The Industrialization of SciML Workshop @ ICERM

# Scaling SciML Algorithms for high-dimensional PDEs

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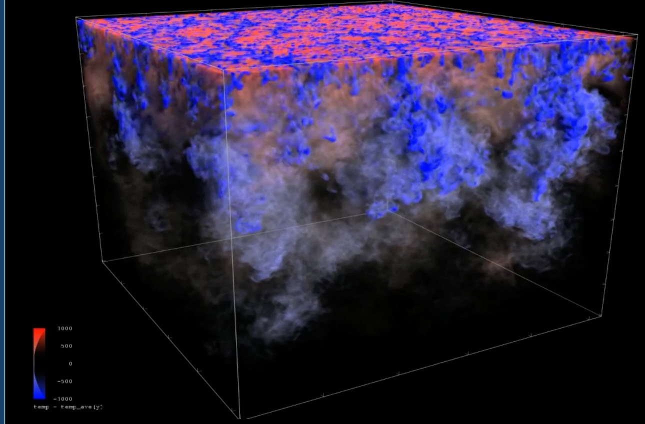
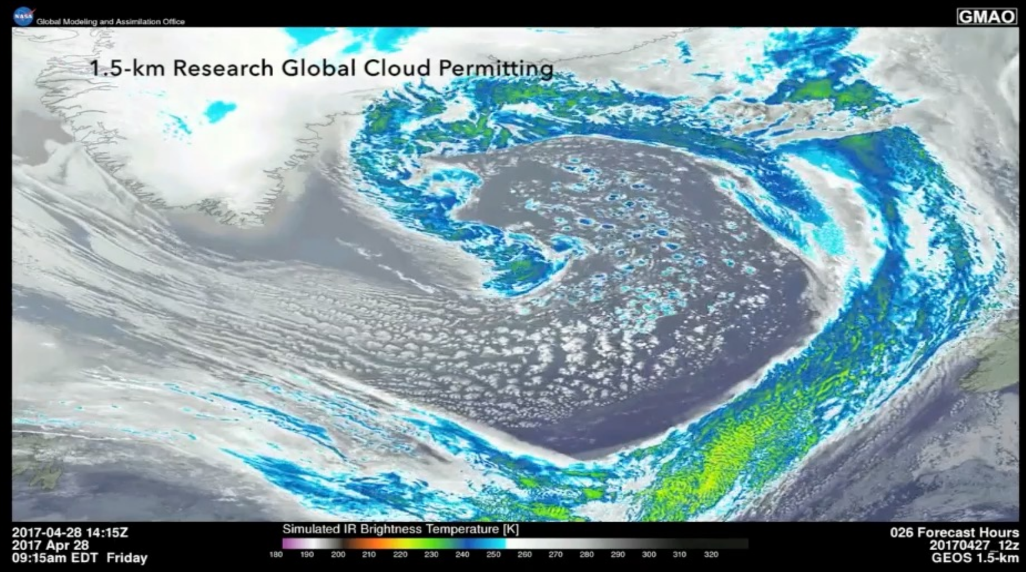
# Physics-based Models

## Represent the **Laws of Nature**

Temperature variations in a star 1.35 times as massive as the Sun (Kelvin)



