Interdisciplinary Scientific Computing Laboratory

JOHNS HOPKINS WHITING SCHOOL of ENGINEERING

Physics-Informed Operator Learning on Latent Spaces

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Interdisciplinary Scientific Computing Laboratory Seminar Series

Centrum IntelliPhysics

- Mission: Develop machine learning tools to accelerate engineering innovation
- Focus: Physics-Informed Machine Learning
  - Efficient training strategies for neural operators
  - Developing hybrid solvers (operators + solvers)
- Applications: Multiscale Modeling in Materials, Engineering and Biomedical Systems







Physics-based Models

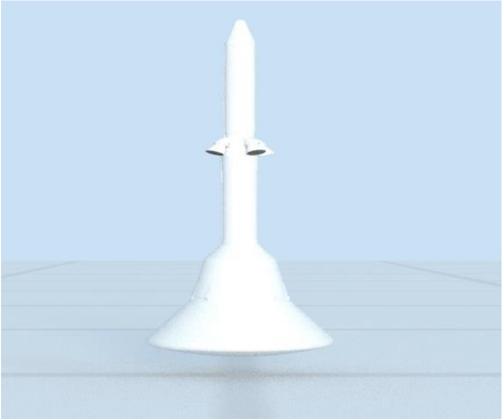
Can represent the **Processes of Nature**

- Physics-based models are approximated via **ODEs/PDEs**

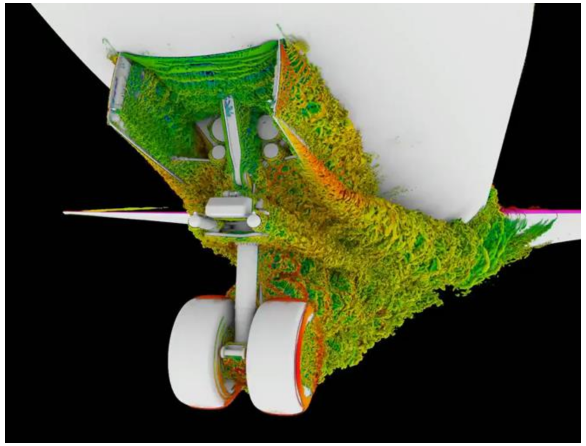
To model earthquake: $m\dfrac{d^2u}{dt^2} + \mathrm{k}\dfrac{du}{dt} + F_0 = 0$

To model waves: $\dfrac{\partial^2 u}{\partial t^2} - v^2\left(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}\right) = 0$

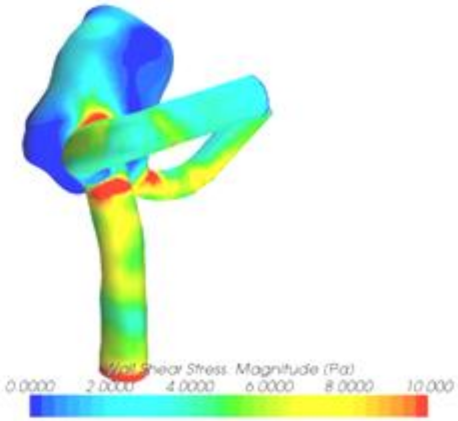
- Computational Mechanics helps us simulate these equations.



Simulation of Orion Spacecraft Launch Abort System (NASA Ames)



Detailed flow around an Aircraft's landing gear (NASA Ames)



CFD Simulation of a Patient-Specific Intracranial Aneurysm

Challenges with Numerical Methods

- Require knowledge of conservation laws, and boundary conditions
- Time consuming and strenuous simulations.
- Difficulties in mesh generation.
- Solving inverse problems or discovering missing physics can be prohibitively expensive.

Develop Physics-based surrogate models for these systems to create a fast-to-evaluate alternative.

Surrogate Modeling Techniques

- Discretized Data
- Discretization dependent
- Queries on mesh
- Learning functions between vector spaces

- Functional Data
- Discretization Invariant
- Continuous quantities
- Learning operators between function spaces

Data-driven

PCA

Auto-encoders

K-PCA

Diffusion maps

f-PCA

DeepONet

LNO

FNO

WNO

F-RKHS

Finite Dimensional

Infinite Dimensional

Physics Informed

PINNs

PI-DeepONet

PINO

Outline

Physics-Informed Operator Learning on Latent Spaces

Part – I: Efficient algorithms beyond the existing ones

Part – II: Data-driven operator learning on reduced spaces

Part – III: Integrating physics and data to learn operator on reduced spaces

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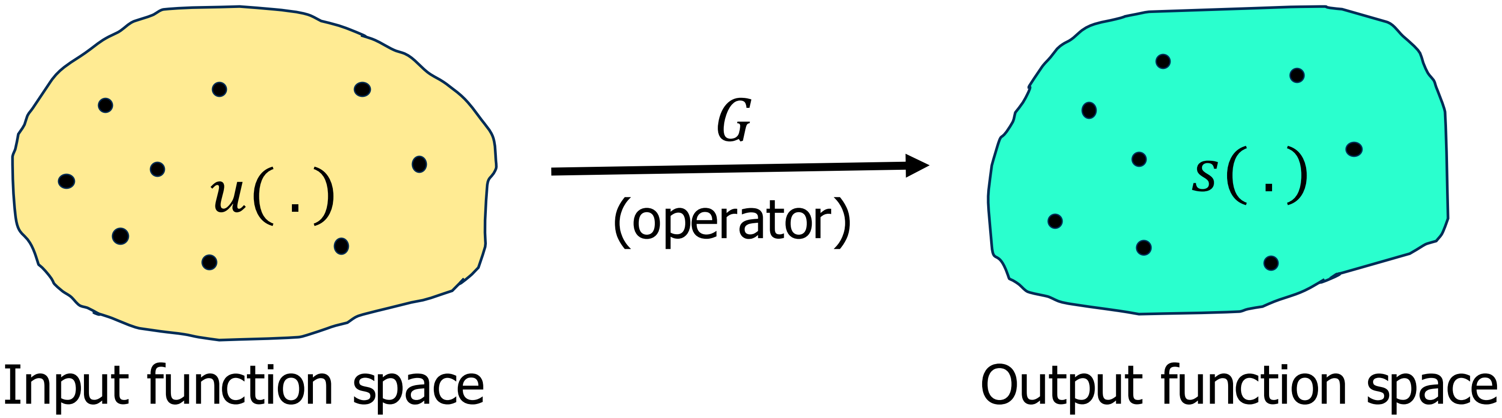
Operator Learning Framework

Input-output map

$$\Phi : \mathcal{U} \rightarrow \mathcal{S}$$

Data $\{\mathcal{U}_n, \mathcal{S}_n\}_{n=1}^{N}$and/or Physics

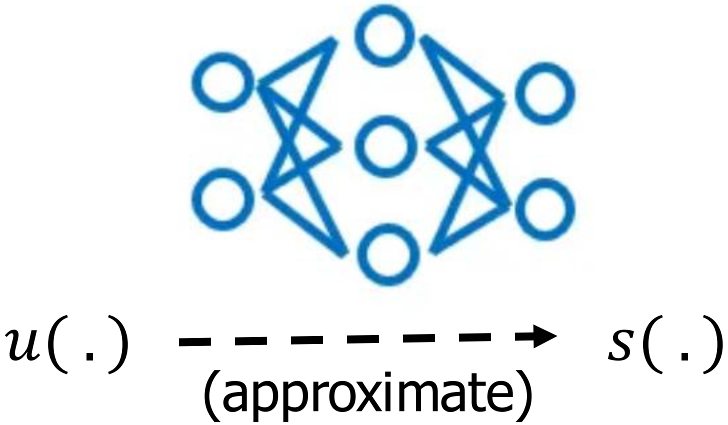
$\mathcal{S}_n = \Phi(\mathcal{F}_n)$, $\mathcal{F}_n \sim \mu \; i.i.d$



Operator learning

$$\Psi : \times \, \Theta \rightarrow \mathcal{S} \text{ such that } \Psi(., \theta^*) \approx \Phi$$

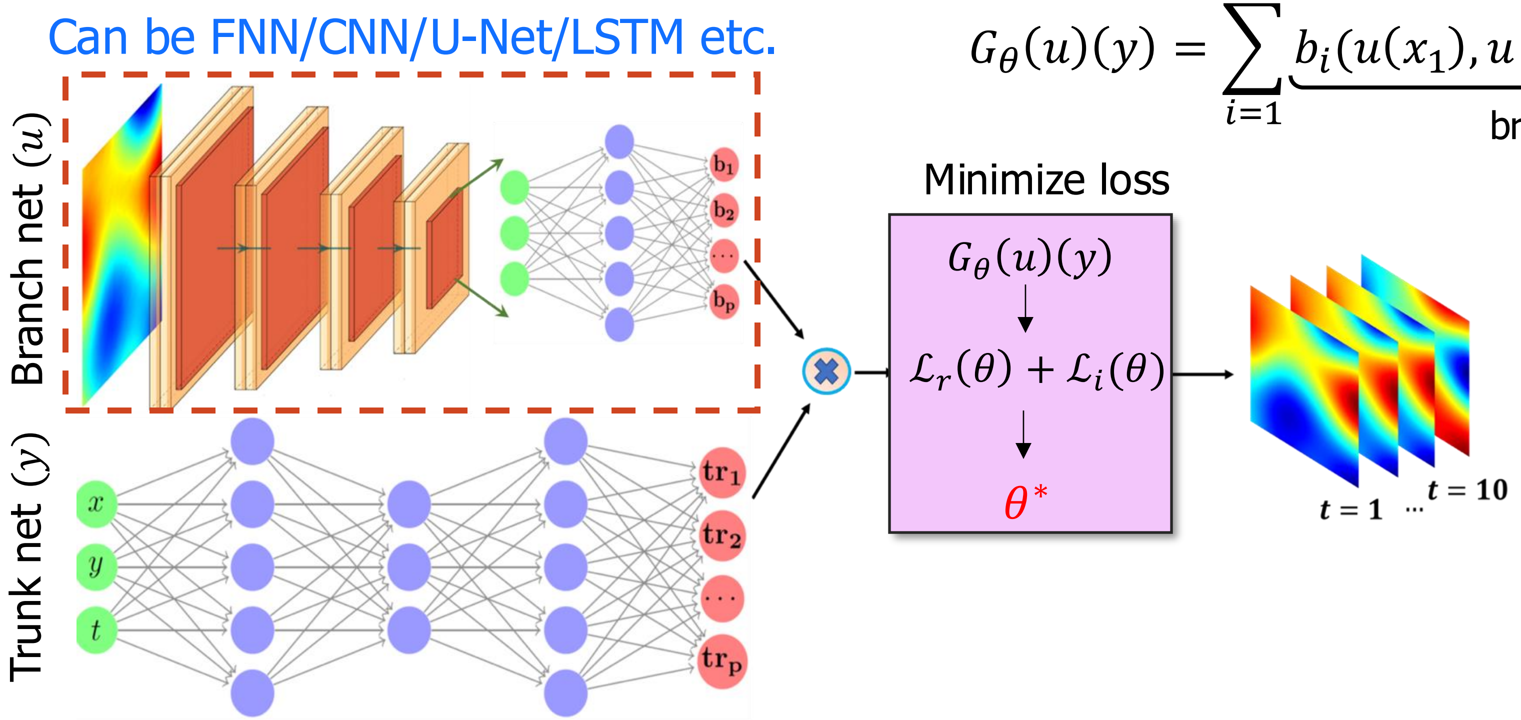
Training $\theta^* = \mathrm{argmin}_\theta \, l(\{\mathcal{U}_n, \Psi(\mathcal{S}_n, \theta)\})$



Deep Operator Network (DeepONet)

- Generalized Universal Approximation Theorem for Operator [Chen '95, Lu et al. '19]
- **Branch net**: Input $\{u(x_i)\}_{i=1}^{m}$, output: $\left[b_1, b_2, .., b_p\right]^T \in \mathbb{R}^p$
- **Trunk net**: Input y, output: $\left[t_1, t_2, .., t_p\right]^T \in \mathbb{R}^p$
- Input u is evaluated at the fixed locations $\{y_i\}_{i=1}^{m}$

$$G_\theta(u)(y) = \sum_{i=1}^{p} \underbrace{b_i(u(x_1), u\,(x_2), \ldots, u\,(x_m))}_{\text{branch net}} \cdot \underbrace{tr_i(y)}_{\text{trunk net}}$$



Data-Driven Training of DeepONet

$\nabla\big(K(\boldsymbol{x})\nabla u(\boldsymbol{x})\big) = 1 \; u(\boldsymbol{x}) = 0 \; \forall \; \boldsymbol{x} \in \partial\Omega$

Nonlinear operator $\mathcal{G} : \mathcal{K} \rightarrow \mathcal{U}$

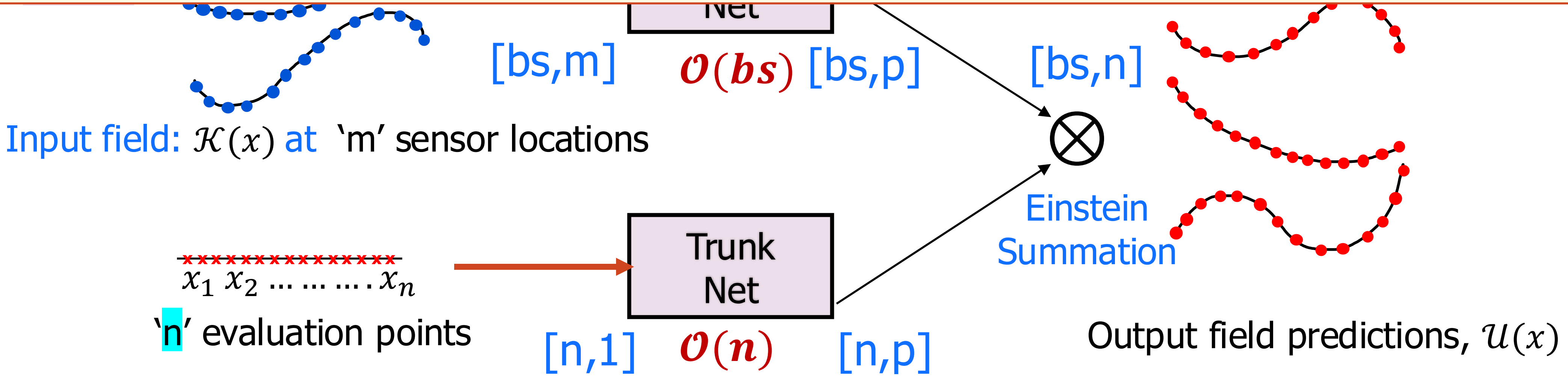
Neural operator $\mathcal{G}_\theta : \mathcal{K} \rightarrow \mathcal{U}, \quad \theta \in \Theta$

