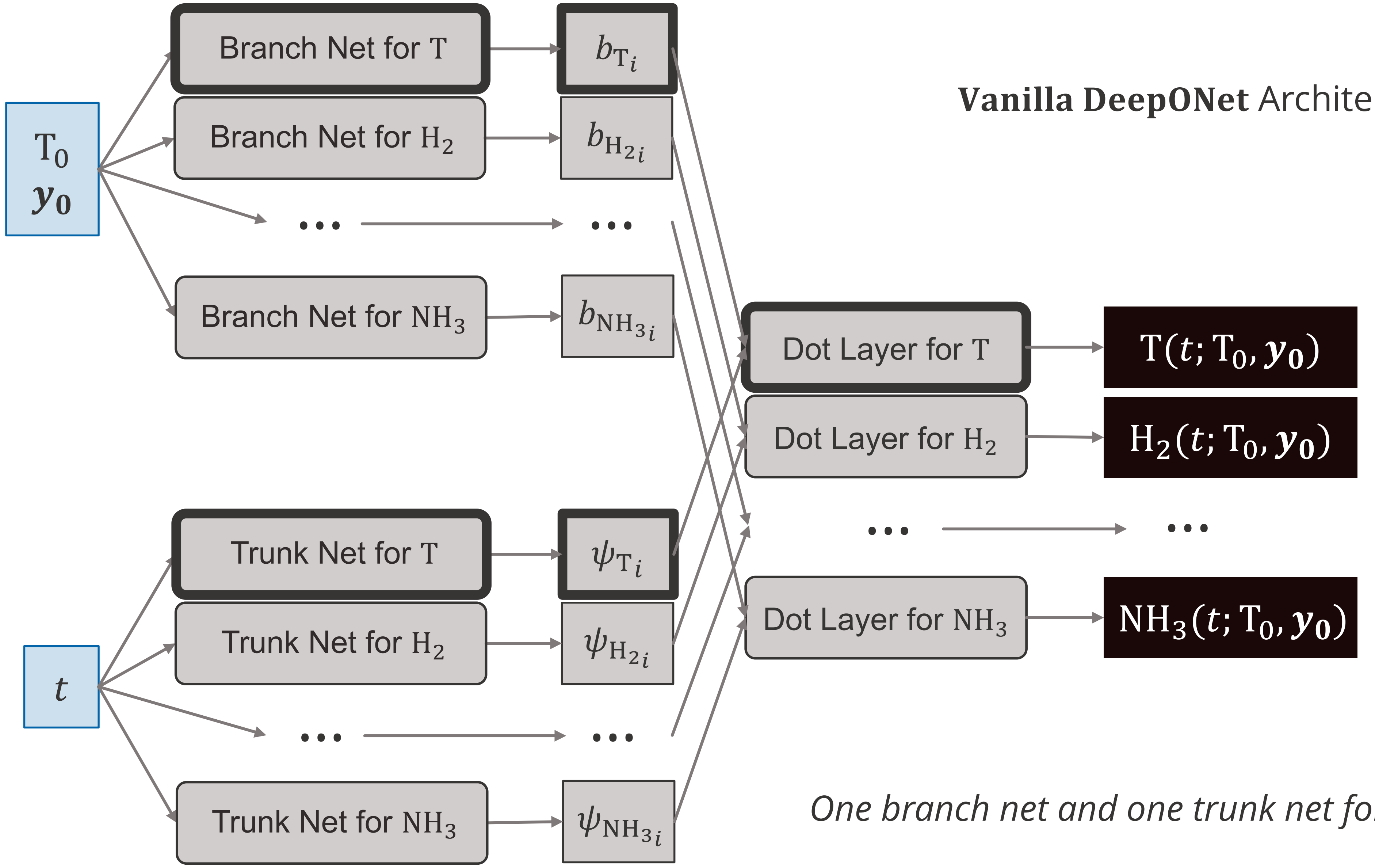
Vanilla DeepONet Architecture



One branch net and one trunk net for each state variable

Application: Isobaric 0D Reactor, H_2 Ignition