Flow field around the nose landing gear of a Boeing 777




Evolution of an Icelandic Low in the North Atlantic Ocean over three days

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

$$\frac{D\mathbf{u}}{Dt} = \frac{1}{\rho}\nabla \cdot \boldsymbol{\sigma} + g$$

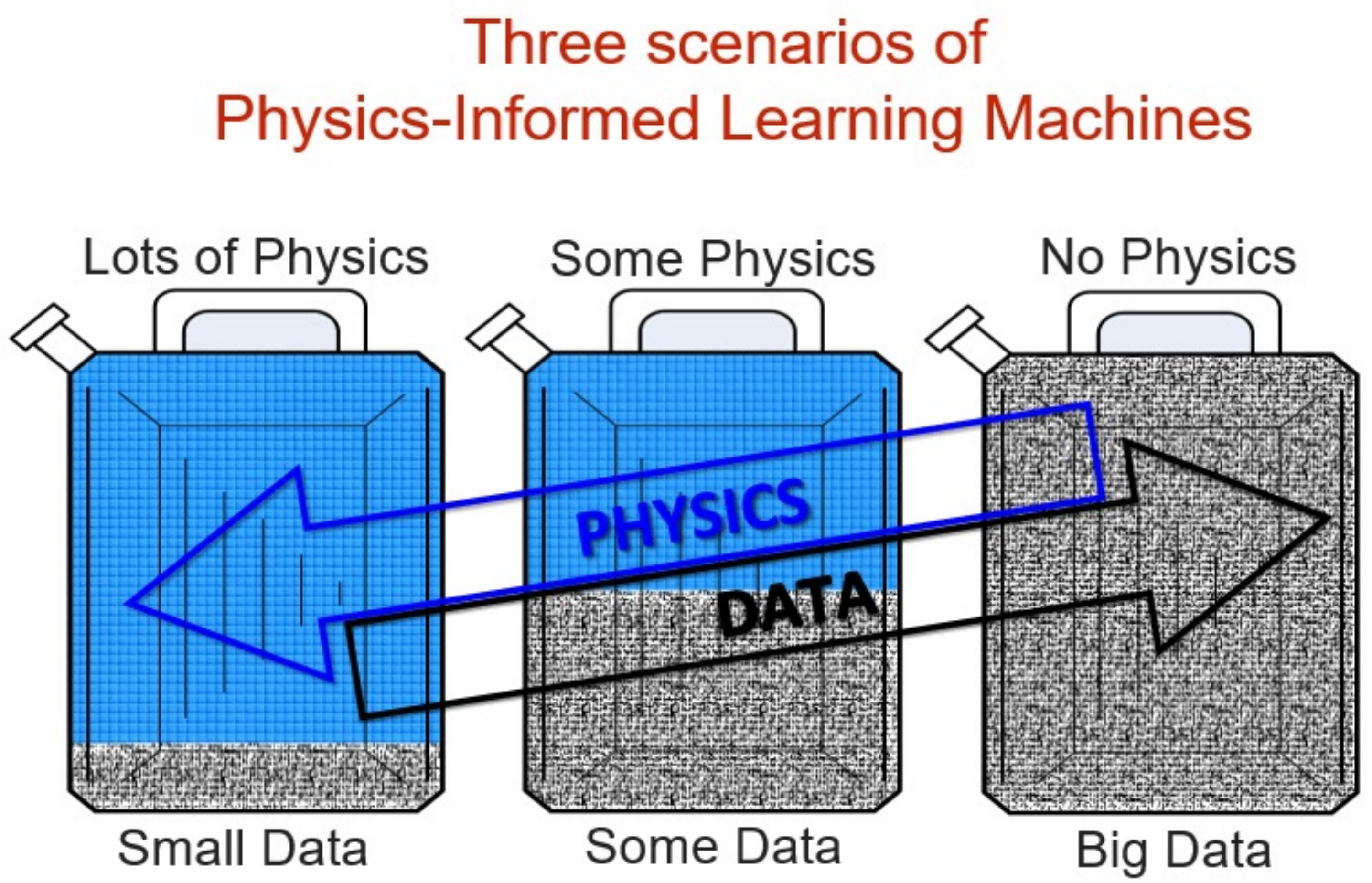
(e.g., Cauchy momentum equation for fluids – momentum transport in continuums)

- **POWERFUL** but computationally **EXPENSIVE**

*Source*: https://www.nas.nasa.gov/SC17/ (NASA)