Training data $\{\mathbf{x}_i, \boldsymbol{y}_i\}_{i=1}^{N}$

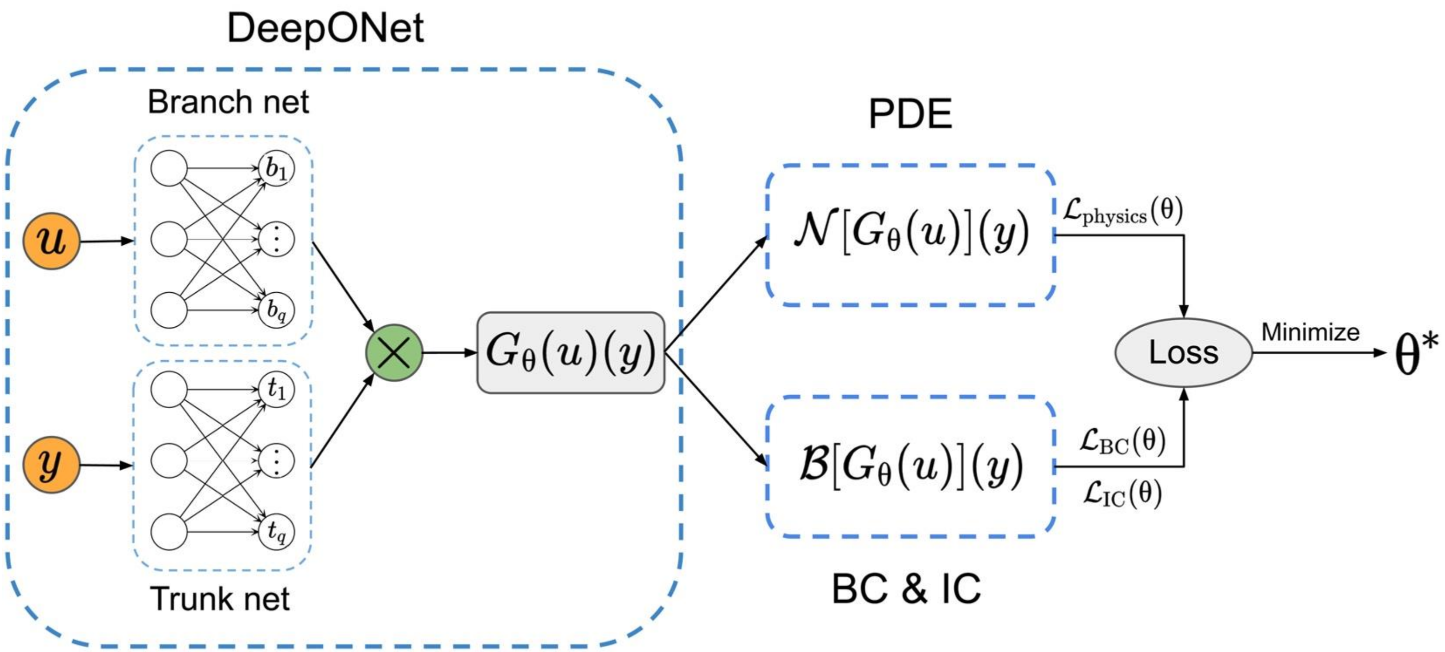
Training Dataset

S.No	Input field data	Output field data
1	$k^1(x_1), \mathrm{k}^1(x_2), \cdots\cdots\cdots, k^1(x_m)$	$\mathrm{u}^1(x_1), \mathrm{u}^1(x_2), \cdots\cdots\cdots, \mathrm{u}^1(x_n)$
2	$k^2(x_1), \mathrm{k}^2(x_2), \cdots\cdots\cdots, \mathrm{k}^2(x_m)$	$u^2(x_1), \mathrm{u}^2(x_2), \cdots\cdots\cdots, \mathrm{u}^2(x_n)$
.	.	.
N	$k^{\mathrm{N}}(x_1), \mathrm{k}^{\mathrm{N}}(x_2), \cdots\cdots\cdots, \mathrm{k}^{\mathrm{N}}(x_m)$	$u^N(x_1), u^N(x_2), \cdots\cdots\cdots, \mathrm{u}^{\mathrm{N}}(x_n)$

Extremely data-hungry.

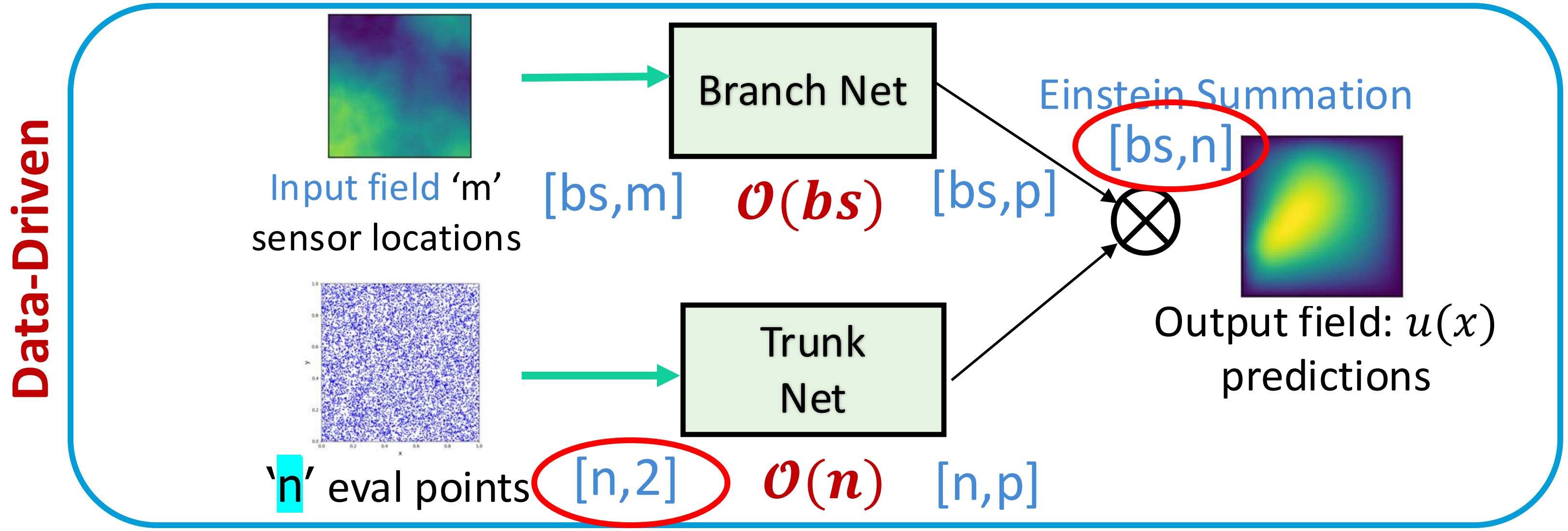


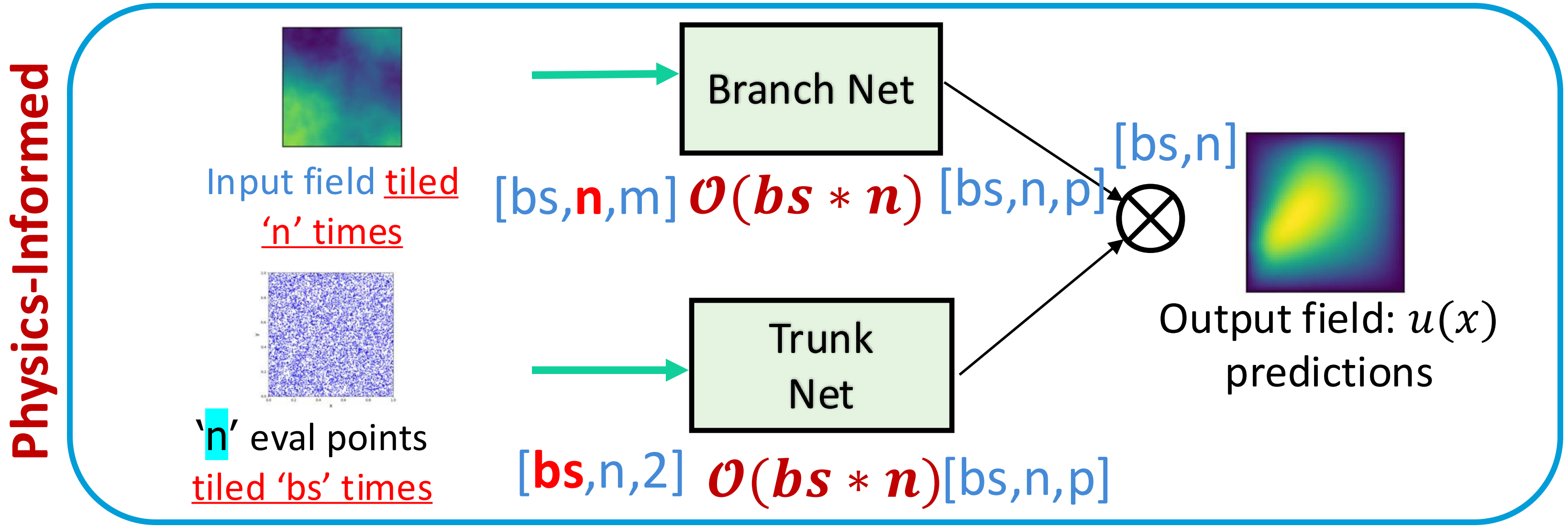
Physics-Informed DeepONet



- Sifan Wang, Hanwen Wang, and Paris Perdikaris. Learning the solution operator of parametric partial differential equations with physics-informed DeepONets. Science Advances, 7(40), October 2021.
- Somdatta Goswami, Yin, M., Yu, Y., & Karniadakis, G. E. (2022). A physics-informed variational DeepONet for predicting crack path in quasi-brittle materials. Computer Methods in Applied Mechanics and Engineering, 391, 114587.

Frameworks for $\nabla(K(\boldsymbol{x})\nabla u(\boldsymbol{x})) = 1$ $u(\boldsymbol{x}) = 0\ \forall\ \boldsymbol{x} \in \partial\Omega$ and $\boldsymbol{x} = (x, y)$





Derivatives

$$\frac{\partial \mathcal{L}}{\partial \theta}$$

$$\frac{\partial \mathcal{L}}{\partial \theta}, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \cdots$$

Reverse-mode autodiff

$$J = [bs * n, bs * n]$$

Shortcomings

↑

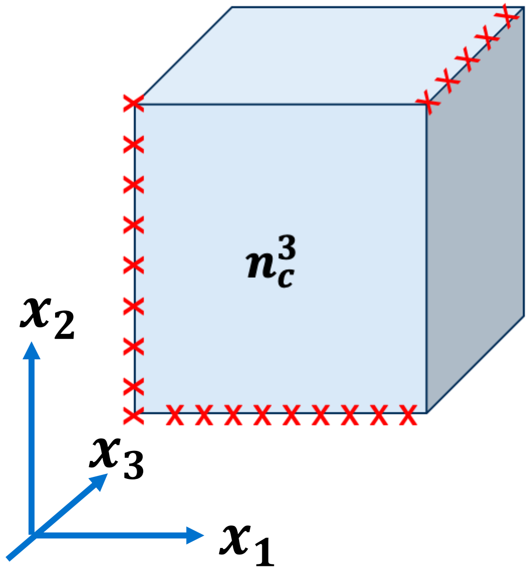
Training is extremely expensive. So, never made it to common practice.