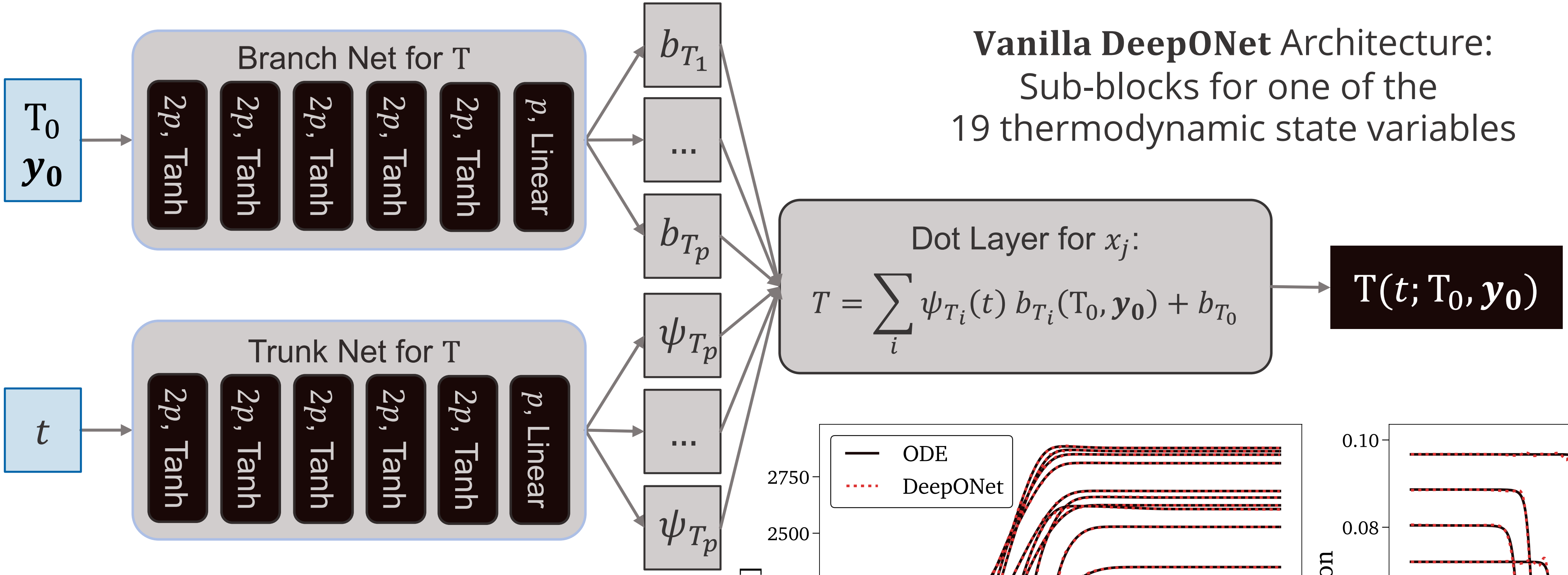
Vanilla DeepONet Architecture



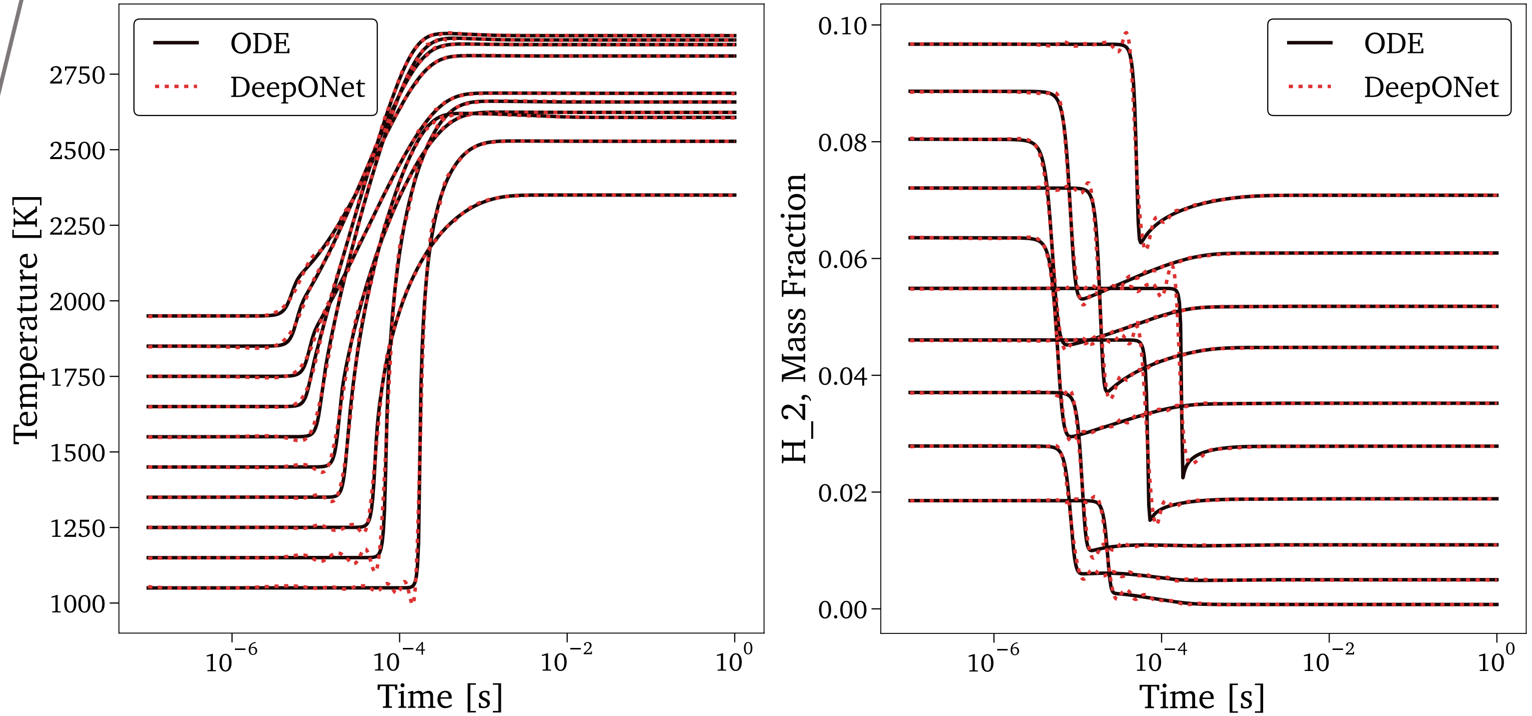
One branch net and one trunk net for each state variable

