Physics-informed reduced order model with conditional neural fields

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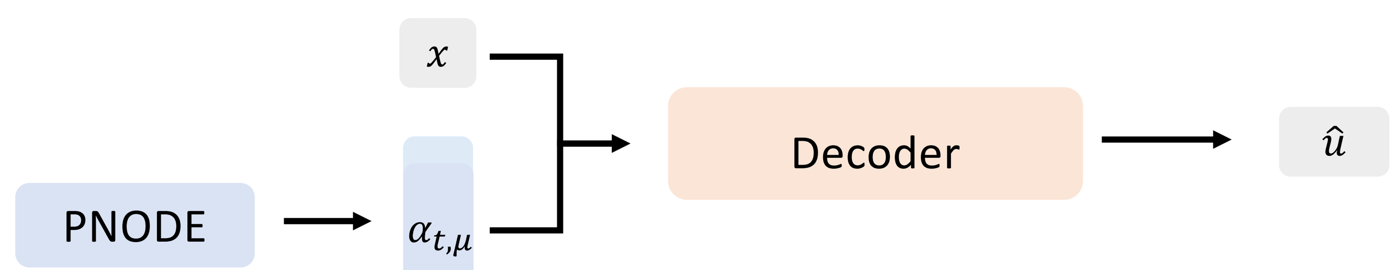
Summary: We introduce **CNF-ROM structure** and its **physics-informed learning objective** to produce approximate solutions of spatio-temporal governing PDEs parametrized by μ.

Proposed Method

CNF-ROM structure

- Learn coordinate-based NN to approximate parametrized PDE solution.



- The coordinate-based solution (decoder output) is conditionally defined based on the low-dimensional latent state $\alpha \in \mathbb{R}^{d_\alpha}$. ([3])
- The parametrized neural ODE (PNODE) learns different velocities (trajectories) of latent states for each μ. ([1])

PINNs objective

- PDE residual loss is available for CNF-ROM: automatic differentiation for spatial derivatives and the chain rule for time derivatives!

$$\frac{\partial D_\psi(x, \alpha_{t,\mu})}{\partial t} = \frac{\partial D_\psi(x, \alpha_{t,\mu})}{\partial \alpha_{t,\mu}} f_\theta(\alpha_{t,\mu}, t, \mu)$$

Chain Rule for time derivatives!