Our Proposed framework

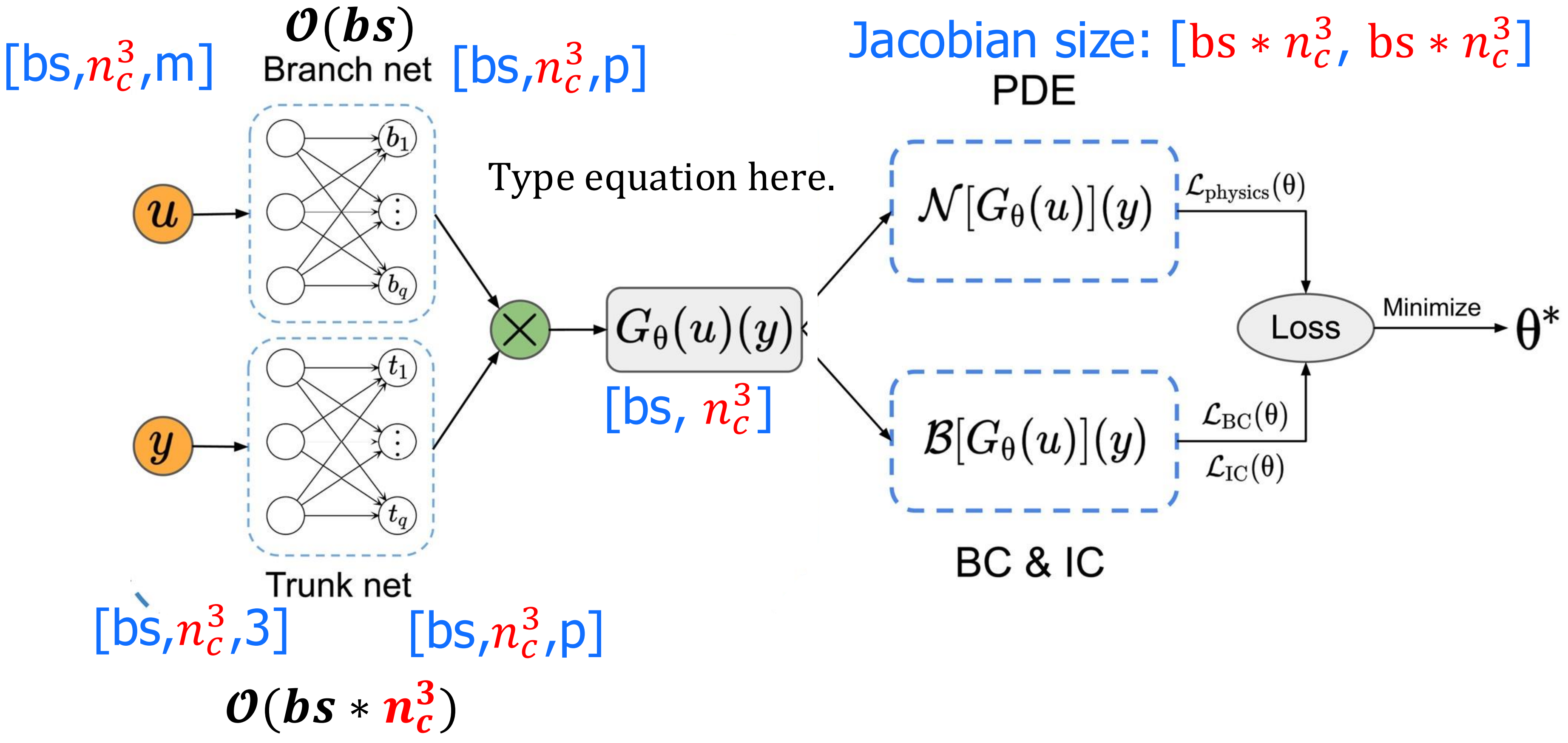
Separable DeepONet: Breaking the Curse of Dimensionality in Physics-Informed Machine Learning

Mandl, Luis, Somdatta Goswami, Lena Lambers, and Tim Ricken. "Separable DeepONet: Breaking the Curse of Dimensionality in Physics-Informed Machine Learning." *arXiv preprint arXiv:2407.15887* (2024).

Vanilla – Physics Informed DeepONet

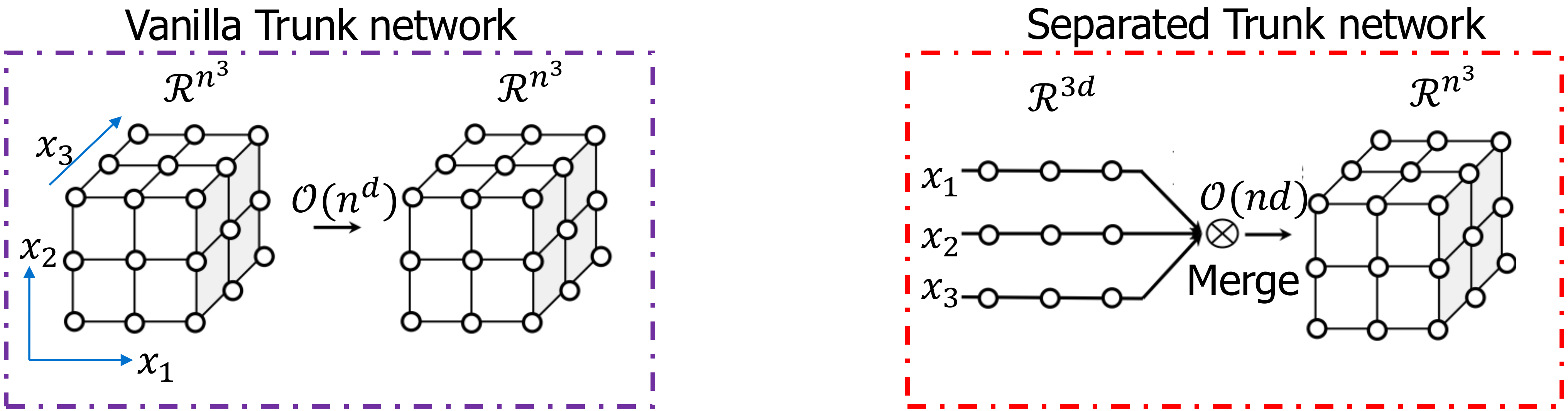


$n_{x_1} = n_{x_2} = n_{x_3} = n_c$



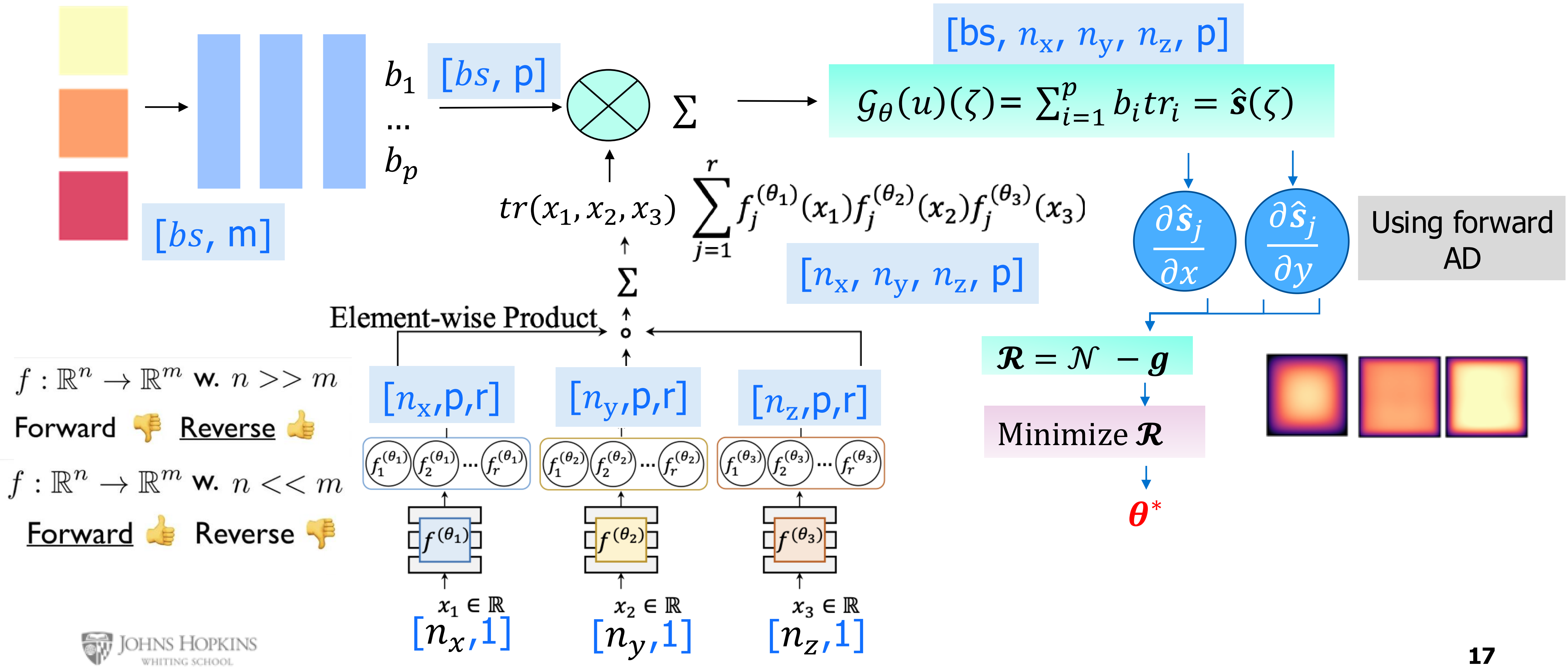
Sifan Wang, Hanwen Wang, and Paris Perdikaris. Learning the solution operator of parametric partial differential equations with physics-informed DeepONets. Science Advances, 7(40), October 2021.

Introducing Separation of Variables



Introduced in PINNs : Cho, J., Nam, S., Yang, H., Yun, S. B., Hong, Y., & Park, E. (2022). Separable PINN: Mitigating the curse of dimensionality in physics-informed neural networks. ArXiv preprint - 2211.08761.

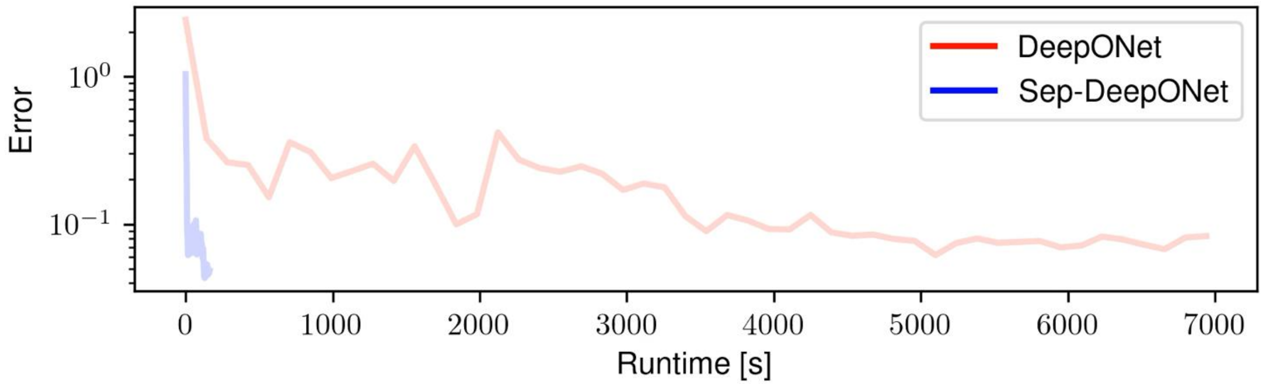
Separable DeepONet Framework



Numerical Examples

Problem	**Model**	**d**	**Relative $\mathcal{L}_2$ error**	**Run-time** (ms/iter.)
Burgers Equation	Vanilla	2	5.1e-2	136.6
	Separable (Ours)		6.2e-2	3.64
Consolidation Biot's Theory	Vanilla	2	7.7e-2	169.43
	Separable (Ours)		7.9e-2	3.68
Parameterized Heat Equation	Vanilla	4	-	10,416.7
	Separable (Ours)		7.7e-2	91.73

Burgers' Equation

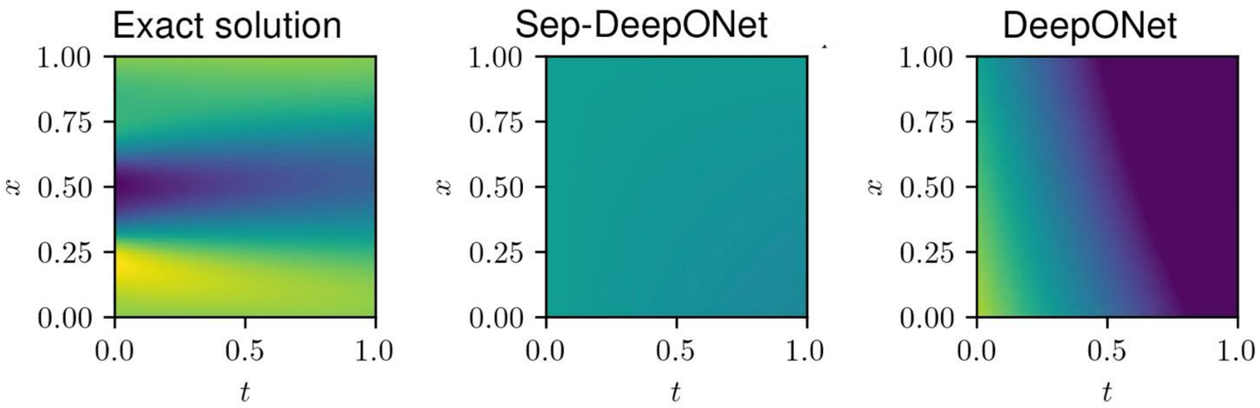


$$\frac{\partial s(x,t)}{\partial t} + s\frac{\partial s(x,t)}{\partial x} - \nu \frac{\partial^2 s(x,t)}{\partial x^2} = 0.$$

$$s(0,t) = s(1,t),$$

$$\frac{\partial s(0,t)}{\partial x} = \frac{\partial s(1,t)}{\partial x},$$

$$s(x,0) = u(x), \quad x \in [0,1]$$



Model	Branch	Trunk	p	r	Parameters	$\mathcal{L}_2$ rel. err.	Runtime [s]	Runtime improvment
Vanilla PI-DeepONet	6×[100]	6×[100]	100	-	131,701	5.14e-2	6,829.2	-
Sep-PI-DeepONet	6×[100]	6×[100]	50	50	672,151	6.24e-2	182.1	97,33%
	6×[100]	6×[100]	20	20	244,921	6.04e-2	197.8	97,10%
	6×[100]	6×[50]	20	20	129,221	6.46e-2	197.0	97,12%