Application: Isobaric 0D Reactor, H_2 Ignition

Vanilla DeepONet Architecture:
Sub-blocks for one of the
19 thermodynamic state variables



With $p = 20$
(total of **297,160** parameters)
noticeable inaccuracies



Application: Isobaric 0D Reactor, H_2 Ignition

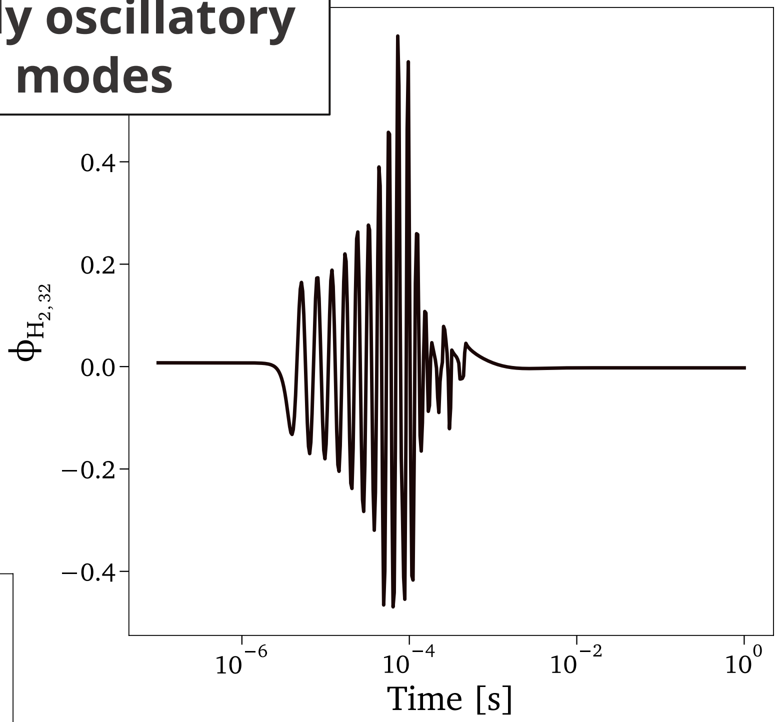
Scenario-Aggregated Snapshot Matrix

$$\mathbf{H_2} = \begin{bmatrix} | & | & & | & | \\ \mathbf{H_2}_1 & \mathbf{H_2}_2 & \cdots & \mathbf{H_2}_{499} & \mathbf{H_2}_{500} \\ | & | & & | & | \end{bmatrix}$$