# Data + Laws of Physics

**The 5D Law**: Dinky, Dirty, Dynamic, Deceptive Data



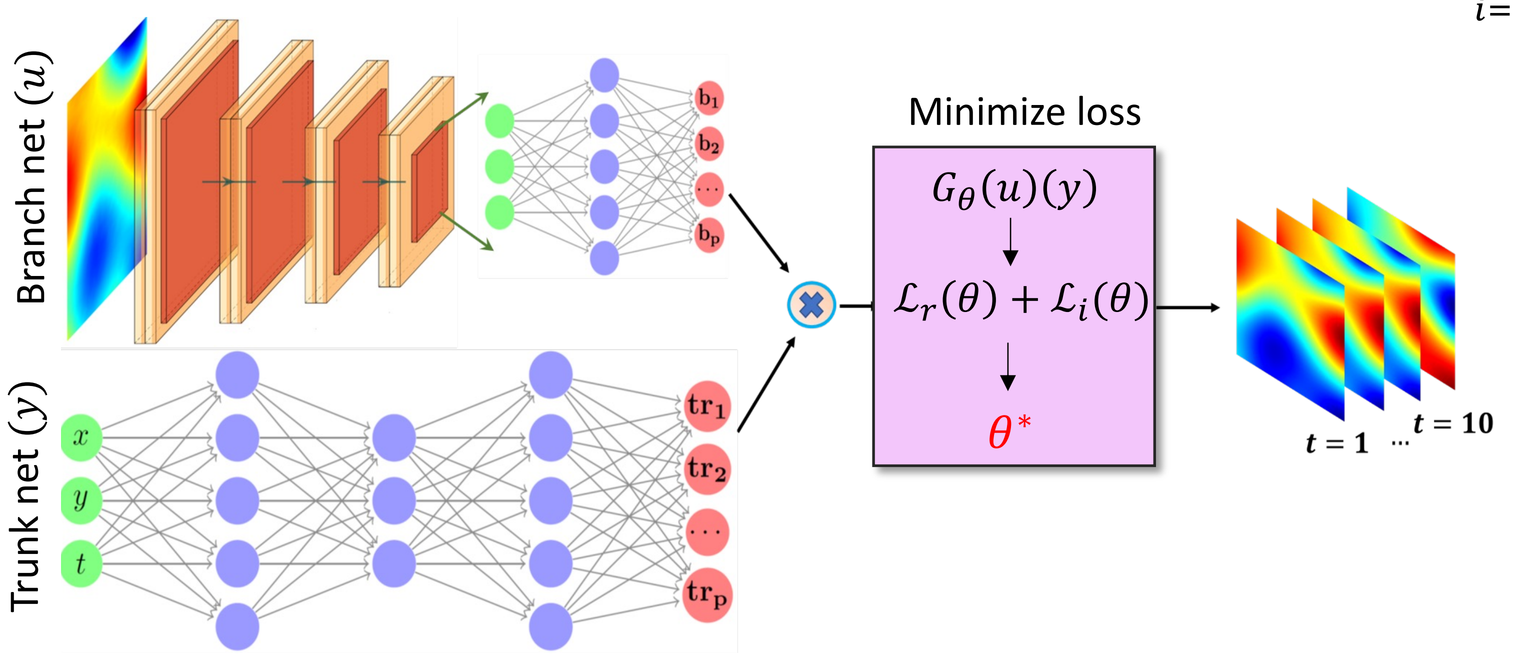

**FEM** **PINNs** **Neural Operators**

# Neural Operators

## 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 $\{y_i\}_{i=1}^{m}$

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




Other neural operators

- Fourier neural operator [1]
- Wavelet neural operator [2]
- Laplace neural operator [3]

[1] Li, Z. et al. (2020), [2] Tripura, T. and Chakraborty, S. (2022), [3] Cao, Q. and Goswami S. (2023).

# Brusselator reaction-diffusion system

Autocatalytic chemical reaction:

$$A \xrightarrow{k_1} X,$$
$$B + X \xrightarrow{k_2} Y + D,$$
$$2X + Y \xrightarrow{k_3} 3X,$$
$$X \xrightarrow{k_4} E,$$

$u = \{X\}$
$v = \{Y\}$

2D time-dependent rate equations

$$\frac{\partial u}{\partial t} = D_0\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + a - (1+b)u + vu^2,$$
$$\frac{\partial v}{\partial t} = D_1\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) + bu - vu^2, \quad \mathrm{x} \in [0,1]^2,\ t \in [0,1],$$

$D_0, D_1, a, b$: diffusivity and reaction rate parameters

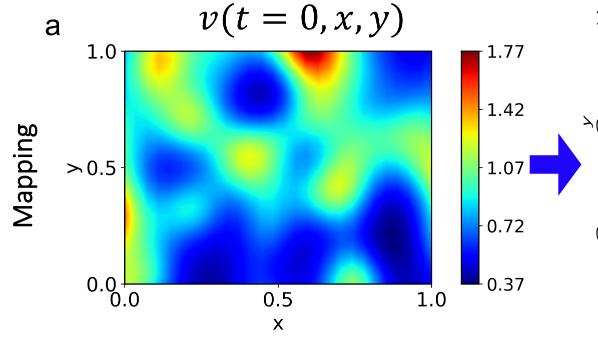
Initial conditions

$$u(x,y,t=0) = h_1(x,y) \geq 0,$$
$$v(x,y,t=0) = h_2(x,y) \geq 0,$$

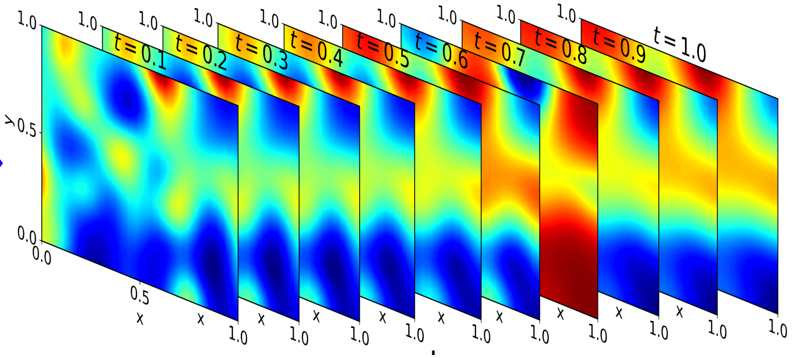
Mapping:

