Neural Closure Models for Dynamical Systems[1]

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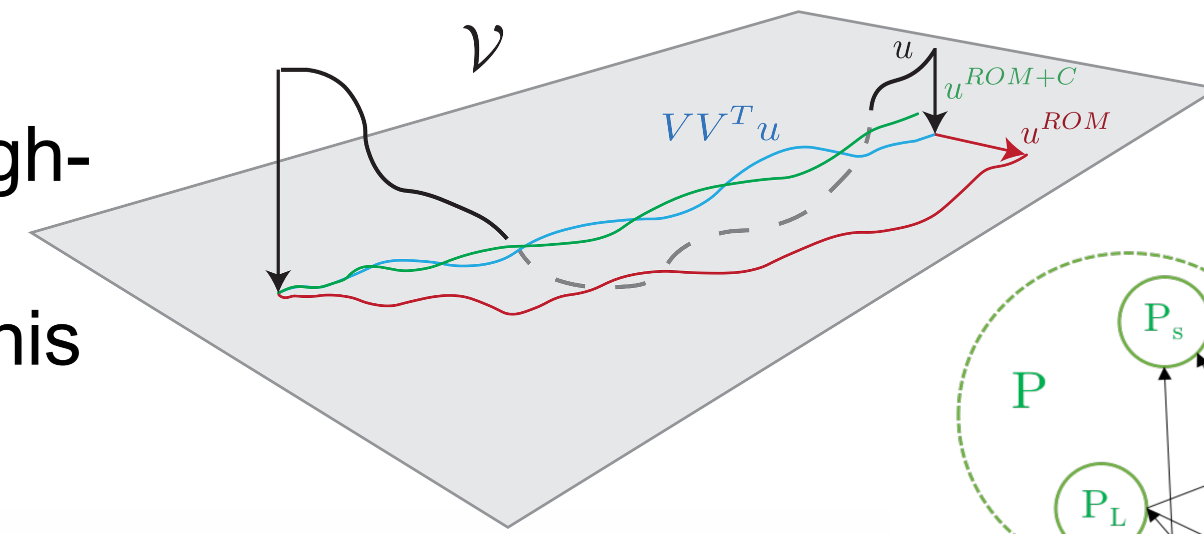
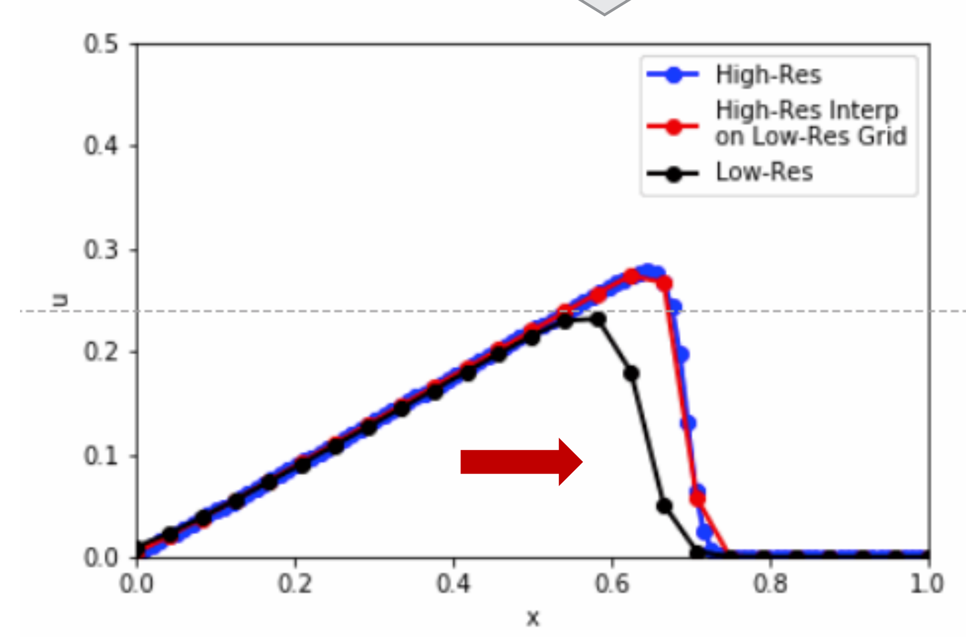
Introduction