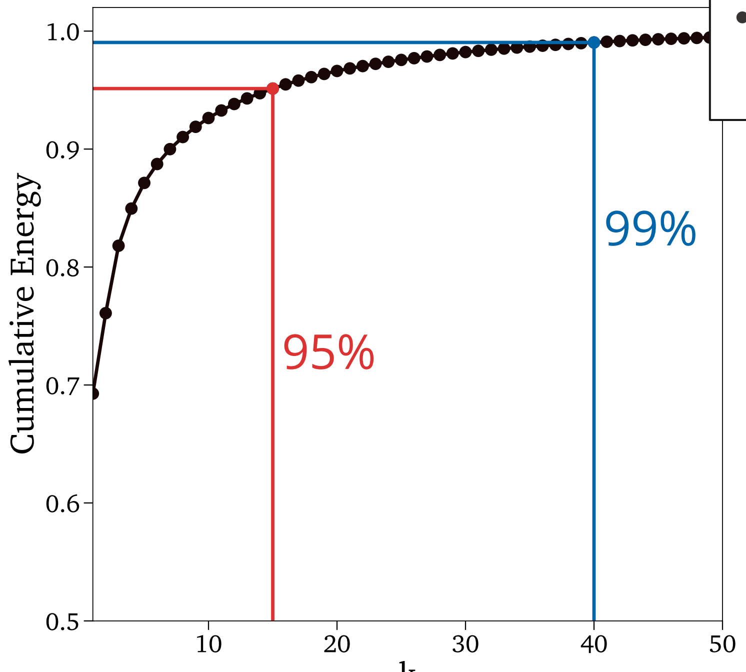
SVD

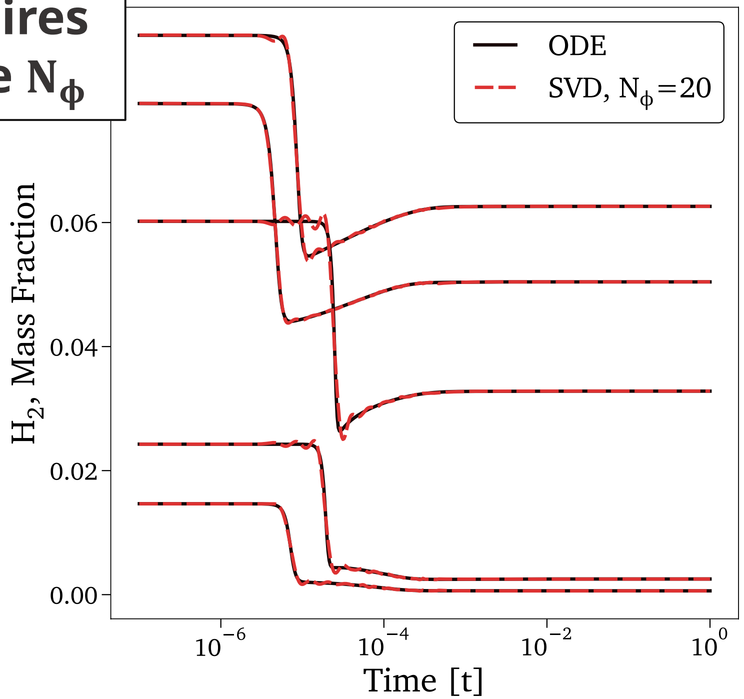
$$\mathbf{H_2} = \mathbf{\Phi}_{H_2} A_{H_2}^T$$

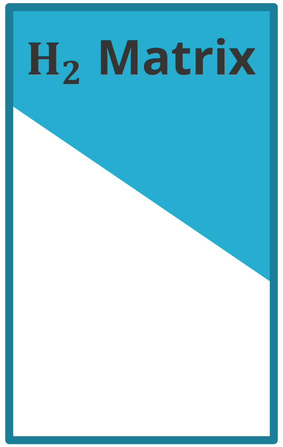
- **Highly oscillatory modes**



- **Requires large N_ϕ**







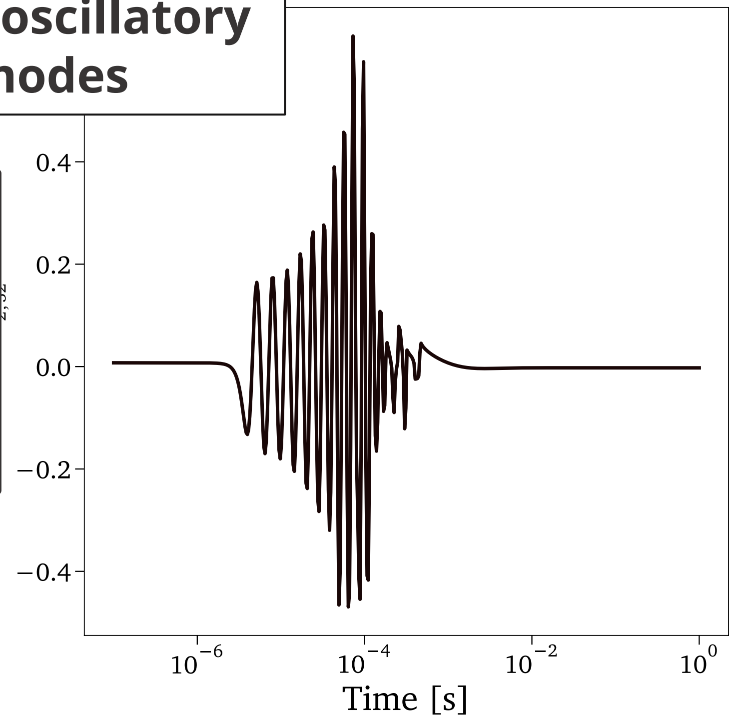
Application: Isobaric 0D Reactor, H_2 Ignition