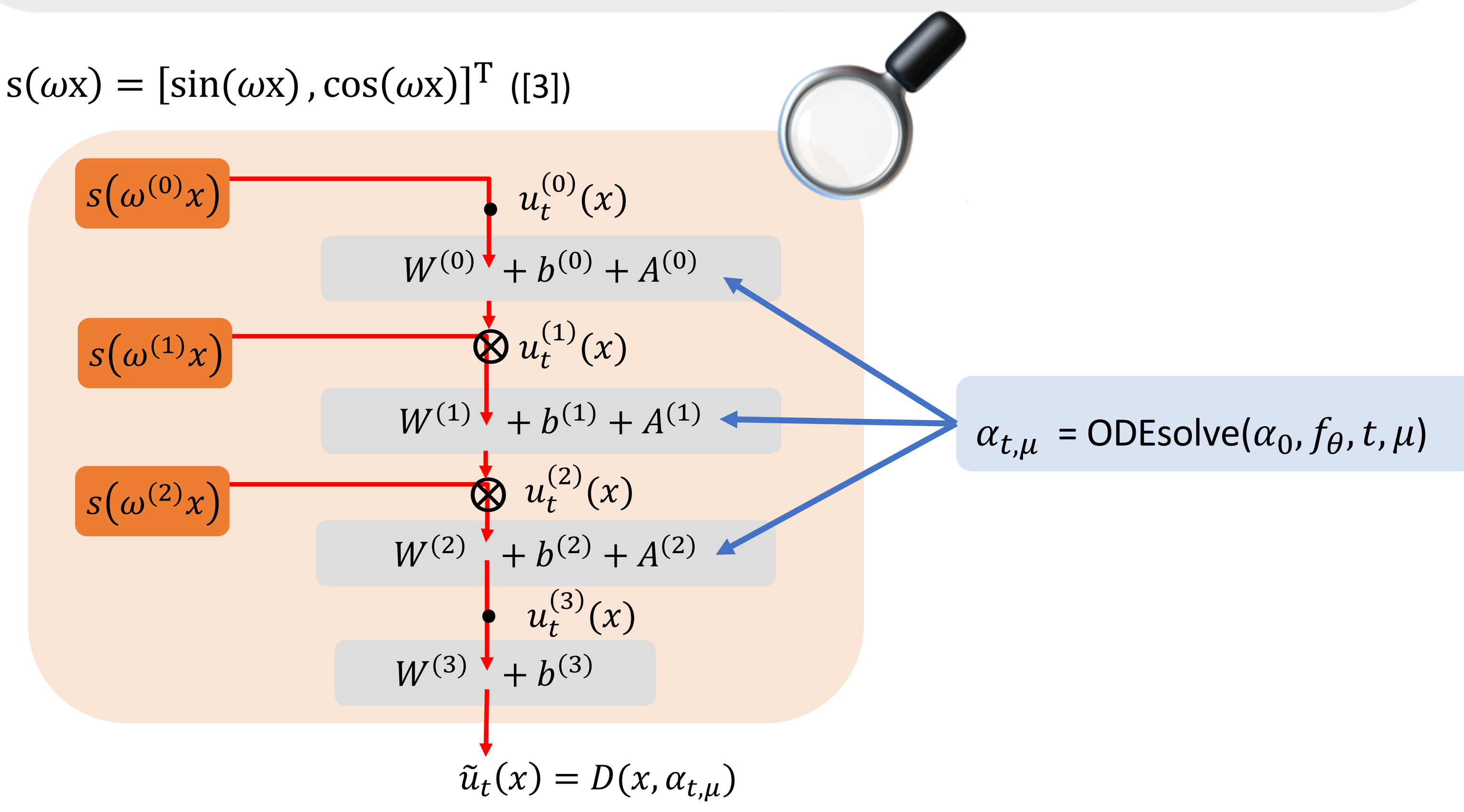
MODEL

CNF-ROM

DECODER $D_\psi(x, \alpha_{t,\mu}) = \sum_{k=1}^{K} c_{\psi_{1,k}}(\alpha_{t,\mu}) s_{\psi_{2,k}}(x) + \text{bias}$

PNODE $\frac{d\alpha_{t,\mu}}{dt} = f_\theta(\alpha_{t,\mu}, t, \mu)$

$s(\omega x) = [\sin(\omega x), \cos(\omega x)]^T$ ([3])



Trade-offs in imposing exact IC/BC ([2])

Limitation of Physics-informed Neural Networks (PINNs)

- Initial and boundary conditions (IC, BC) are not strictly met when added as loss terms.

➥ We introduce an approximate distance function to impose hard constraints.

Limitation of R-function-based approximate distance function (ADF, ϕ)

- The second and higher-order derivatives of ϕ explode at the joining points of boundaries.

➥ We introduce an auxiliary CNF-ROM $v(x,t,\mu)$ to learn the first derivatives of $\hat{u}$.

➥ Any second or higher-order derivatives of $\hat{u}$ are approximated using the derivatives of v.

Imposing exact initial and boundary conditions

$$\hat{u}(x,t,\mu;\psi,\theta) = \phi(x,t) D_\psi(x, \alpha_{t,\mu}(\theta)) + u_0(x)$$

- $\phi(x,t) = 0$ holds on initial and boundary sets
- ψ, θ: parameters for decoder and PNODE, respectively
- C_d: collocation points C_o: inner collocation points
- N_d: # collocation points N_o: # inner collocation points

➤ Train $v(x,t,\mu) = D_\xi(x, \beta_{t,\mu})$ via

$$L_{\text{deriv}}(\xi,\theta) = \frac{1}{N_o} \sum_{(x,t,\mu)\in C_o} \left\| D_\xi(x, \beta_{t,\mu}(\theta)) - \partial_x \hat{u} \right\|^2$$

➤ Derivatives of $v(x,t)$ do not suffer from ADF issue anymore.