Biot’s Consolidation

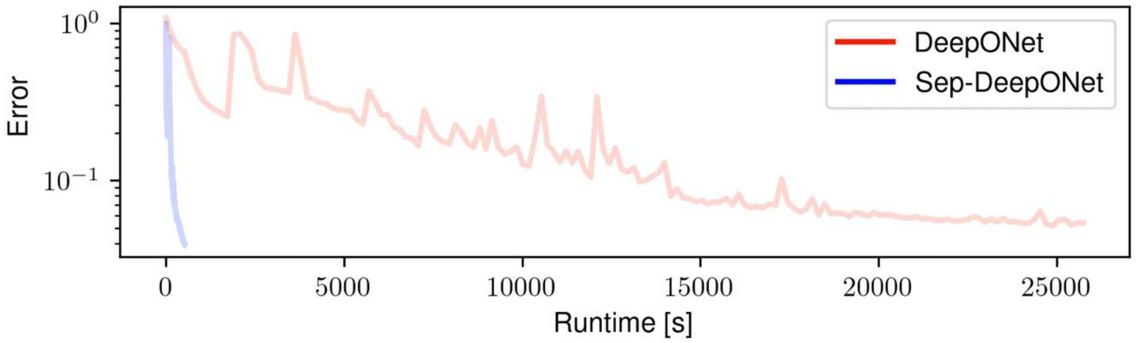
$$(\lambda + 2\mu)\frac{\partial^2 u(z,t)}{\partial z^2} - \frac{\partial p(z,t)}{\partial z} = 0$$

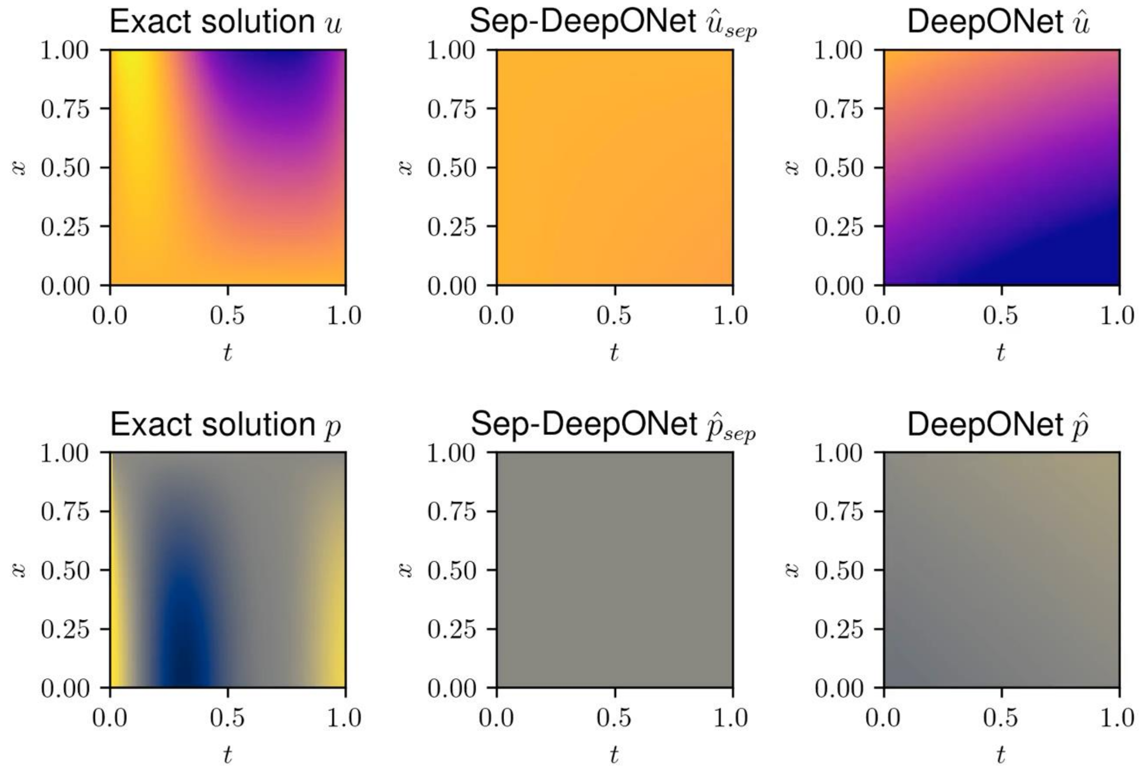
$$\frac{\partial^2 u(z,t)}{\partial t \partial z} - \frac{k}{\rho g}\frac{\partial^2 \tilde{p}(z,t)}{\partial z^2} = 0,$$

$$u(z,0) = 0, \qquad p(0,t) = 0,$$

$$p(z,0) = f(0), \qquad u(L,t) = 0,$$

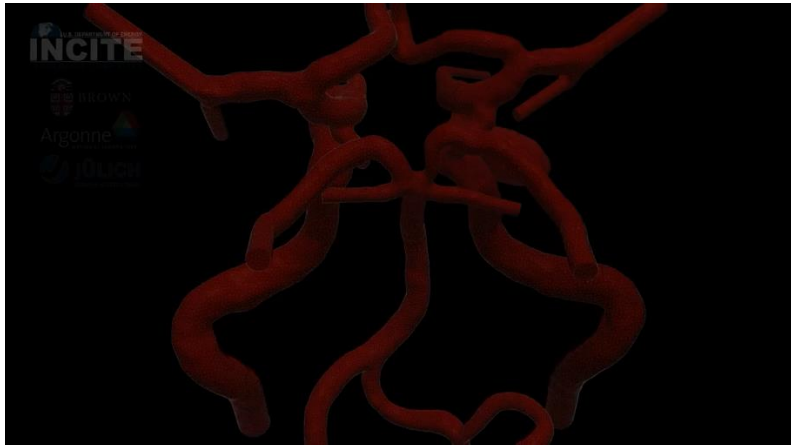
$$\sigma(0,t) = -f(t), \qquad \frac{\partial p(L,t)}{\partial z} = 0,$$

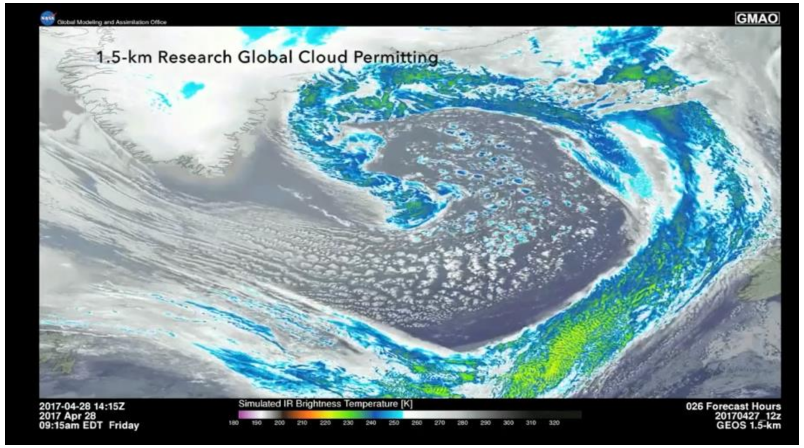


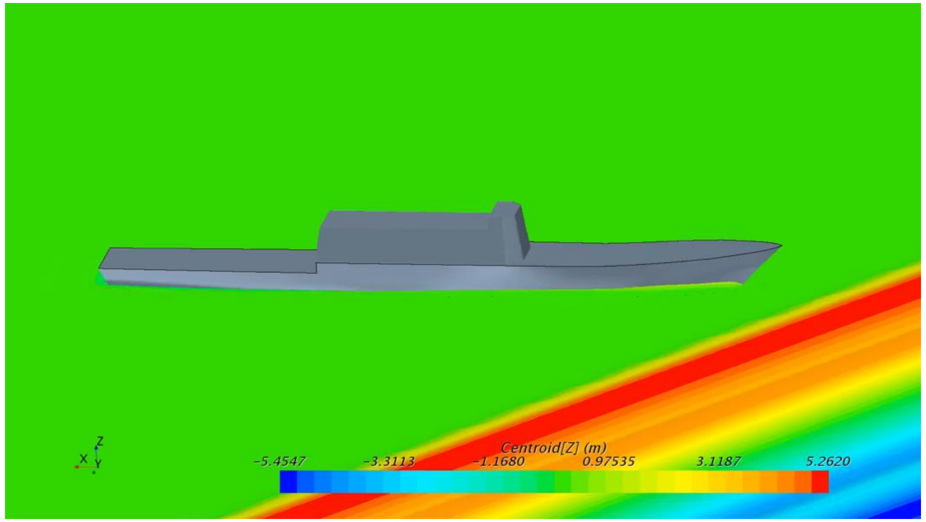


Implementing Physics-Informed DeepONet is not an easy task for complicated systems

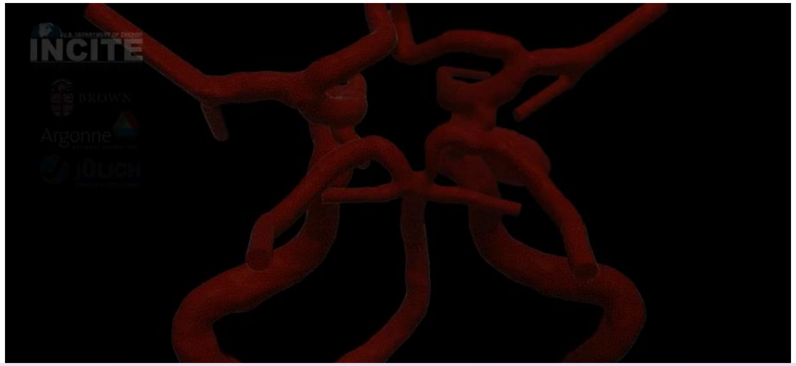
Can we harness the explosion of data to extract knowledge, insight and decision?

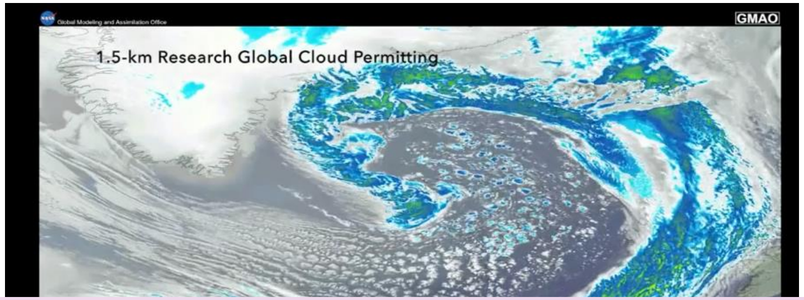

INCITE
Argonne


Global Modeling and Assimilation Office
GMAO
1.5-km Research Global Cloud Permitting
2017-04-28 14:15Z
2017 Apr 28
09:15am EDT Friday
Simulated IR Brightness Temperature [K]
180 190 200 210 220 230 240 250 260 270 280 290 300 310 320
026 Forecast Hours
20170427_12z
GEOS 1.5-km


Centroid[Z] (m)
-5.4547 -3.3113 -1.1680 0.97535 3.1187 5.2620

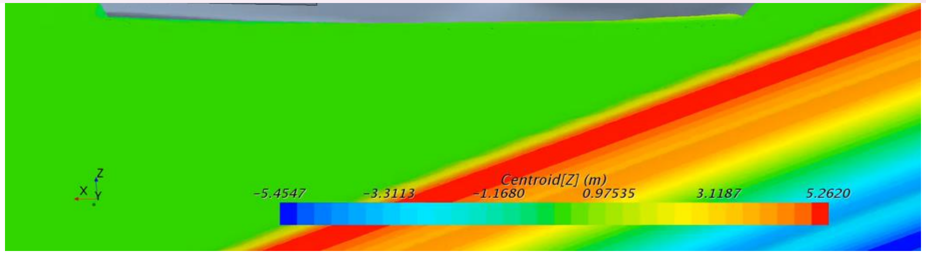

StreamTime LIVE - Baltimore, MD 2024-03-26 01:28:45 EDT





BIG Decisions need BIG MODELS

But we have: sparse high-dimensional datasets



Outline

Physics-Informed Operator Learning on Latent Spaces

Part – I: Efficient algorithms beyond the existing ones

Part – II: Data-driven operator learning on reduced spaces

Part – III: Integrating physics and data to learn operator on reduced spaces

Our Proposed framework

nature communications

Article

https://doi.org/10.1038/s41467-024-49411-w

Learning nonlinear operators in latent spaces for real-time predictions of complex dynamics in physical systems

Viscous Shallow water equation

- Model the dynamics of large-scale atmospheric flows
- Perturbation is used to induce the development of barotropic instability

$$\frac{\mathrm{d}\boldsymbol{V}}{\mathrm{d}t} = -f\boldsymbol{k} \times \boldsymbol{V} - g\nabla h + \nu\nabla^2\boldsymbol{V}$$

$$\frac{\mathrm{d}h}{\mathrm{d}t} = -h\nabla \cdot \boldsymbol{V} + \nu\nabla^2 h$$

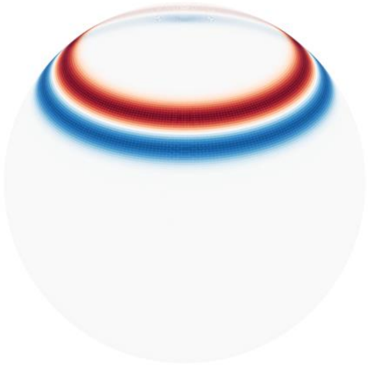
$$h'(\lambda, \phi) = \hat{h}\cos(\phi)\mathrm{e}^{-(\lambda/\alpha)^2}\mathrm{e}^{-[(\phi_2-\phi)/\beta]^2}$$

rvs: $\alpha \sim U[0.\bar{1}, 0.5]$ $\beta \sim U[0.0\bar{3}, 0.2]$

Operator: $\mathcal{G}: h'(\lambda, \varphi, t = 0) \longmapsto u(\varphi, \lambda, t)$