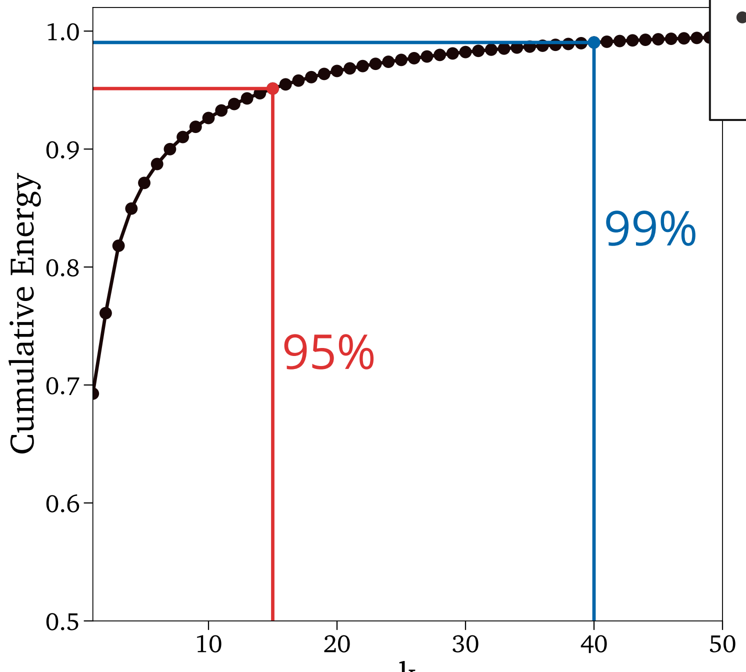
Scenario-Aggregated Snapshot Matrix

H_2

Due to SVD's inefficiencies in compressing data characterized by symmetries (i.e., shifts, stretches, and rotations)