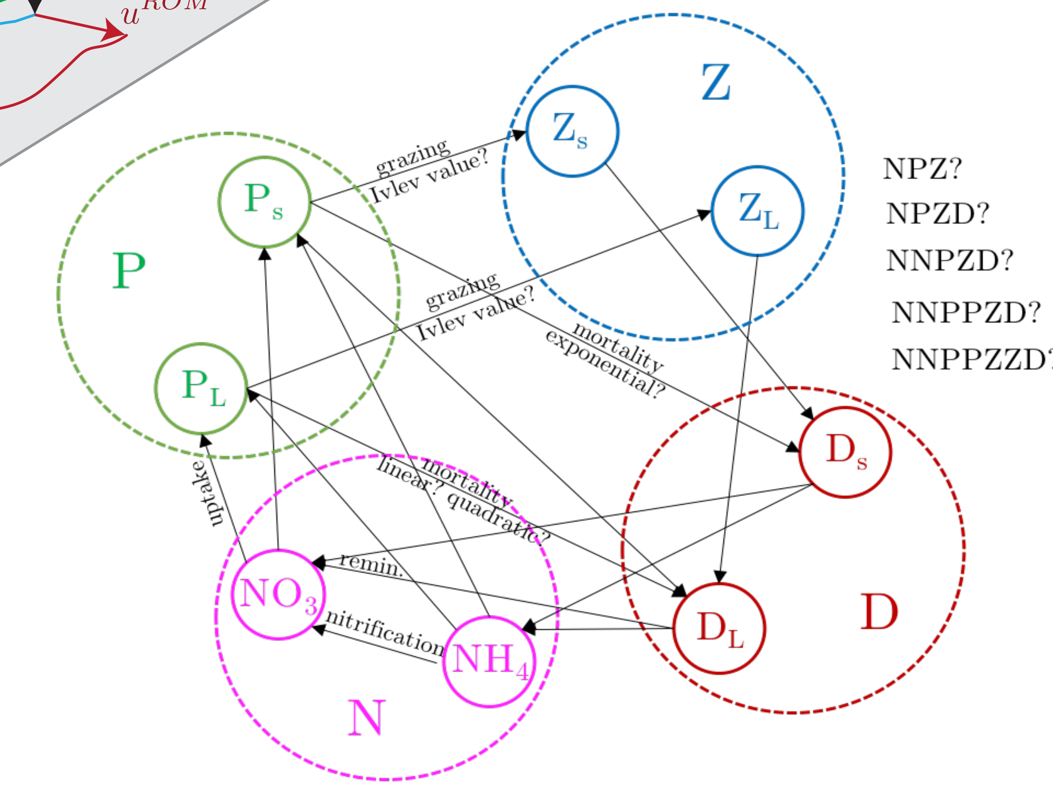
Problem: High computational costs associated with high-fidelity simulations leads to low-fidelity models with truncated scales, processes, and variables; however, this often limits the reliability and usefulness of simulations



Low-Fidelity Models:

- Reduced order models
- Coarse resolution models
- Models with smaller/aggregated number of state variables





Biogeochemical models of various complexities

Goal: Learn *closure models* from high-fidelity data

Background

Mori-Zwanzig Formulation: Proves the need for a *non-Markovian closure* term

$$\frac{\partial}{\partial t}\hat{u}(\hat{u}_0,t) = \underbrace{PR(\hat{u}(\hat{u}_0,t))}_{\text{Low-Fidelity}} + \underbrace{P\int_0^t K(\hat{u}(\hat{u}_0,t-s),s)ds}_{\text{Memory}}$$