How to train?

We propose simultaneous learning objectives for both decoder and PNODE parameters.

1. Data matching Loss $L_{\text{data}}(\psi,\theta) = \frac{1}{N_d} \sum_{(x,t,\mu)\in C_d} \| \hat{u}(x,t,\mu;\psi,\theta) - u(x,t,\mu) \|^2$

2. PINN Loss $L_{\text{PDE}}(\psi,\theta) = \frac{1}{N_o} \sum_{(x,t,\mu)\in C_o} \| \mathcal{F}(\hat{u}(x,t,\mu;\psi,\theta), v(x,t,\mu)) \|^2$

- For data loss, solution data $u(x,t,\mu)$ on collocation points are given.
- For PINN loss, $\mathcal{F}$ is PDE residual function and v is used for second or larger order derivatives.

PINN as fine-tuning objective; to learn without data

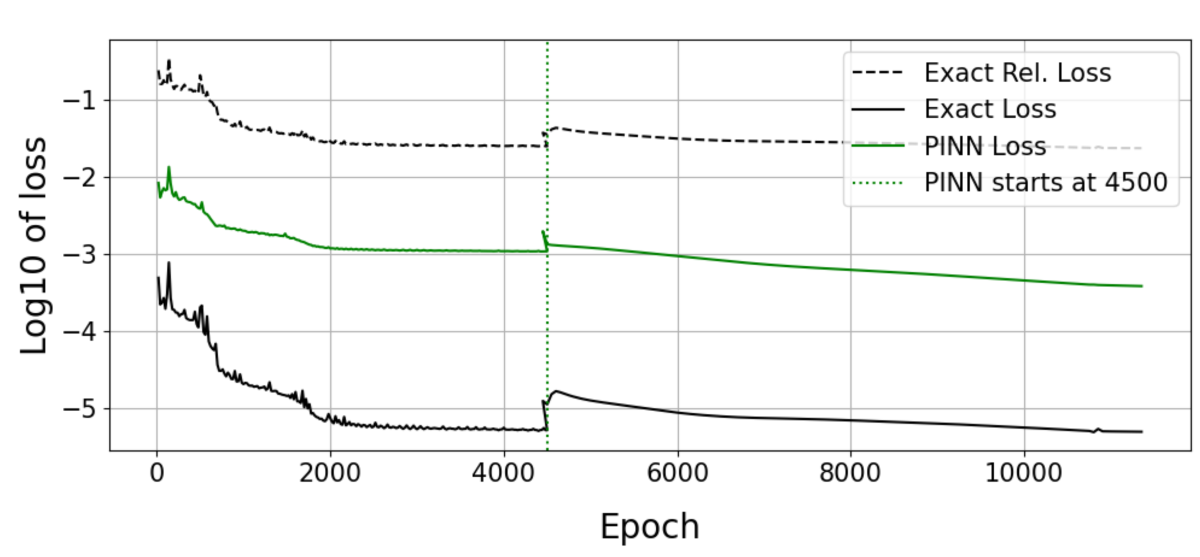
Scenario (a) Pre-training with data: $L_{\text{data}}(\psi,\theta) + L_{\text{deriv}}(\xi,\theta)$

Scenario (b) Fine-tuning with PINN: $L_{\text{PDE}}(\theta) + L_{\text{deriv}}(\theta)$