- **Highly oscillatory modes**





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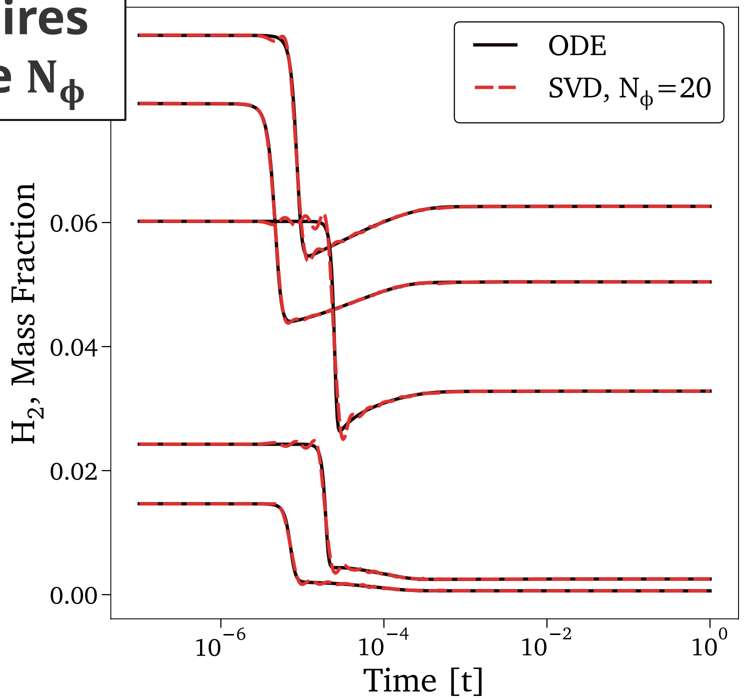
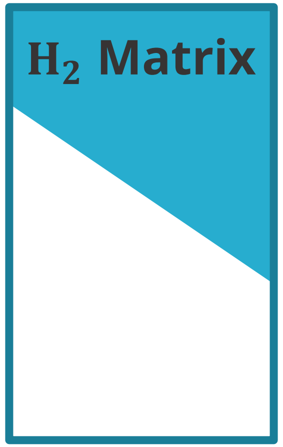
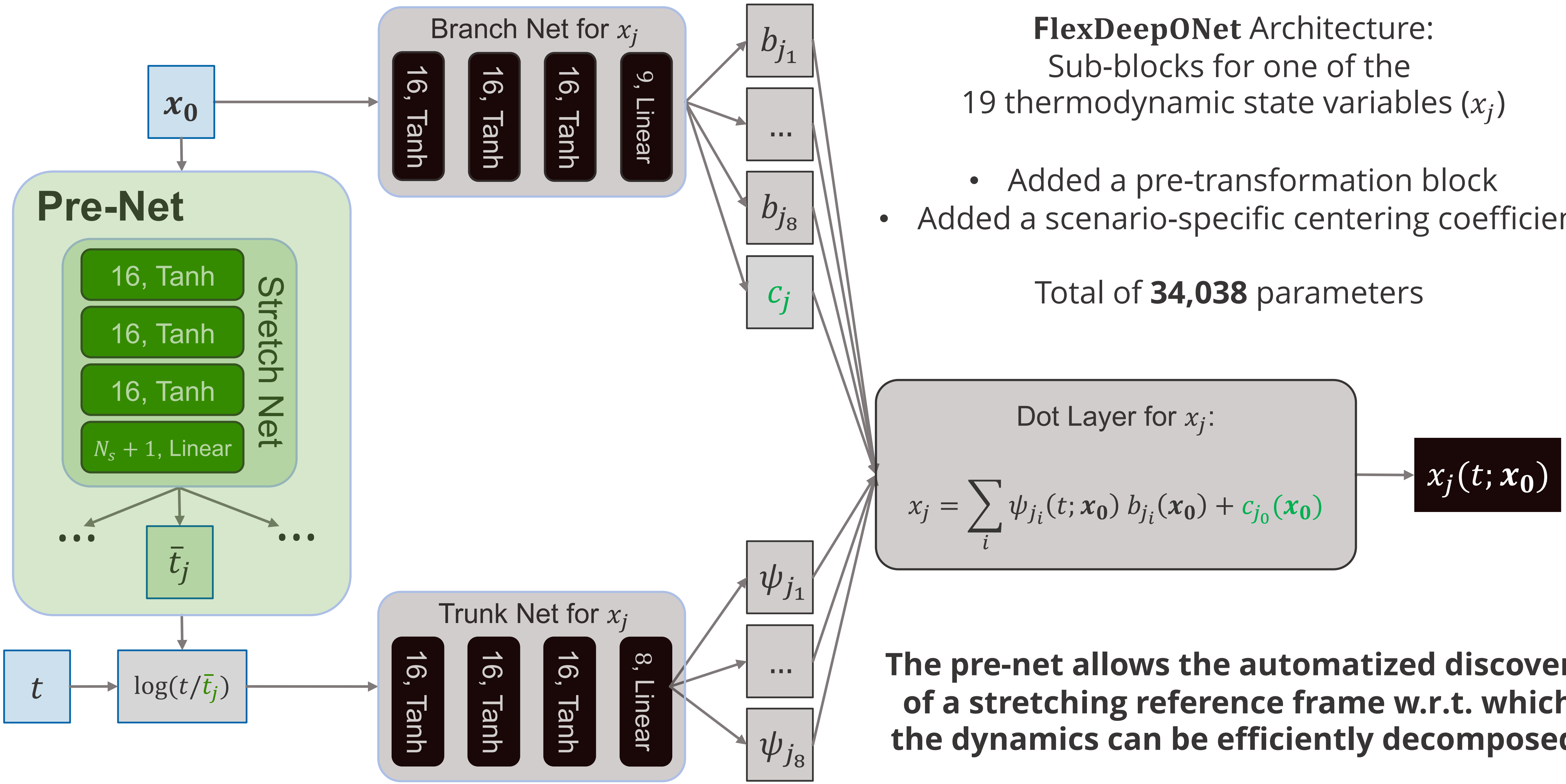




Application: Isobaric 0D Reactor, H_2 Ignition



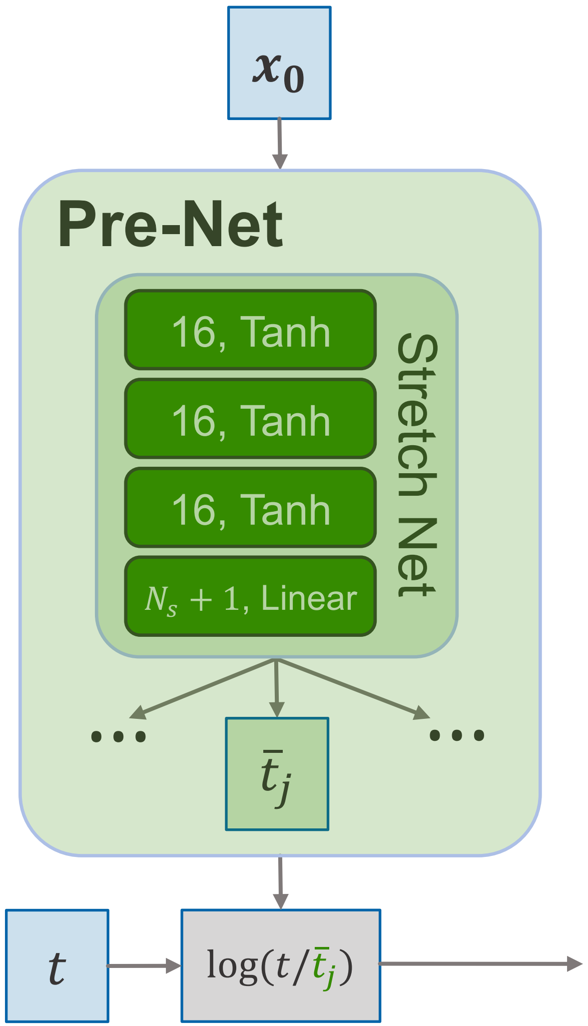
FlexDeepONet Architecture:
Sub-blocks for one of the
19 thermodynamic state variables (x_j)