$$h_2(x,y) \rightarrow v(x,y,t)$$

Objective:




initial field of species Y



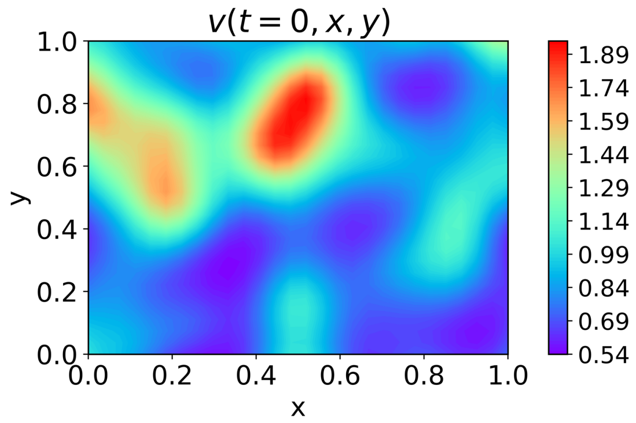

evolution of field of species Y

Initial condition is modeled as GRF:

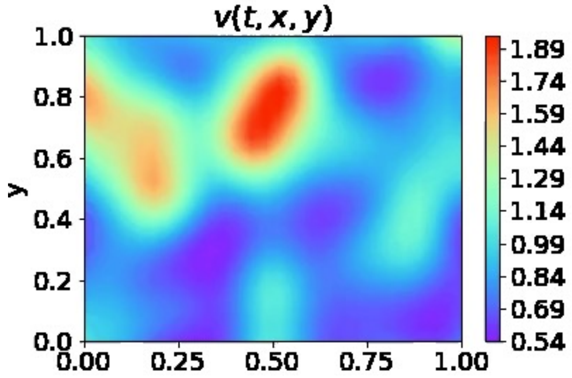
- $v(t=0,\mathrm{x}) \sim \mathcal{GP}\left(\mu(\mathrm{x}), \mathrm{Cov}(\mathrm{x},\mathrm{x}')\right)$

*Solved with a finite difference (FD) solver (discretization: 28x28 grid points)

# Brusselator reaction-diffusion system




DOFs: 28 x 28 = 784




DOFs: 20 x 28 x 28 = 15680

$a = 1, b = 3$

$D_0 = 1, D_1 = 0.5$

# samples = 1600

To achieve an error of 2.41% on the test dataset, the DeepONet model required 0.2 M parameters.

Kontolati, K., Goswami, S., Shields, M.D. and Karniadakis, G.E., 2023. On the influence of over-parameterization in manifold based surrogates and deep neural operators. *Journal of Computational Physics*, *479*, p.112008.