Biological time-scales: Exchange of information occurs on *non-negligible time-scales*, thus introducing explicit delays could eliminate the need for modeling intermediate states

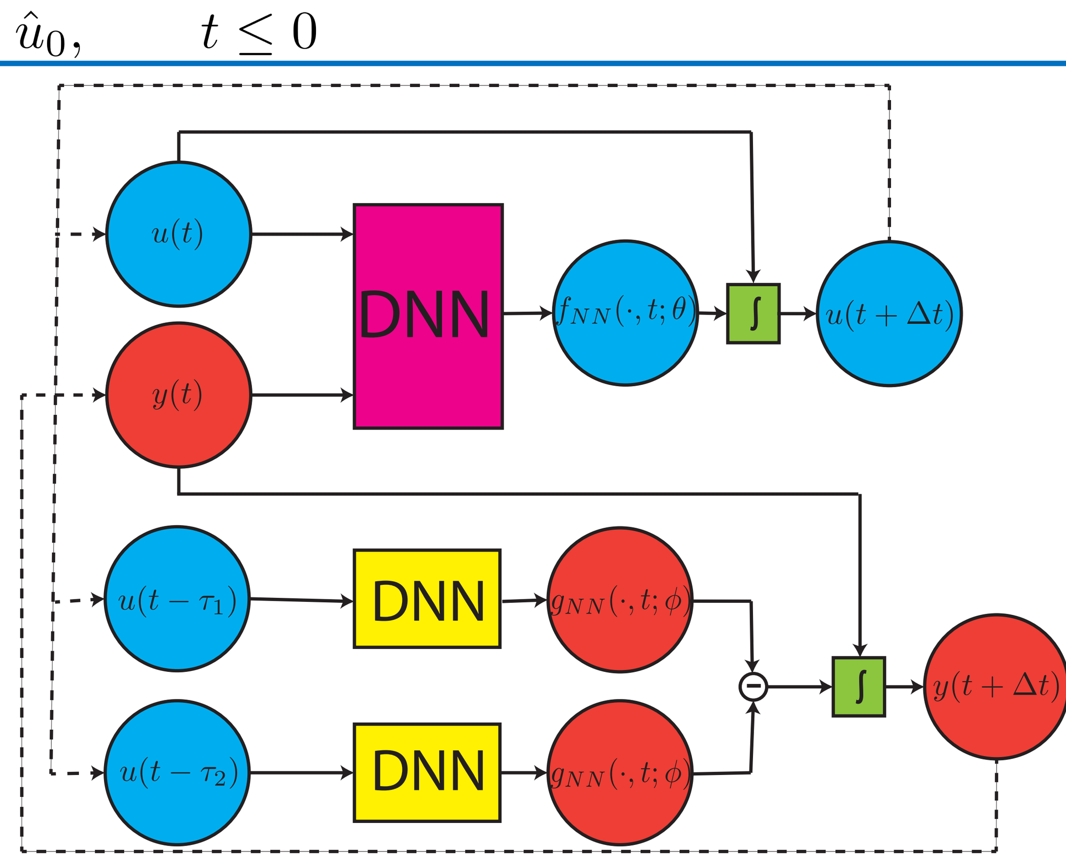
Methodology

Delay Differential Equations (DDEs): Widely used in modeling population dynamics, biology, and medicine

Distributed-nDDEs

$$\frac{\partial \hat{u}(t)}{\partial t} = \underbrace{PR(\hat{u}(t))}_{\text{Low-Fidelity}} + \underbrace{f_{NN}\left(\hat{u}(t), \int_{t-\tau_2}^{t-\tau_1} g_{NN}(\hat{u}(\tau);\phi)d\tau, t;\theta\right)}_{\text{Neural Closure}}$$

$$\hat{u}(0) = \hat{u}_0, \qquad t \leq 0$$



Discrete-nDDEs

$$\frac{\partial \hat{u}(t)}{\partial t} = \underbrace{PR(\hat{u}(t))}_{\text{Low-Fidelity}} + \underbrace{f_{RNN}(\hat{u}(t), \hat{u}(t-\tau_1), ..., \hat{u}(t-\tau_K), t;\theta)}_{\text{Neural Closure}}$$