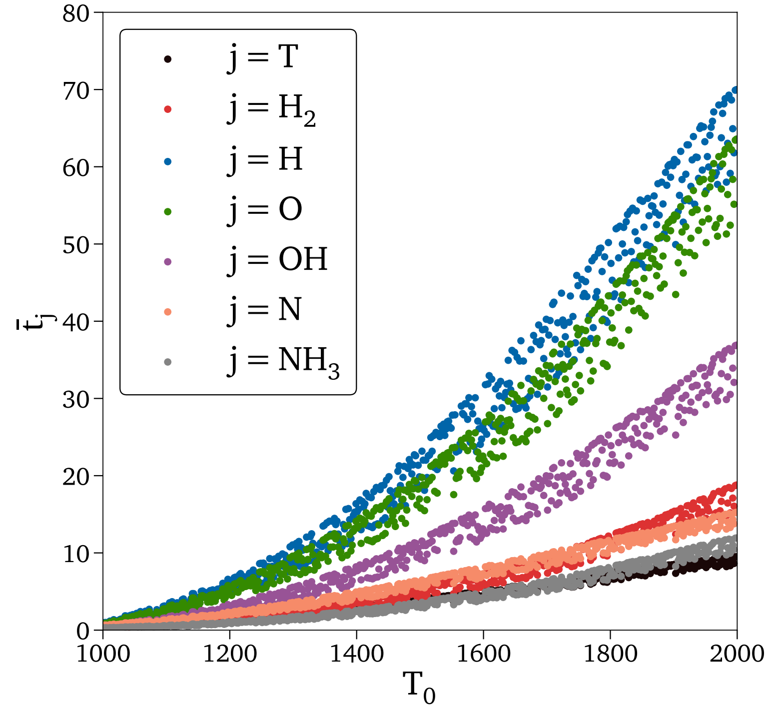
- Added a pre-transformation block
- Added a scenario-specific centering coefficient

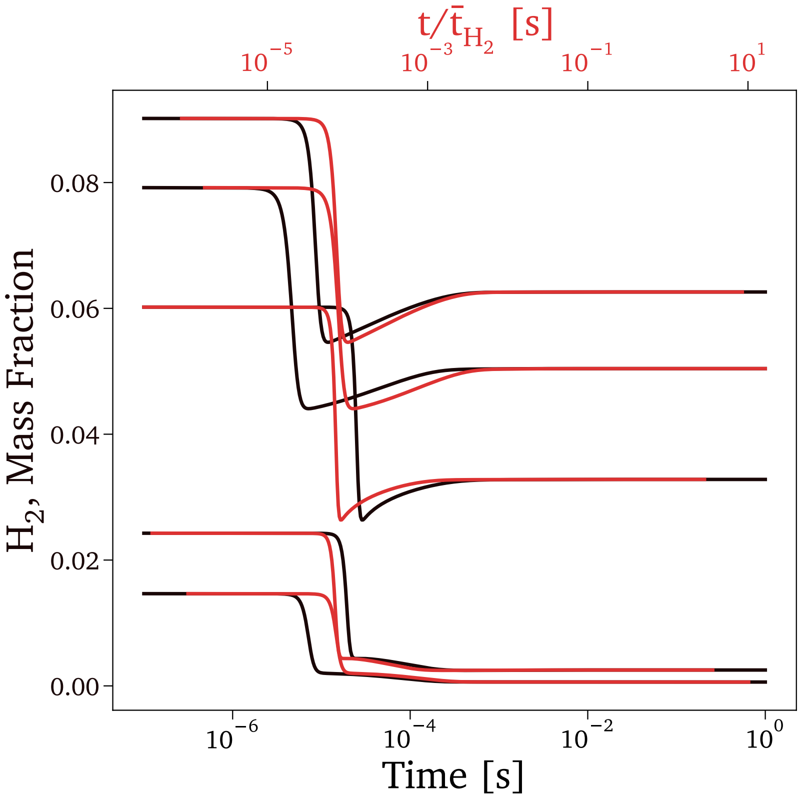
Total of **34,038** parameters

The pre-net allows the automatized discovery of a stretching reference frame w.r.t. which the dynamics can be efficiently decomposed