Input Dimension: 65,536

Gaussian Random Perturbation



Output Dimension: 4,718,592

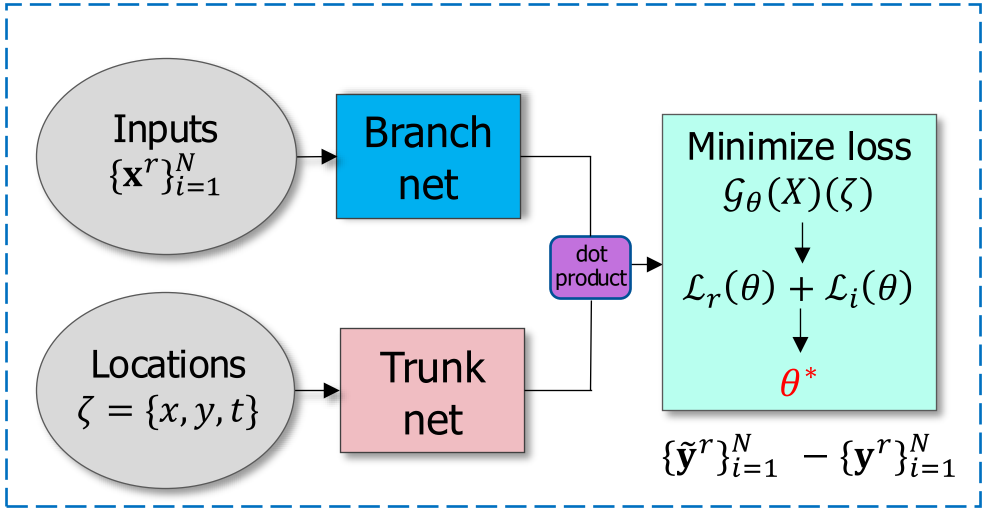
Atmospheric Flow

Latent DeepONet for time-dependent PDEs

Operator $\mathcal{G} : \mathcal{X} \rightarrow \mathcal{Y}$

$\mathcal{G}_\theta : \mathcal{X} \rightarrow \mathcal{Y}, \quad \theta \in \Theta$

Training data $\{\mathbf{x}_i, \boldsymbol{y}_i\}_{i=1}^N$



Latent DeepONet for time-dependent PDEs

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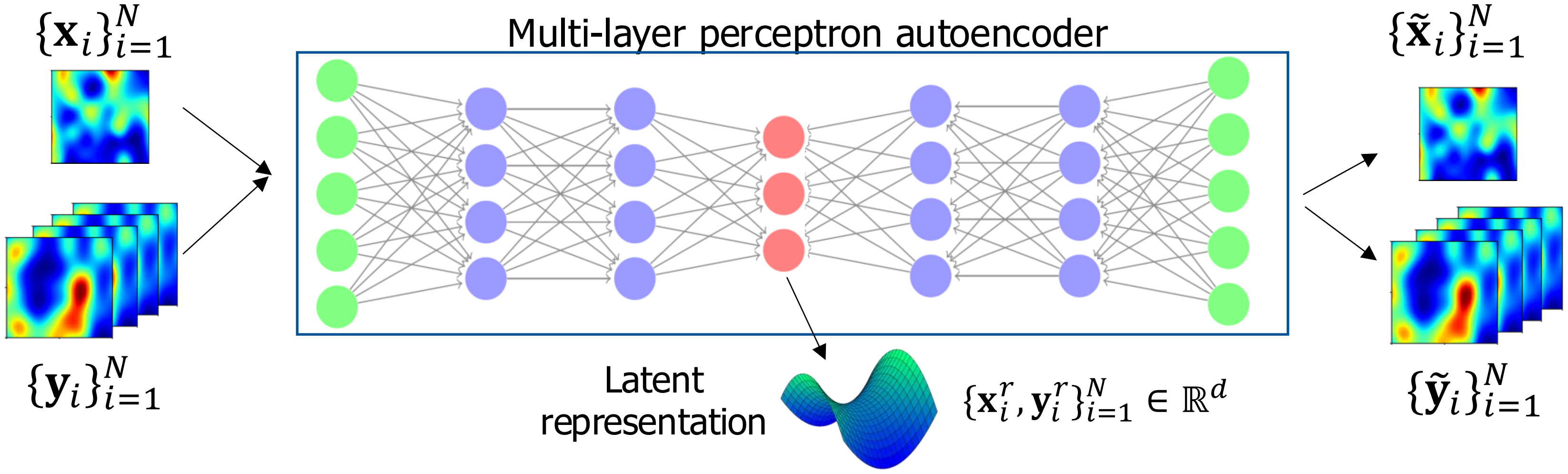
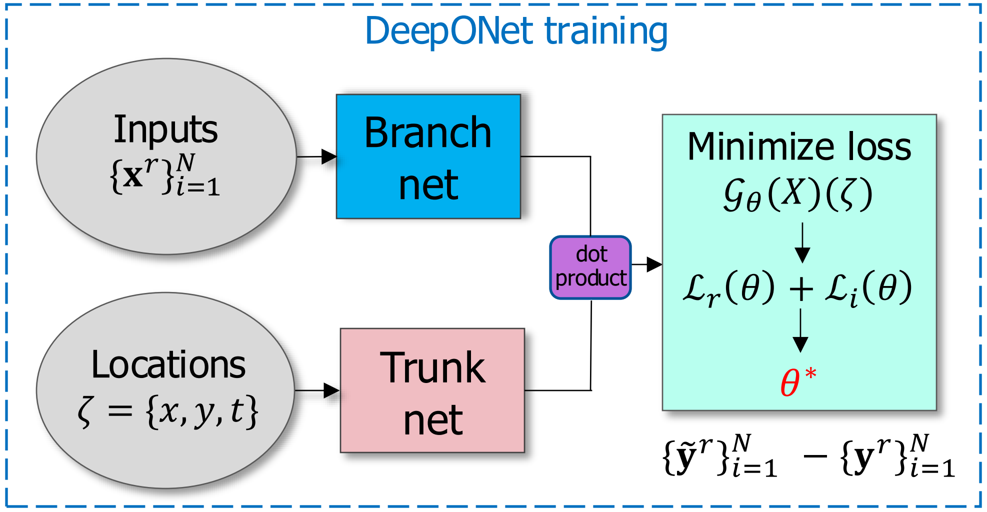
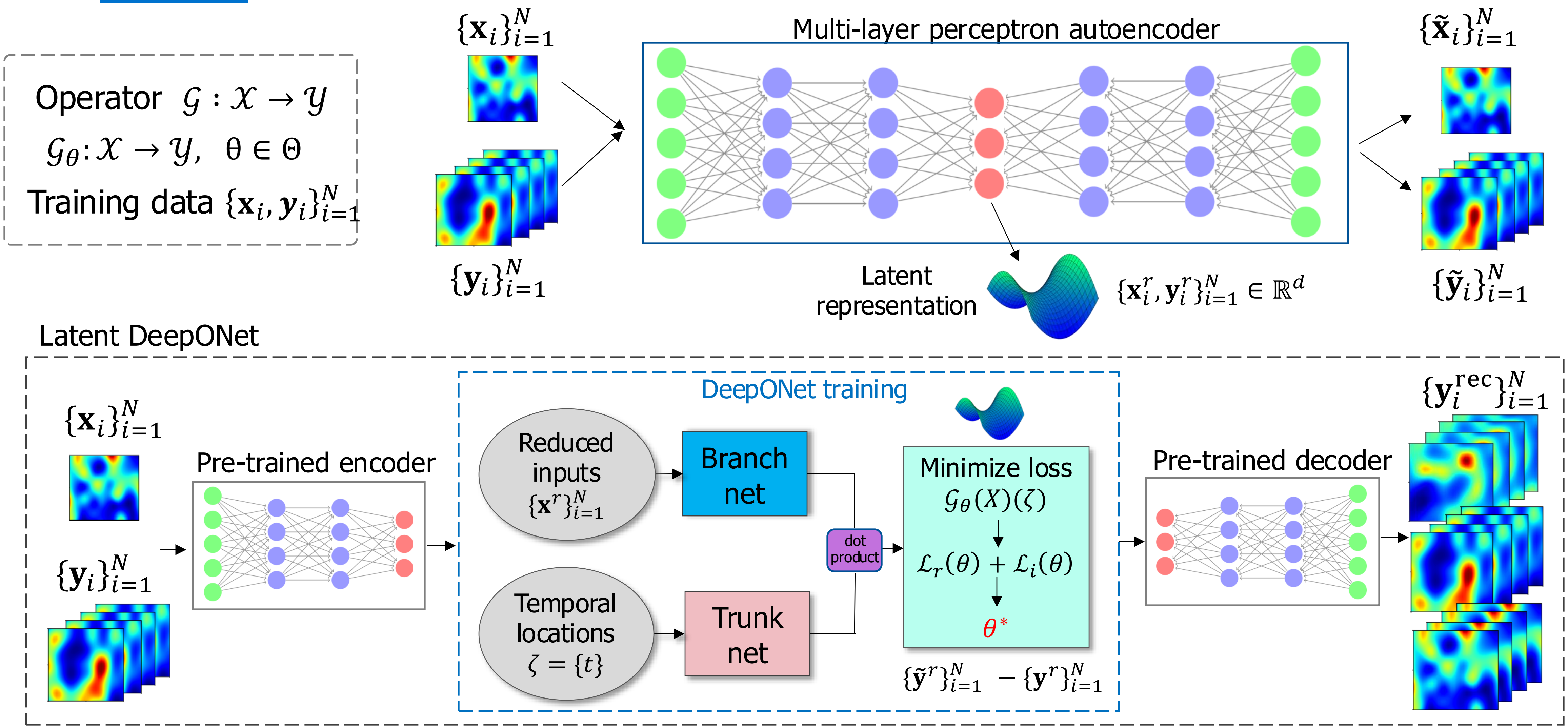




Latent DeepONet for time-dependent PDEs



MLAE: multi-layer autoencoders
PCA: principal component analysis

Consolidated results

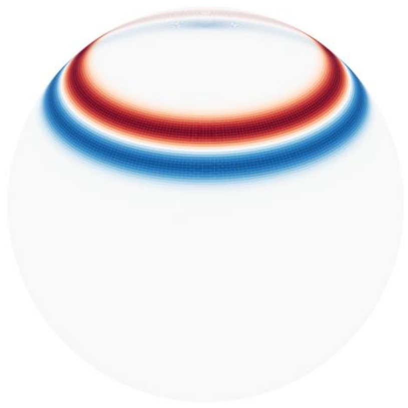
Accuracy of *L-DeepONet for MLAE and PCA*

Application	d	with MLAE	with PCA
Brittle material fracture	9	$3.33 \cdot 10^{-4} \pm 4.99 \cdot 10^{-5}$	$2.71 \cdot 10^{-3} \pm 6.62 \cdot 10^{-6}$
	64	$2.02 \cdot 10^{-4} \pm 1.88 \cdot 10^{-5}$	$3.13 \cdot 10^{-4} \pm 4.62 \cdot 10^{-6}$
Rayleigh-Bénard fluid flow	25	$4.10 \cdot 10^{-3} \pm 8.05 \cdot 10^{-5}$	$3.90 \cdot 10^{-3} \pm 4.73 \cdot 10^{-5}$
	100	$3.55 \cdot 10^{-3} \pm 1.46 \cdot 10^{-4}$	$3.76 \cdot 10^{-3} \pm 4.86 \cdot 10^{-5}$
Shallow water equation	25	$2.30 \cdot 10^{-4} \pm 1.50 \cdot 10^{-5}$	$7.98 \cdot 10^{-4} \pm 8.01 \cdot 10^{-7}$
	81	$2.23 \cdot 10^{-4} \pm 1.83 \cdot 10^{-5}$	$4.18 \cdot 10^{-4} \pm 4.67 \cdot 10^{-6}$

Computational training time in seconds (s) on an NVIDIA A6000 GPU

Application	L-DeepONet	Full DeepONet	FNO-3D
Brittle material fracture	1,660	15,031	128,000
Rayleigh-Bénard fluid flow	2,853	6,772	1,126,400
Shallow water equation	15,218	379,022	–

Spherical shallow water equations



- Model the dynamics of large-scale atmospheric flows
- Barotropically unstable mid-latitude jet (*Ref: Galewsky et al. 2004)*
- Perturbation is used to induce the development of barotropic instability

<u>Shallow-water equations</u>

$$\frac{\mathrm{d}\boldsymbol{V}}{\mathrm{d}t} = -f\boldsymbol{k} \times \boldsymbol{V} - g\nabla h + \nu\nabla^2 \boldsymbol{V}$$

$$\frac{\mathrm{d}h}{\mathrm{d}t} = -h\nabla \cdot \boldsymbol{V} + \nu\nabla^2 h$$

- $\boldsymbol{V} = iu + jv$: velocity vector tangent to the sphere
- h: height field (thickness of the fluid layer)
- $f = 2\Omega\sin\varphi$: Coriolis parameter
- φ: latitude, Ω: angular velocity of Earth, ν: diff. coeff.