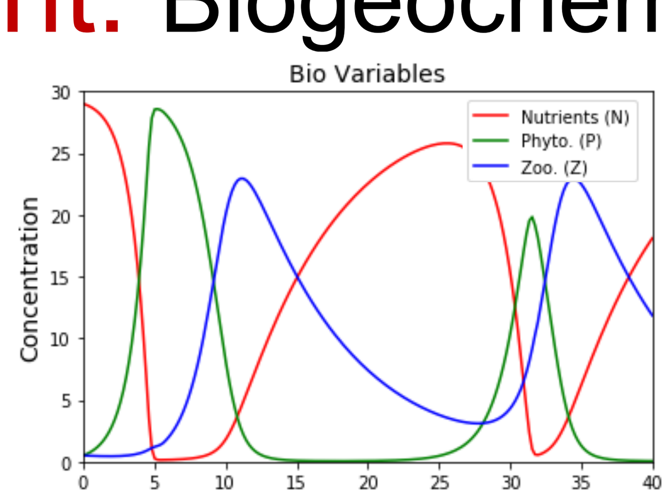
$$\hat{u}(0) = \hat{u}_0, \qquad t \leq 0$$

Key Innovations:

- Unified approach to learn and model any kind of DDE
- Elimination of the need for recurrent networks for modeling memory effects
- Derived adjoint equations to enable efficient training of neural-DDEs in any ML framework

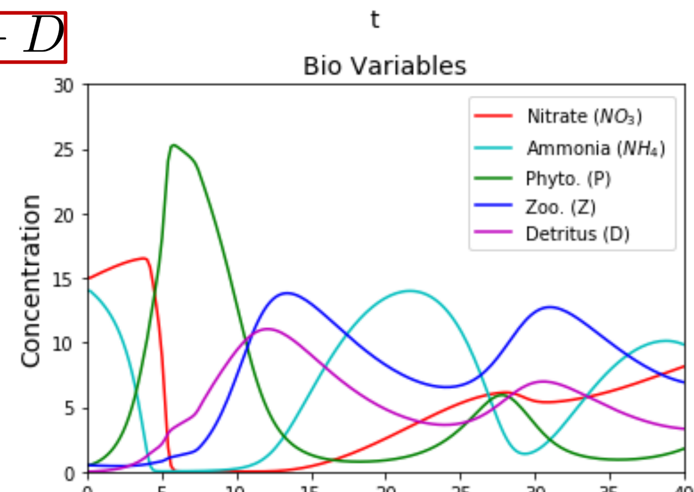
Experiment: Biogeochemical Models

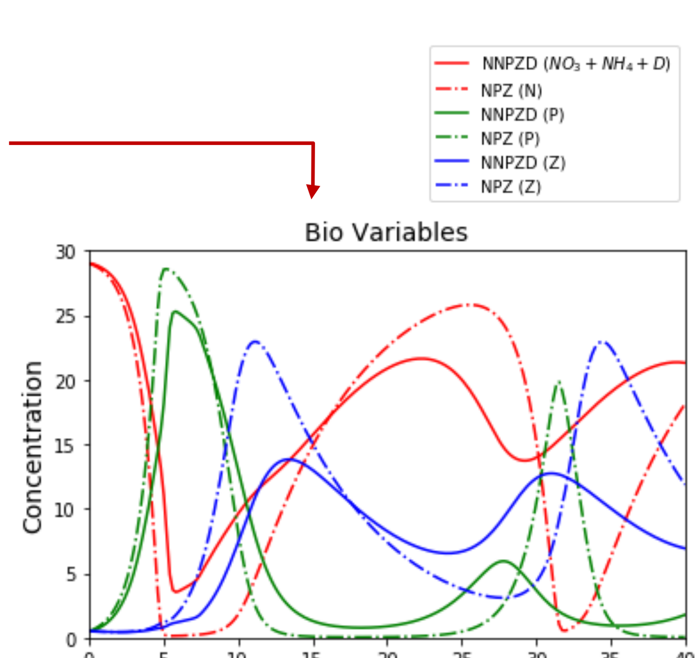
Low-Fidelity: Nutrients-Phytoplankton-Zooplankton (NPZ) model