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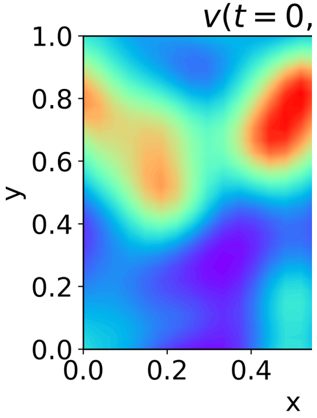
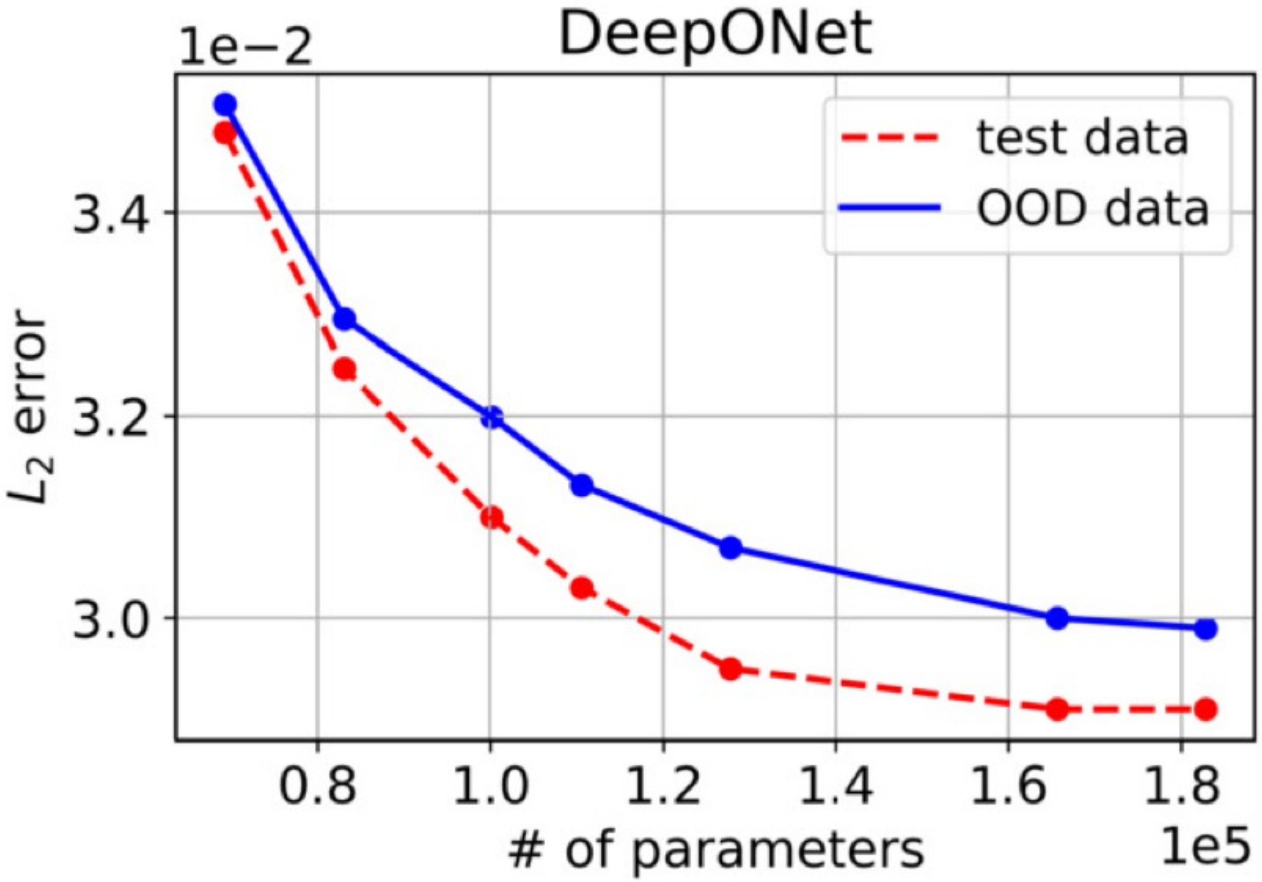



DOFs: 28 x




$a = 1, b = 3$

$D_0 = 1, D_1 = 0.5$

\# samples = 1600

0

To achieve an error ... ed 0.2 M parameters.

# Viscous Shallow water equation

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

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

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

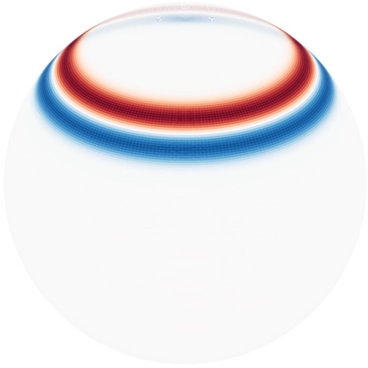
$$h'(\lambda, \phi) = \hat{h}\cos(\phi)\mathrm{e}^{-(\lambda/\alpha)^2}\mathrm{e}^{-[(\phi_2-\phi)/\beta]^2}$$