<u>Initial condition</u>

$$u(\phi) = \begin{cases} 0 & \text{for} \quad \phi \leq \phi_0 \\ \frac{u_{\max}}{e_n} \exp\left[\frac{1}{(\phi - \phi_0)(\phi - \phi_1)}\right] & \text{for} \ \phi_0 < \phi < \phi_1 \\ 0 & \text{for} \quad \theta \geq \phi_1 \end{cases}$$

$$h'(\lambda, \phi) = \hat{h}\cos(\phi)\mathrm{e}^{-(\lambda/\alpha)^2}\mathrm{e}^{-[(\phi_2 - \phi)/\beta]^2}$$

rvs: $\alpha \sim U[0.\overline{1}, 0.5]$ $\quad \beta \sim U[0.0\overline{3}, 0.2]$

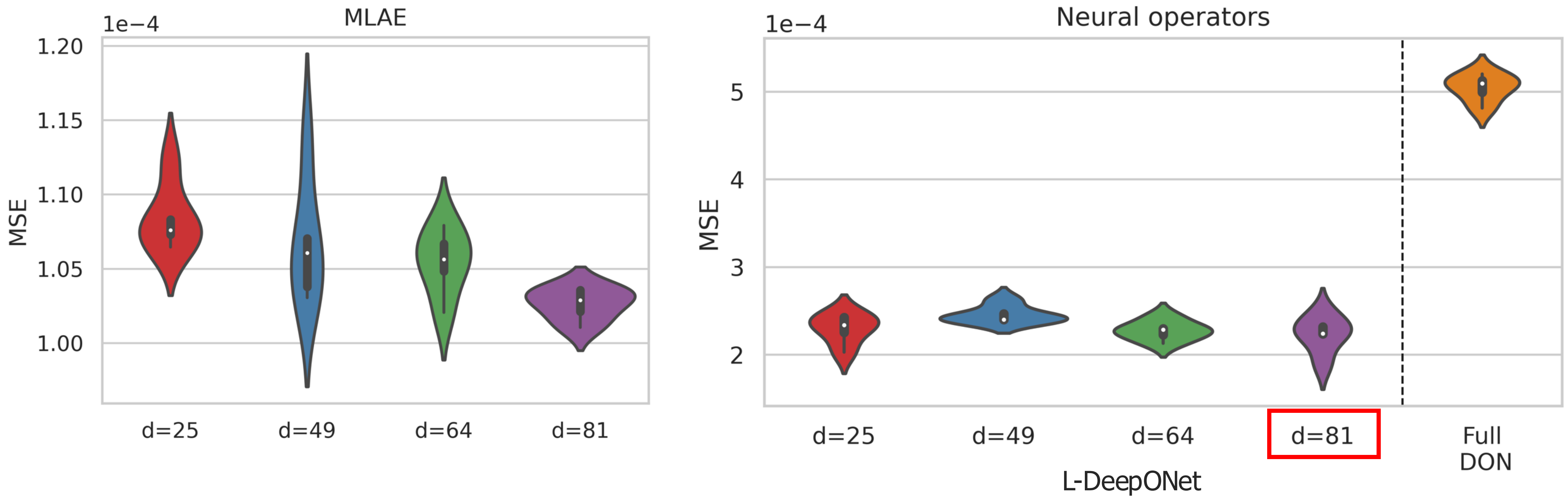
Operator: $\mathcal{G}: h'(\lambda, \varphi, t = 0) \longmapsto u(\varphi, \lambda, t)$

Results

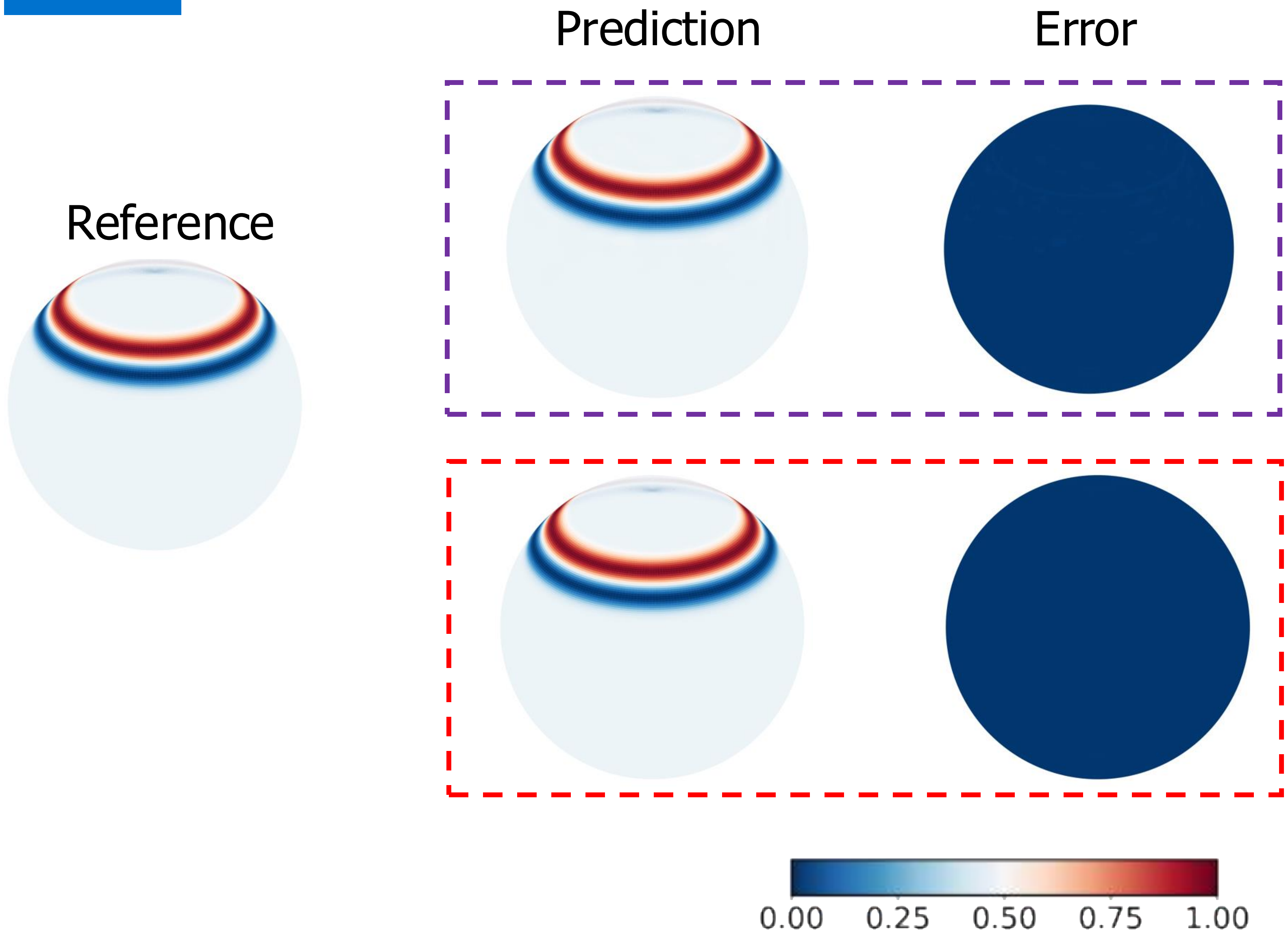
- $\Omega = [0,2\pi]x[0,2\pi]$, $(n_x \; x \; n_y) = (256x256)$ mesh points
- Output dimensionality: $72x256x256 = 4{,}718{,}592$
- Simulation: $t = [0{,}360h], \delta t = 0.1\bar{6}h$, Time steps: $n_t = 72$

Training Time (seconds)

MLAE + Latent DON: 15, 218
Full DON: 379,022



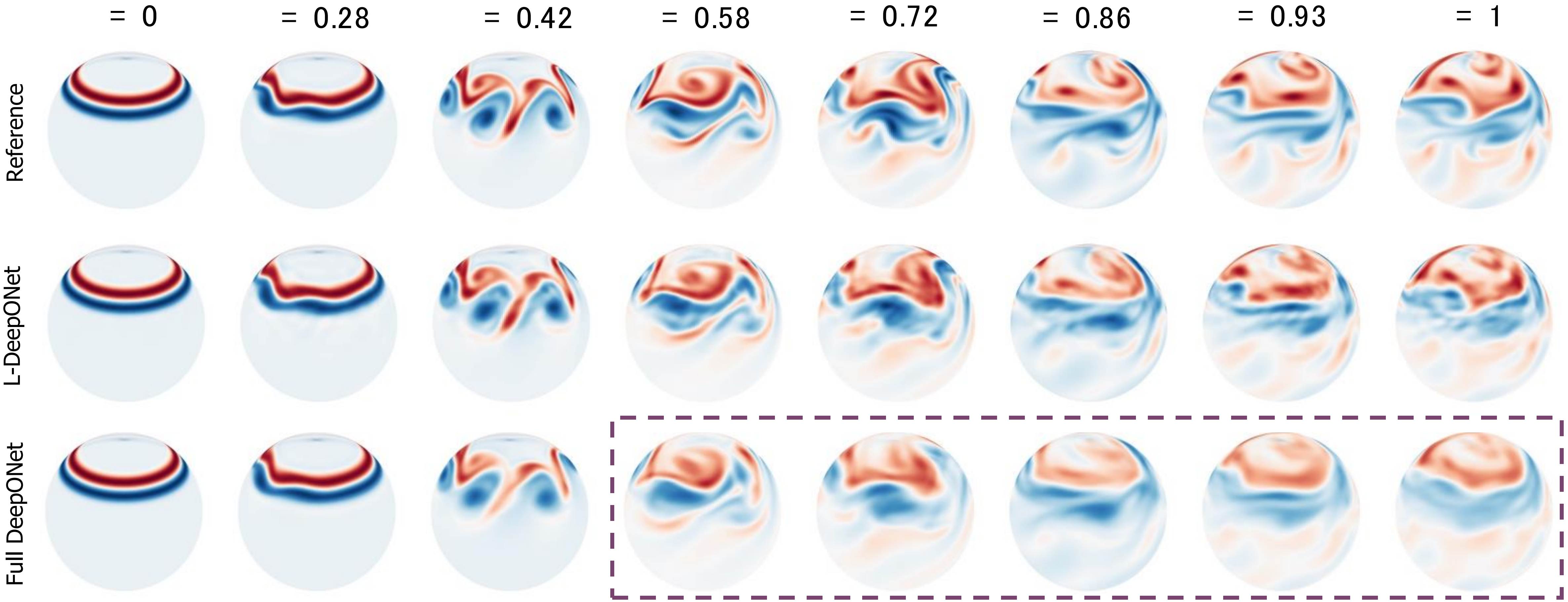
Results



Latent DeepONet
(275,475 Parameters)

DeepONet
(327,872 Parameters)

Latent DeepONet and Full DeepONet



Shortcomings

↑

The framework requires voluminious training data.

Since it’s a two-stage training, the governing physics cannot be incorporated.

Outline

Physics-Informed Operator Learning on Latent Spaces

Part – I: Efficient algorithms beyond the existing ones

Part – II: Data-driven operator learning on reduced spaces

Part – III: Integrating physics and data to learn operator on reduced spaces

Our Proposed framework

Physics-Informed Latent Neural Operator: Integrating Physics and Data using Reduced Order Modeling

Manuscript in preparation

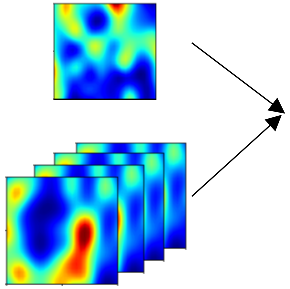
One-shot Learning: Physics Informed Latent Neural Operator

Operator $\mathcal{G} : \mathcal{X} \to \mathcal{Y}$

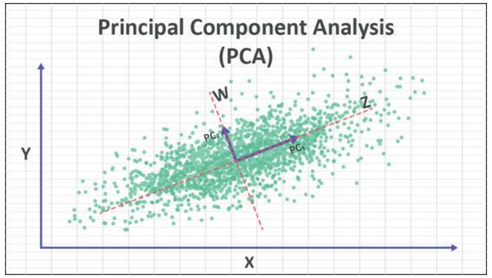
$\mathcal{G}_\theta : \mathcal{X} \to \mathcal{Y}, \quad \theta \in \Theta$

Training data $\{\mathbf{x}_i, \boldsymbol{y}_i\}_{i=1}^{N}$

N(way less than data-driven)