Application: Isobaric 0D Reactor, H_2 Ignition







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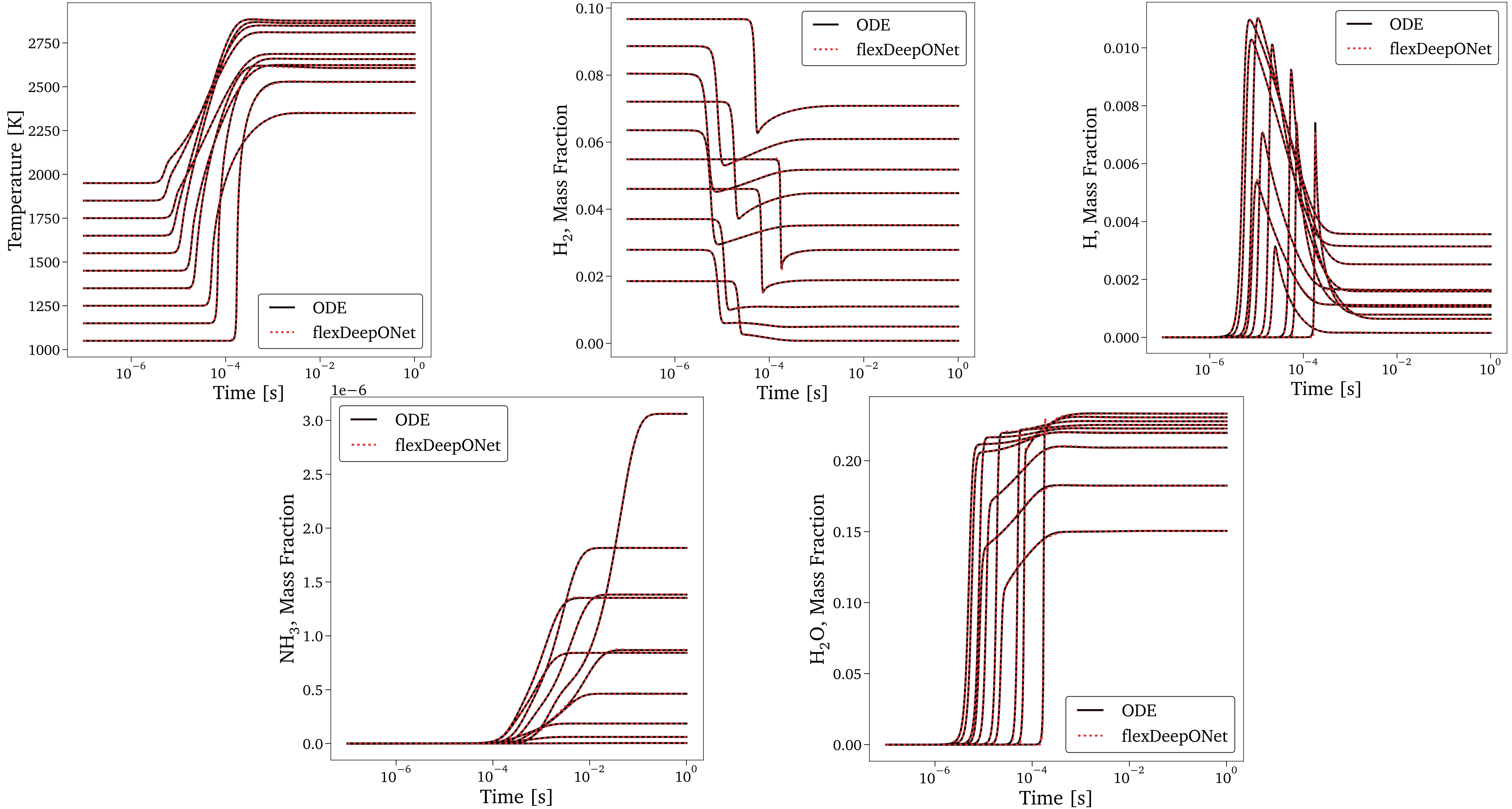

Summary

- In the context of a linear subspace reduced order models for reacting flows, constructed a reduced order operator surrogate model for advancing chemical state using DeepONets
- Preliminary studies show an operator surrogate built on 10 modes (of 20 in the FOM) can reconstruct solutions with little error
- Expanding to higher dimensional models, expanding the space of initial conditions to surrogate general chemical evolution
- Investigating interpretability of the DeepONet projections, utilization of different embeddings, enforcement of physics within the network, combine with manifold learning methods
- Broadly construct universal surrogates for chemistry advancement to avoid expensive time integration

Acknowledgements

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