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

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

Input Dimension: 65,536

Gaussian Random Perturbation



Output Dimension: 4,718,592

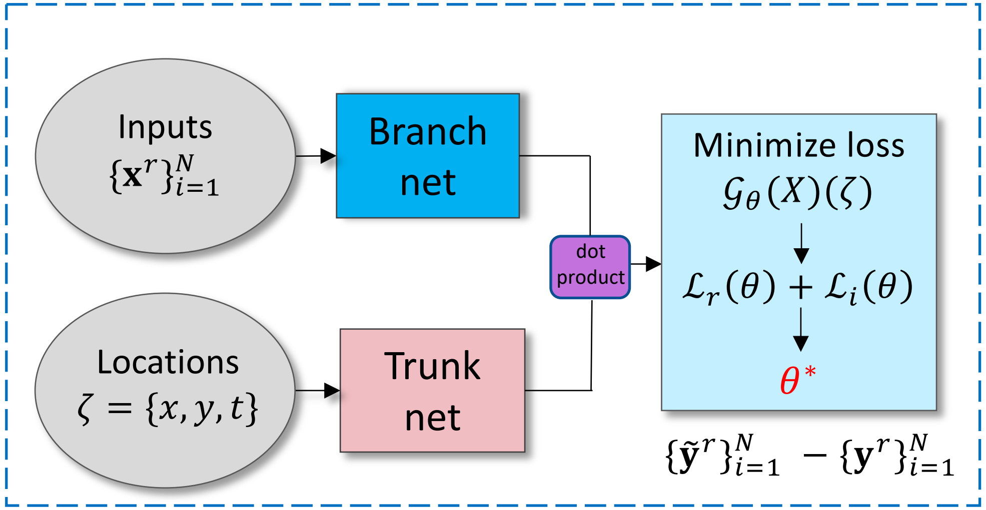
Atmospheric Flow

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



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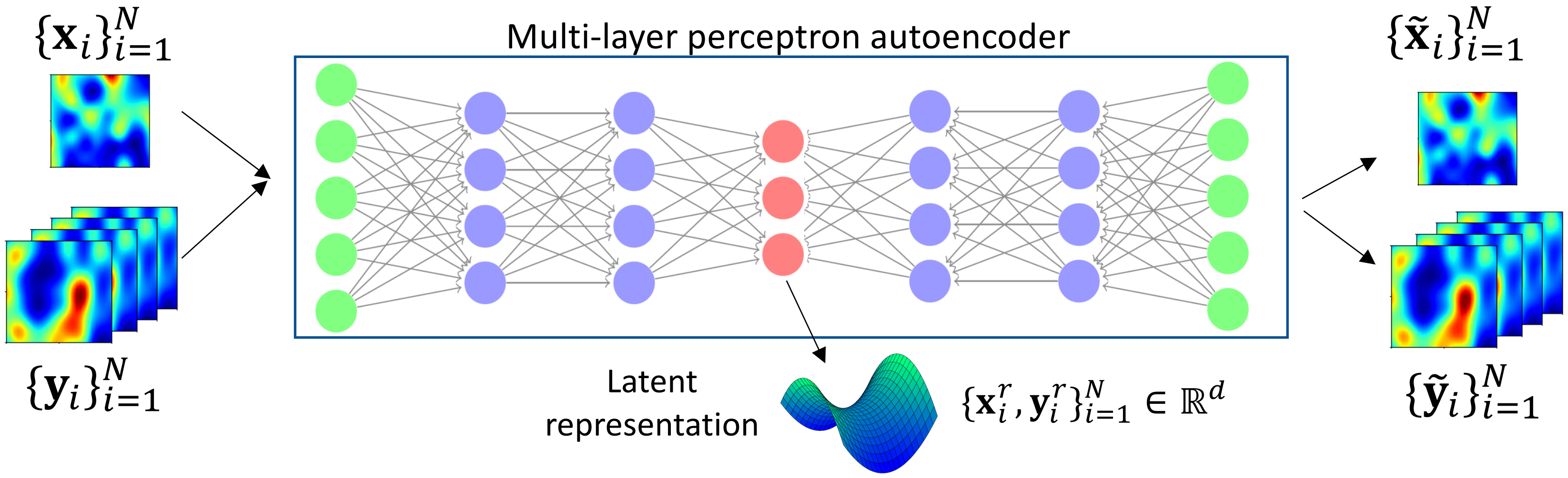