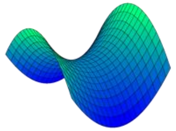


$\{\mathbf{y}_i\}_{i=1}^{N}$

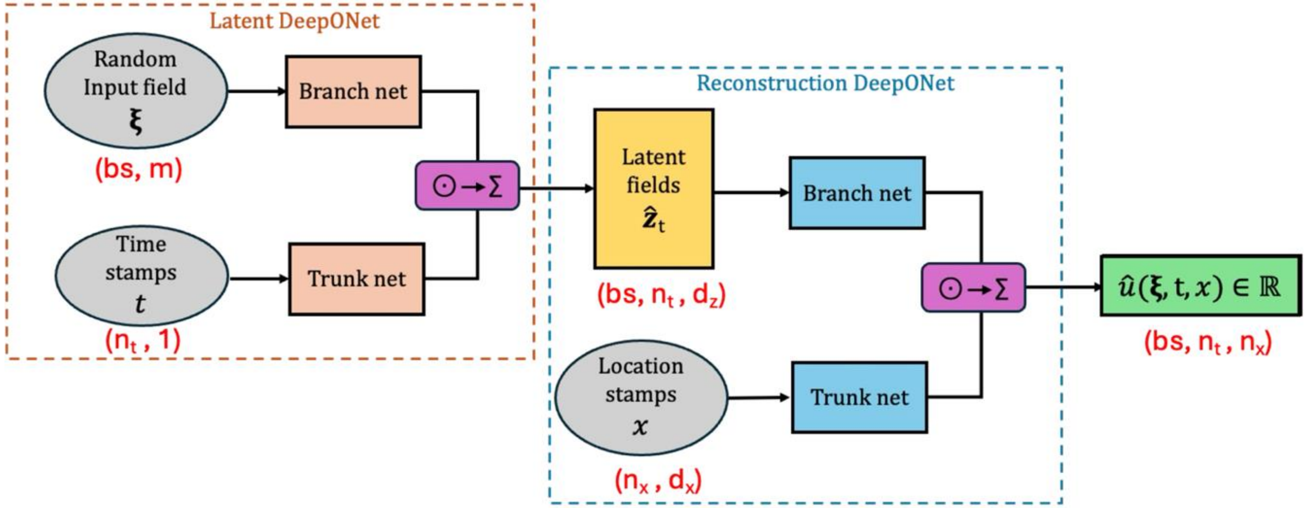


Or Autoencoder

Latent representation



$\{\mathbf{x}_i^r, \mathbf{y}_i^r\}_{i=1}^{N} \in \mathbb{R}^d$

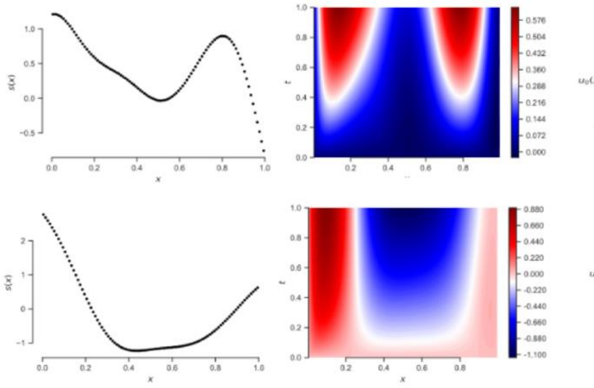
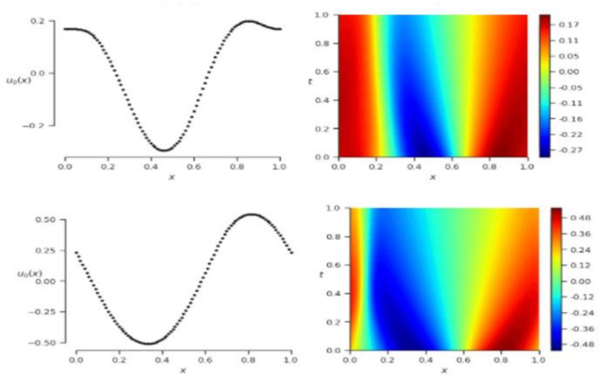
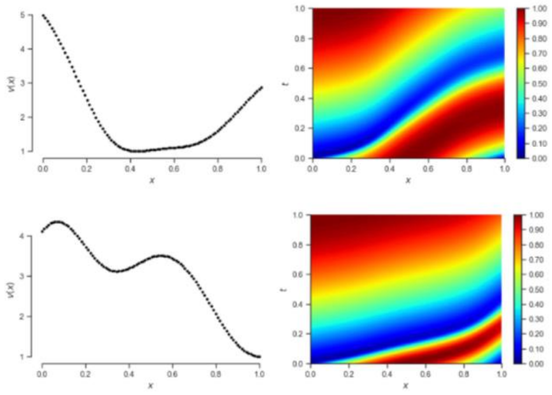


$$\mathcal{L}(\boldsymbol{\theta}) = \mathcal{L}_{\text{data-driven}}(\boldsymbol{\theta}) + \mathcal{L}_{\text{physics-informed}}(\boldsymbol{\theta}),$$

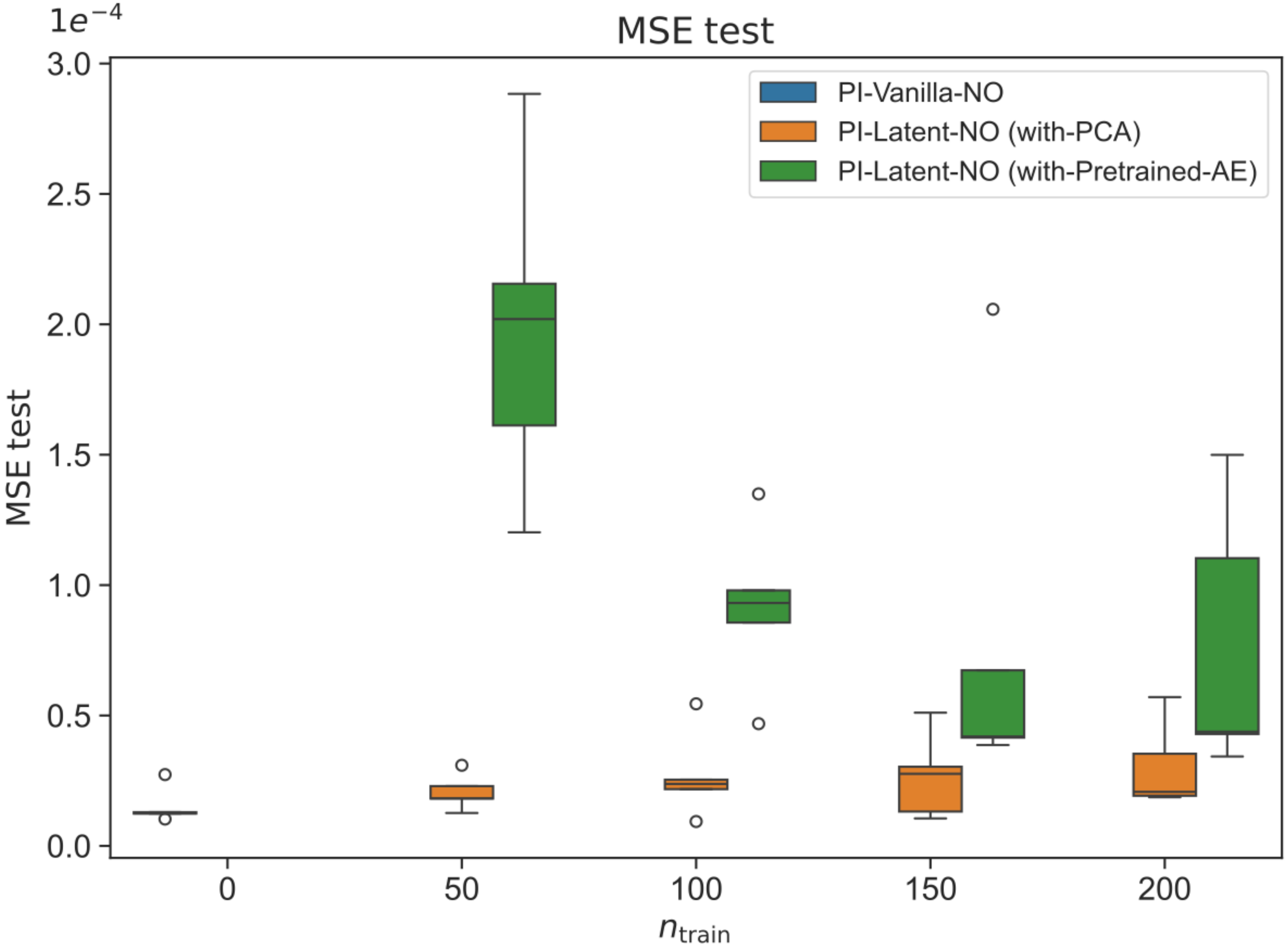
$$\mathcal{L}_{\text{data-driven}}(\boldsymbol{\theta}) = \frac{1}{n_{\text{train}}(n_t+1)} \sum_{i=1}^{n_{\text{train}}} \sum_{j=0}^{n_t} \left\| \mathbf{z}(\boldsymbol{\xi}^{(i)}, j\Delta t) - \hat{\mathbf{z}}(\boldsymbol{\xi}^{(i)}, j\Delta t) \right\|_2^2$$

$$+ \frac{1}{n_{\text{train}}(n_t+1)n_{\boldsymbol{x}}} \sum_{i=1}^{n_{\text{train}}} \sum_{j=0}^{n_t} \sum_{k=1}^{n_{\boldsymbol{x}}} \left(u(\boldsymbol{\xi}^{(i)}, j\Delta t, \boldsymbol{x}^{(k)}) - \hat{u}(\boldsymbol{\xi}^{(i)}, j\Delta t, \boldsymbol{x}^{(k)}) \right)^2,$$

$$\mathcal{L}_{\text{physics-informed}}(\boldsymbol{\theta}) = \mathcal{L}_r(\boldsymbol{\theta}) + \mathcal{L}_{bc}(\boldsymbol{\theta}) + \mathcal{L}_{ic}(\boldsymbol{\theta}).$$

Case	Diffusion-reaction dynamics	Burgers' transport dynamics	Advection
PDE	$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + ku^2 + s(x),$ $D = 0.01,\ k = 0.01,$ $(t,x) \in (0,1] \times (0,1],$ $u(0,x) = 0,\ x \in (0,1)$ $u(t,0) = 0,\ t \in (0,1)$ $u(t,1) = 0,\ t \in (0,1)$ $\mathcal{G}_{\boldsymbol{\theta}} : s(x) \to u(t,x).$	$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0,$ $\nu = 0.01,$ $(t,x) \in (0,1] \times (0,1],$ $u(0,x) = g(x),\ x \in (0,1)$ $u(t,0) = u(t,1)$ $\frac{\partial u}{\partial x}(t,0) = \frac{\partial u}{\partial x}(t,1)$ $\mathcal{G}_{\boldsymbol{\theta}} : g(x) \to u(t,x).$	$\frac{\partial u}{\partial t} + s(x)\frac{\partial u}{\partial x} = 0,$ $(t,x) \in (0,1] \times (0,1],$ $u(0,x) = \sin(\pi x)\ \forall\ x \in (0,1),$ $u(t,0) = \sin(0.5\pi t)\ \forall\ t \in (0,1),$ $s(x) = v(x) - \min_x v(x) + 1$ $\mathcal{G}_{\boldsymbol{\theta}} : v(x) \to u(t,x).$
Input Function	$s(x) \sim \mathrm{GP}(0, k(x,x')),$ $\ell_x = 0.2,\ \sigma^2 = 1.0,$ $k(x,x') = \sigma^2 \exp\left\{-\frac{\\|x-x'\\|^2}{2\ell_x^2}\right\}.$	$g(x) \sim \mathcal{N}\left(0, 25^2\left(-\Delta + 5^2 I\right)^{-4}\right),$	$v(x) \sim \mathrm{GP}(0, k(x,x')),$ $\ell_x = 0.2,\ \sigma^2 = 1.0,$ $k(x,x') = \sigma^2 \exp\left\{-\frac{\\|x-x'\\|^2}{2\ell_x^2}\right\}.$
Samples			

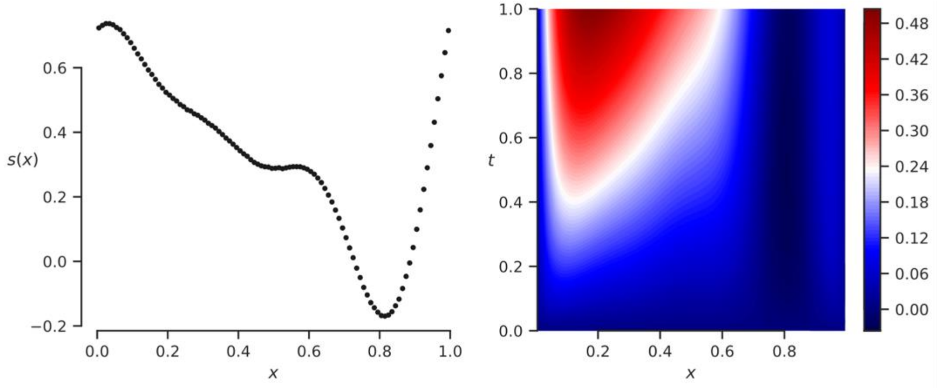
Accuracy Comparison



Reaction Diffusion Dynamics

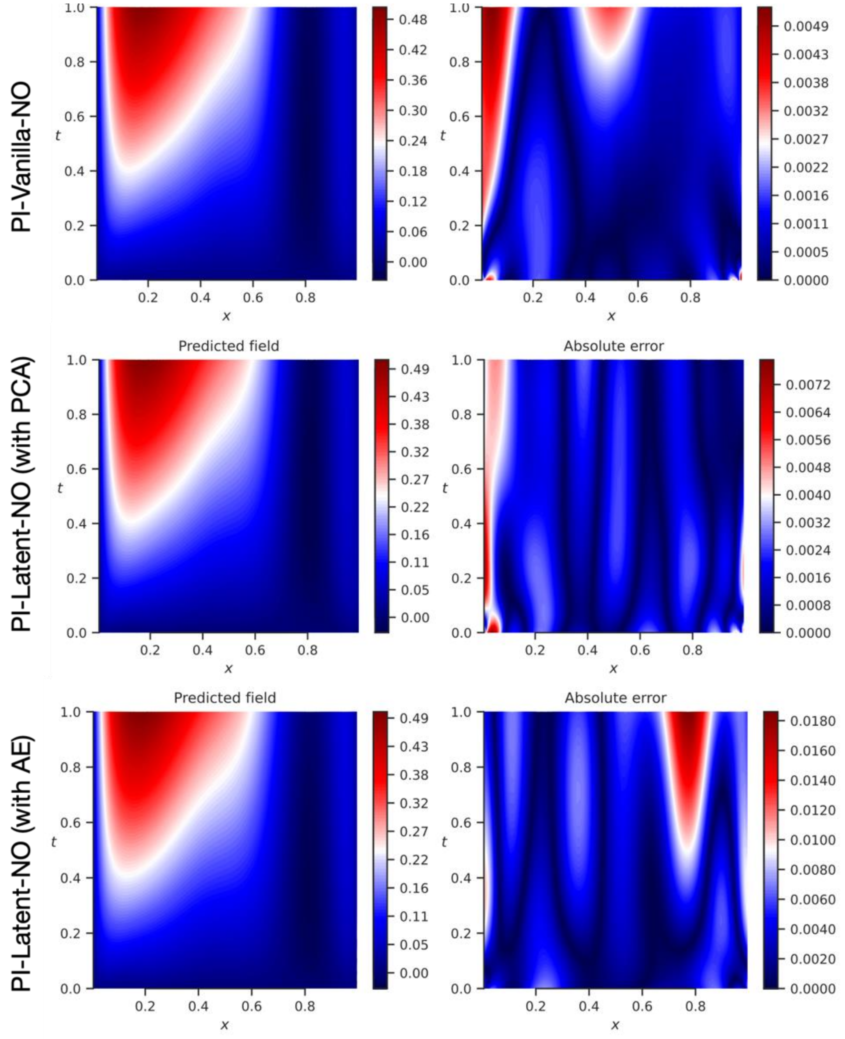
Source
(Input function)