$N \equiv NH_4 + NO_3 + D$

High-Fidelity: Ammonia-Nitrate-Phytoplankton-Zooplankton-Detritus (NNPZD) model

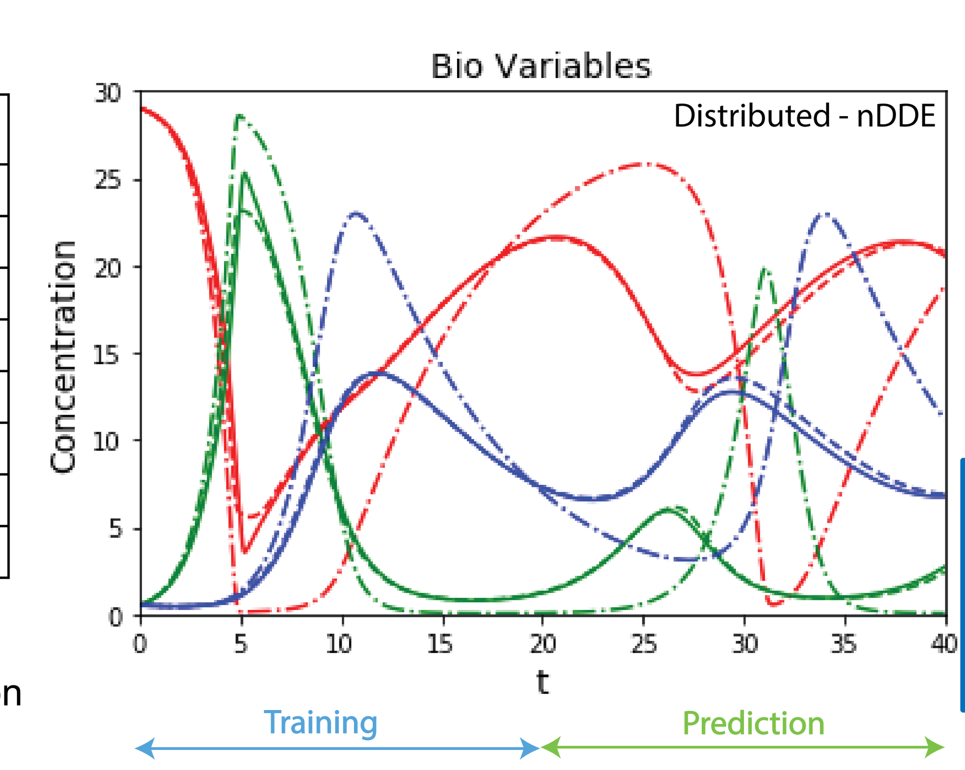




Distributed-nDDE Closure Architecture:

Layers	Act.
f_{NN}	
Input layer with 5 neurons	none
2 FC hidden layer with 7 neurons	tanh
FC output layer with 3 neurons	linear
g_{NN}	
Input layer with 3 neurons	none
2 FC hidden layer with 5 neurons	tanh
FC output layer with 4 neurons	linear

Loss function: Time averaged L_2 error + penalization for state becoming negative + penalization for sum of the states not remaining constant



NPZ with neural closure can emulate NNPZD time-response

Conclusion

Developed a *neural delay differential equations (nDDEs)* based closure modeling framework, motivated by the Mori-Zwanzig formulation and the inherent delays in natural dynamical systems

[1]Gupta and Lermusiaux, arXiv 2020 [https://arxiv.org/abs/2012.13869]