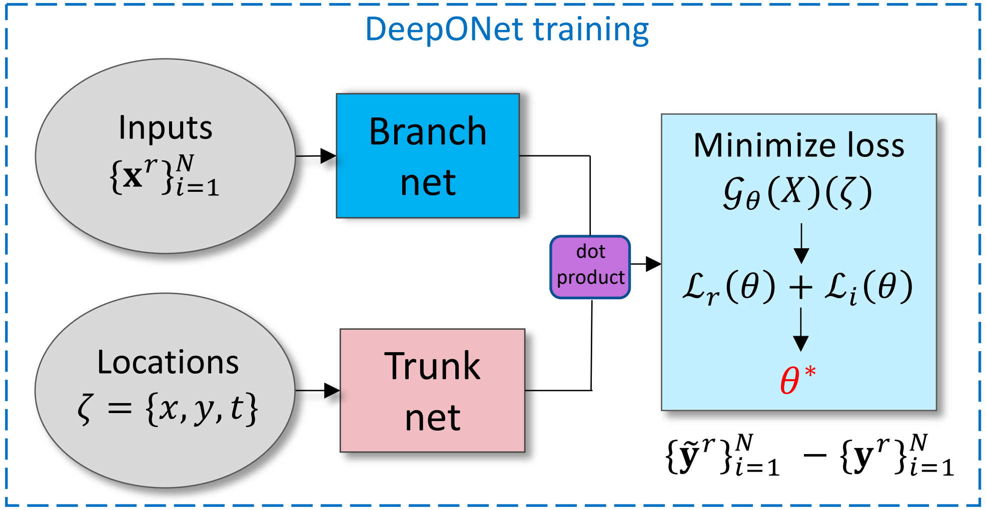

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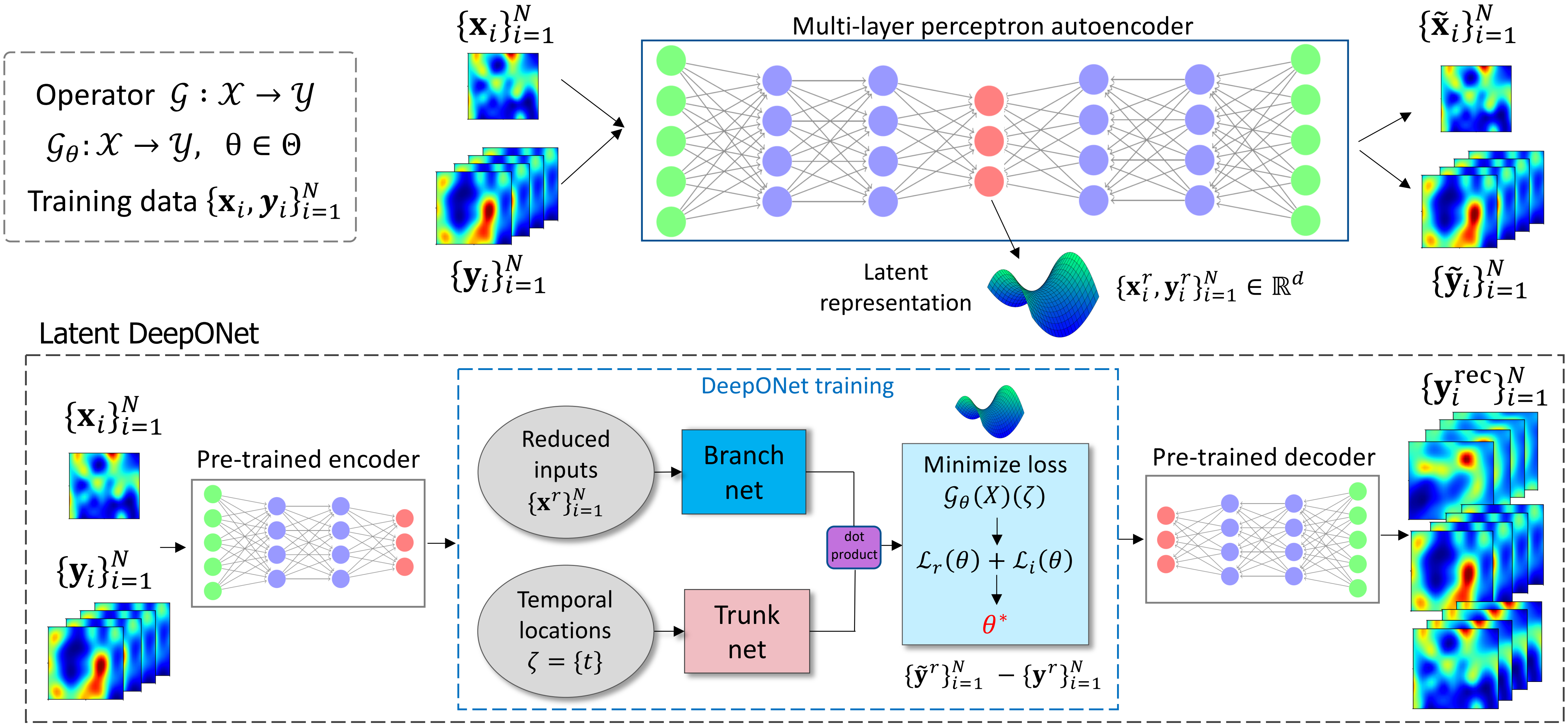