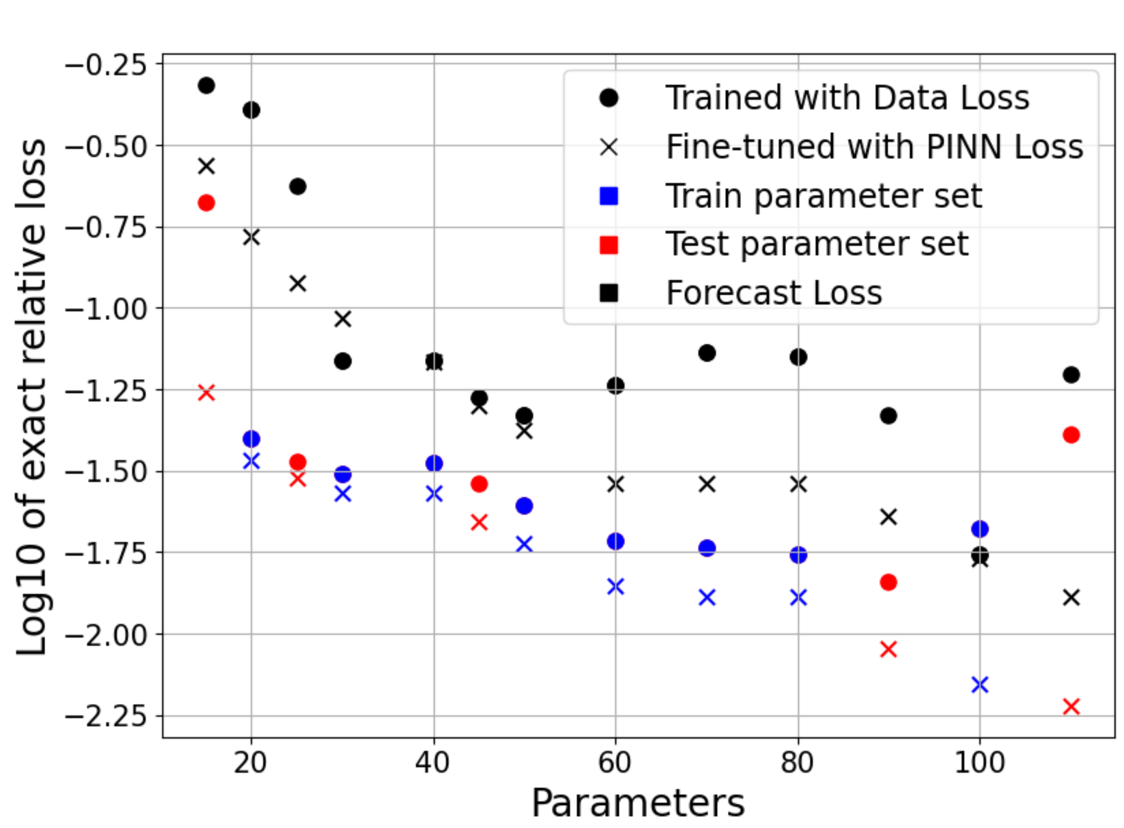
- Only update PNODEs parameter for fine-tuning, with the ROM perspective