Solution
(Ground Truth)

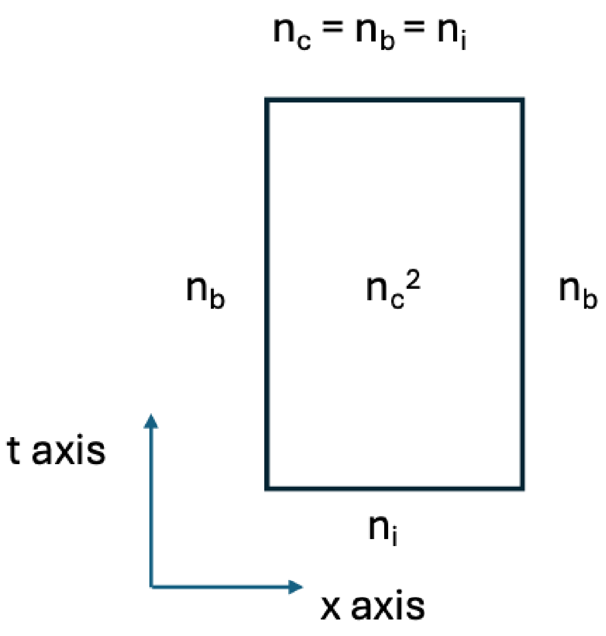


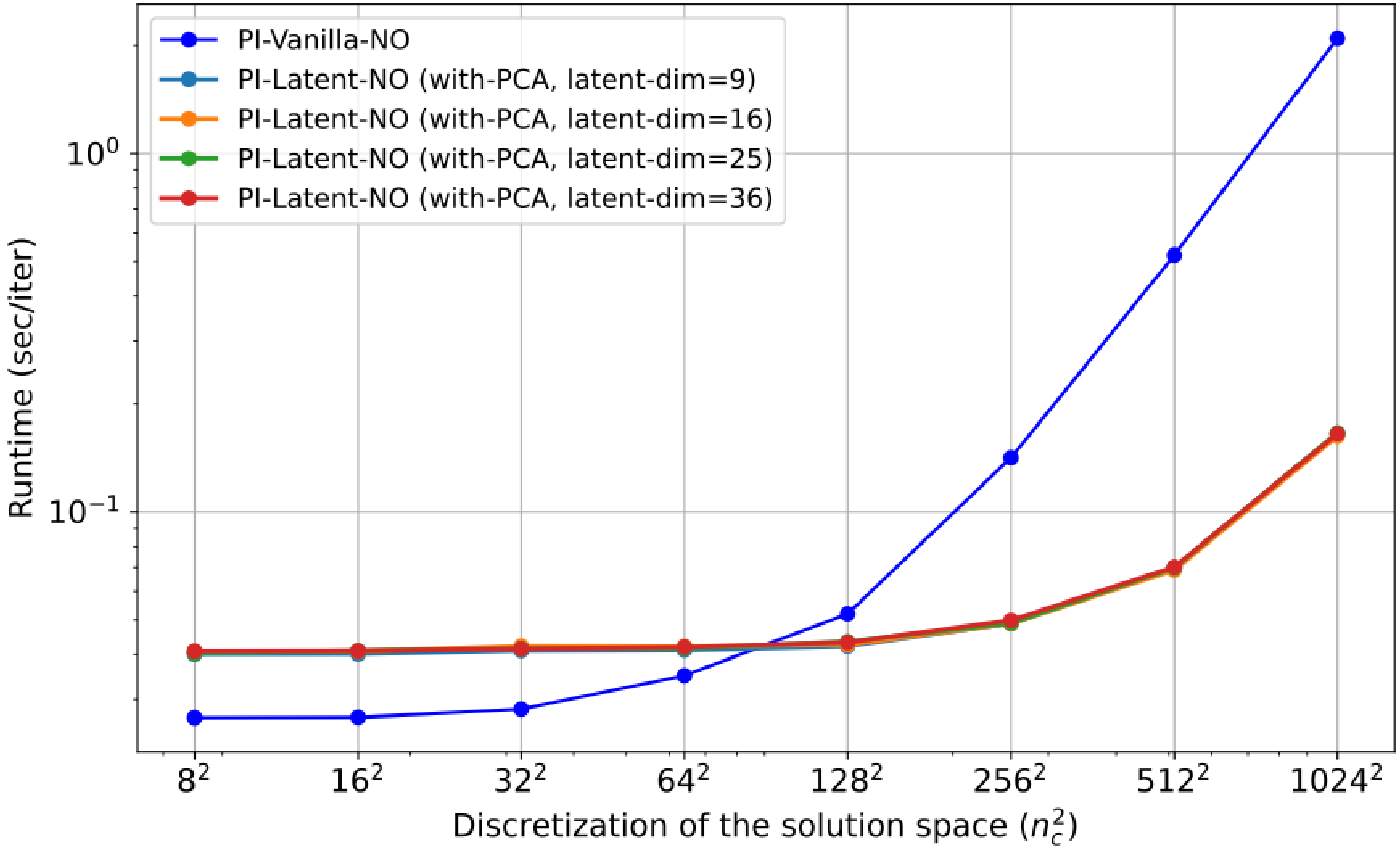
Prediction

Error

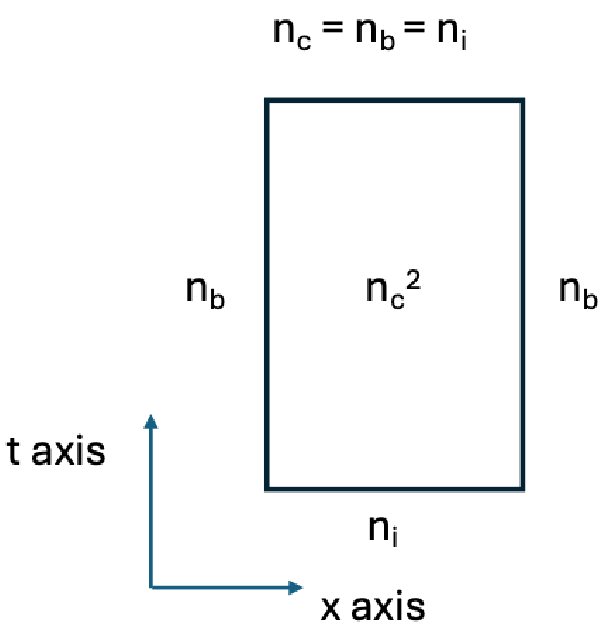


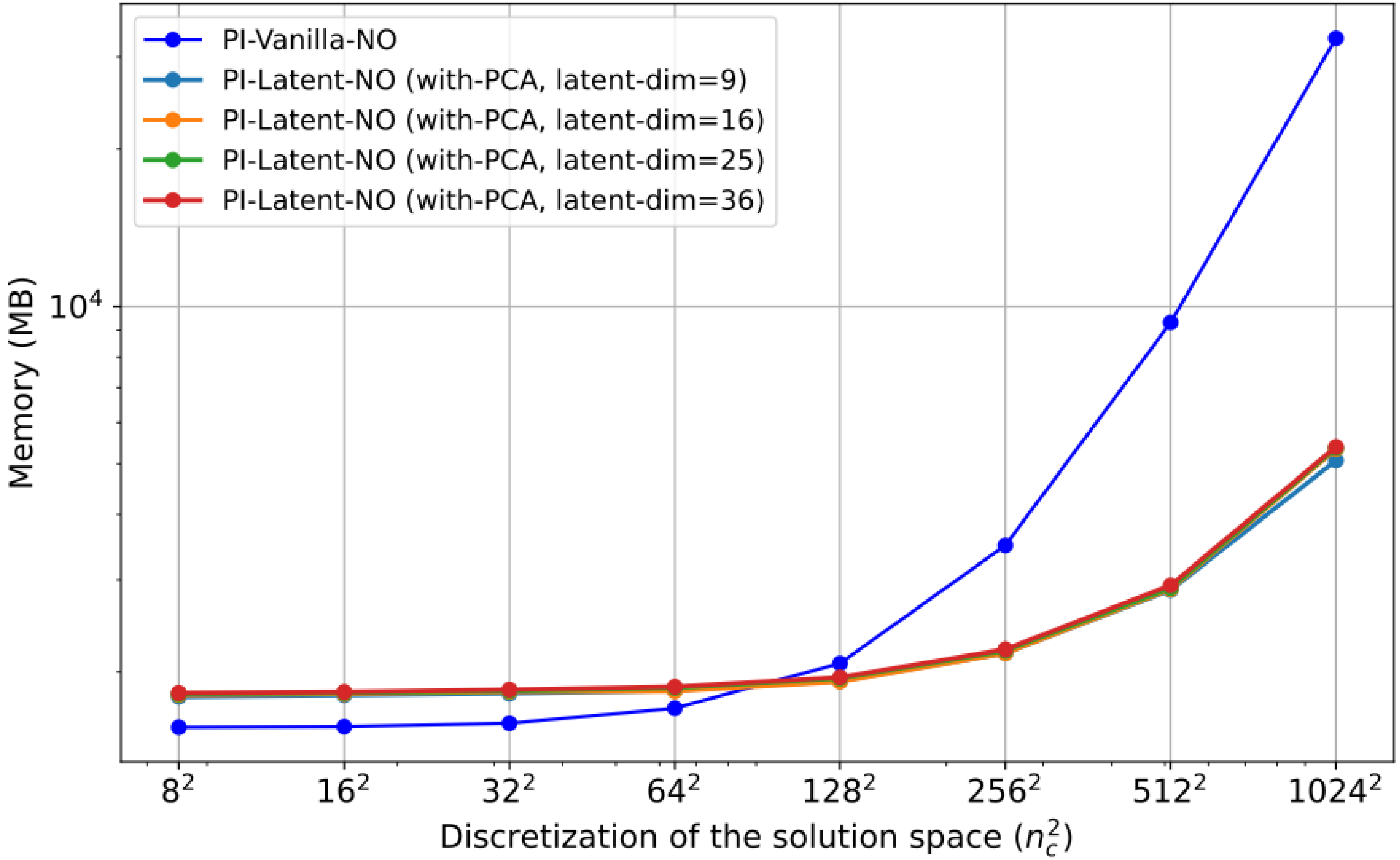
Runtime Scaling





Memory Scaling





More Comparisons

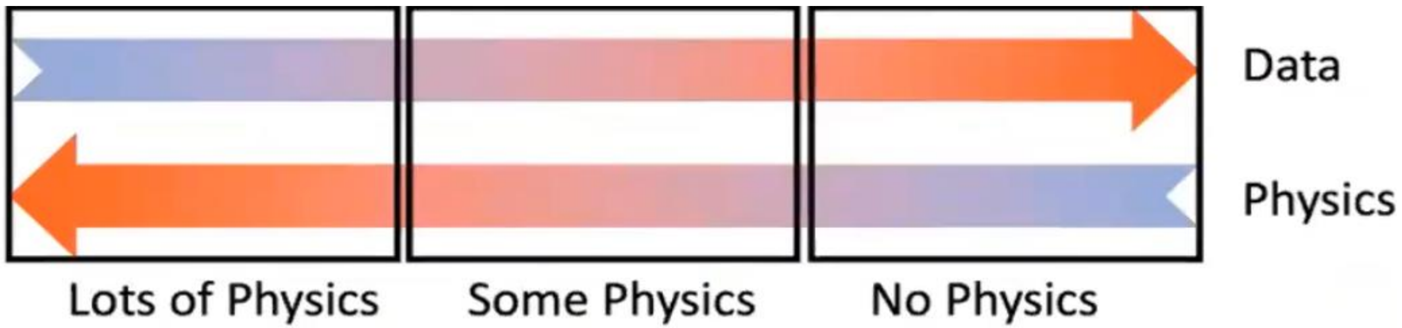
1D Burgers transport dynamics: Performance metrics

Model	n_{train}	MSE_{test}	Training Time (in sec)
PI-Vanilla-NO	0	6.1e-04 $\pm$ 8.4e-05	9236 $\pm$ 101
PI-Latent-NO (with-PCA)	200	5.5e-04 $\pm$ 1.3e-04	13913 $\pm$ 180
PI-Latent-NO (with-Pretrained-AE)	200	6.7e-04 $\pm$ 1.3e-04	14000 $\pm$ 414

1D Advection: Performance metrics

Model	n_{train}	MSE_{test}	Training Time (in sec)
PI-Vanilla-NO	0	5.1e-04 $\pm$ 2.1e-05	5322 $\pm$ 130
PI-Latent-NO (with-PCA)	200	4.7e-04 $\pm$ 6.0e-05	8534 $\pm$ 335
PI-Latent-NO (with-Pretrained-AE)	200	5.7e-04 $\pm$ 4.9e-05	8387 $\pm$ 148

Key Takeaways



- These methods have a niche in real world problems, where partially physics in known and some measurements of quantities of interest are available.
- Separable architecture introduces the possibility of employing physics in neural operators.
- Learning NOs on reduced spaces with data and physics opens up the possibly of exploring large design spaces efficiently.

Acknowledgement








Funding

Thank you!