Results

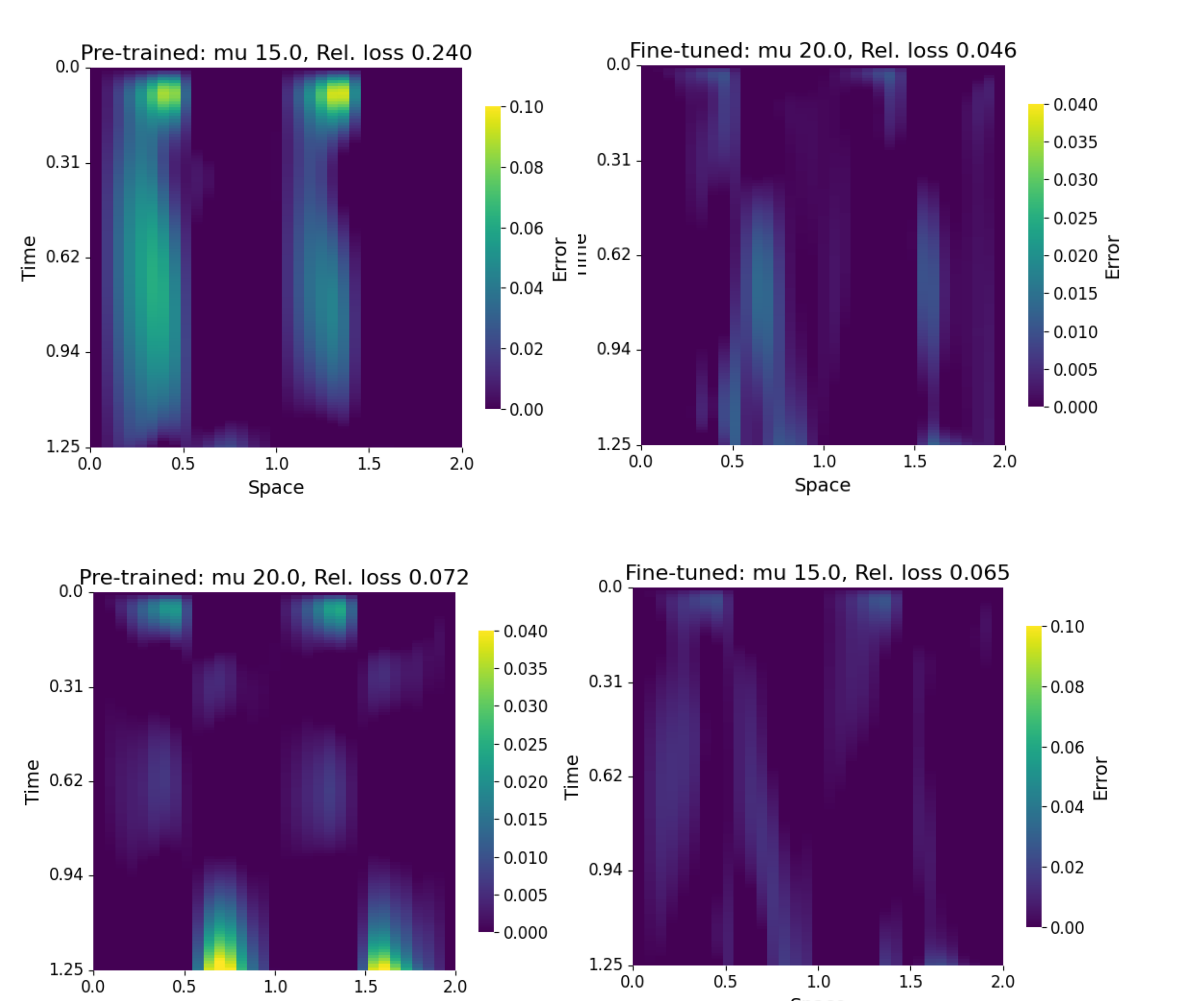
Loss trajectory for (a) → (b)



Fine-tuning performance: parameter inter/extrapolation, time extrapolation



Heatmaps for the loss for (a, left) and (b, right) when μ = 15 (bottom), 20 (top)



- time > 1 corresponds to the time extrapolation region

References

[1] K. Lee and E. J. Parish. Parameterized neural ordinary differential equations: applications to computational physics problems. Proceedings of the Royal Society A, 477(2251):20210162, 2021.

[2] N. Sukumar and A. Srivastava. Exact imposition of boundary conditions with distance functions in physics-informed deep neural networks. *Computer Methods in Applied Mechanics and Engineering*, 389:114333, 2022.

[3] Y. Yin, M. Kirchmeyer, J. Franceschi, A. Rakotomamonjy, and P. Gallinari. Continuous PDE dynamics forecasting with implicit neural representations. In The Eleventh International Conference on Learning Representations, 2023.

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