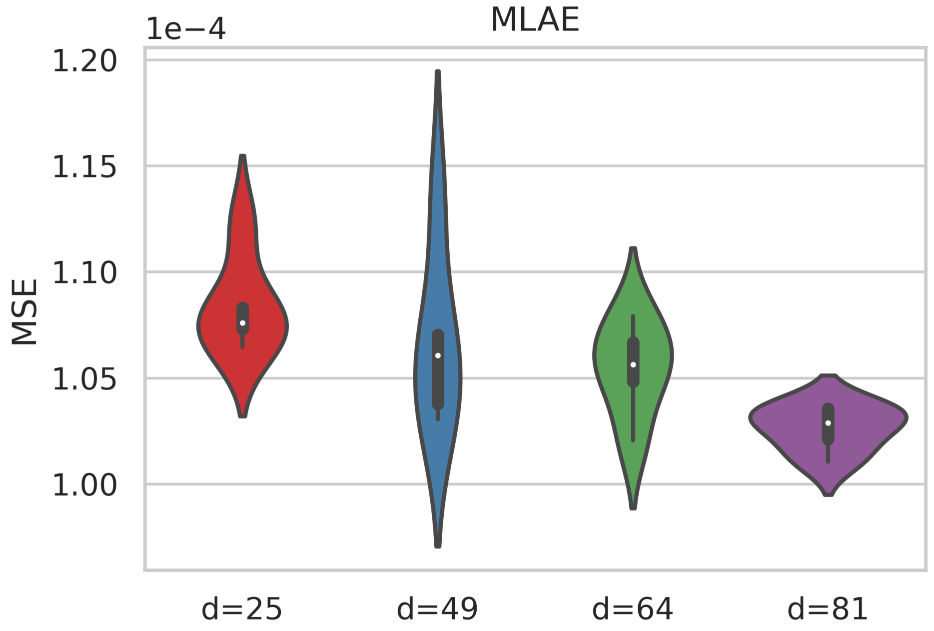

Kontolati, K., Goswami, S., Karniadakis, G.E. and Shields, M.D., 2023. Learning in latent spaces improves the predictive accuracy of deep neural operators. *arXiv preprint arXiv:2304.07599*.

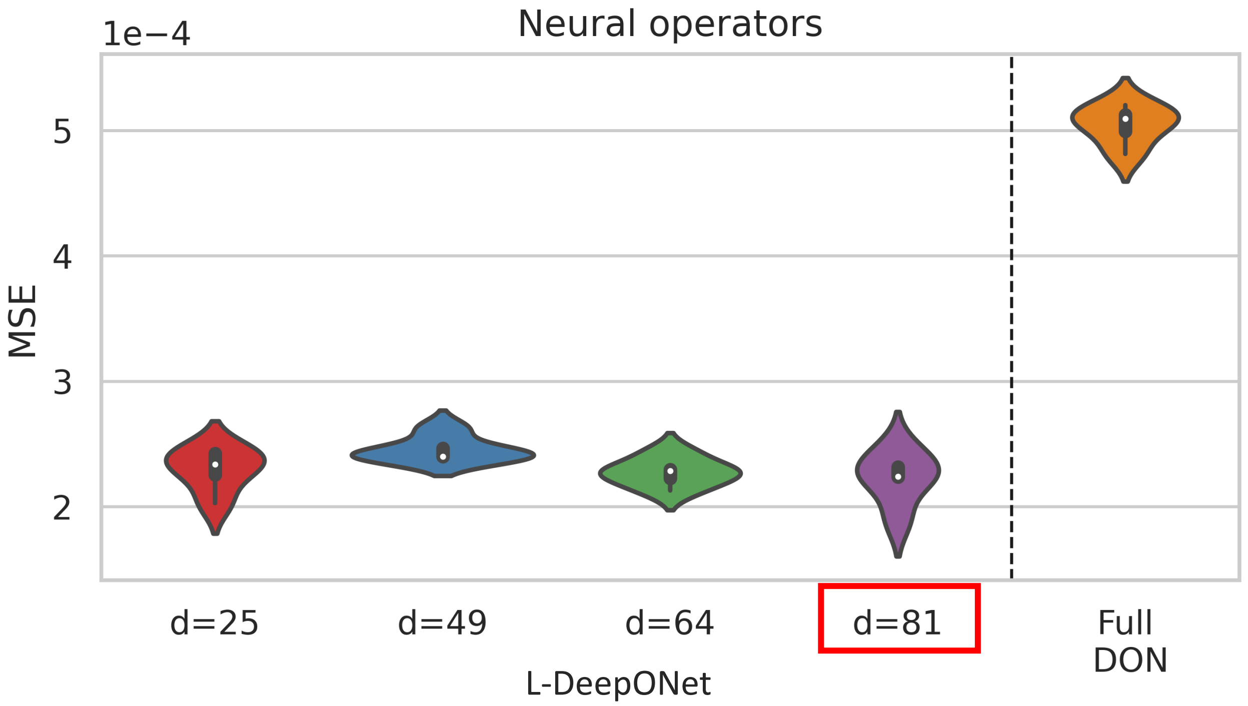
# Results

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

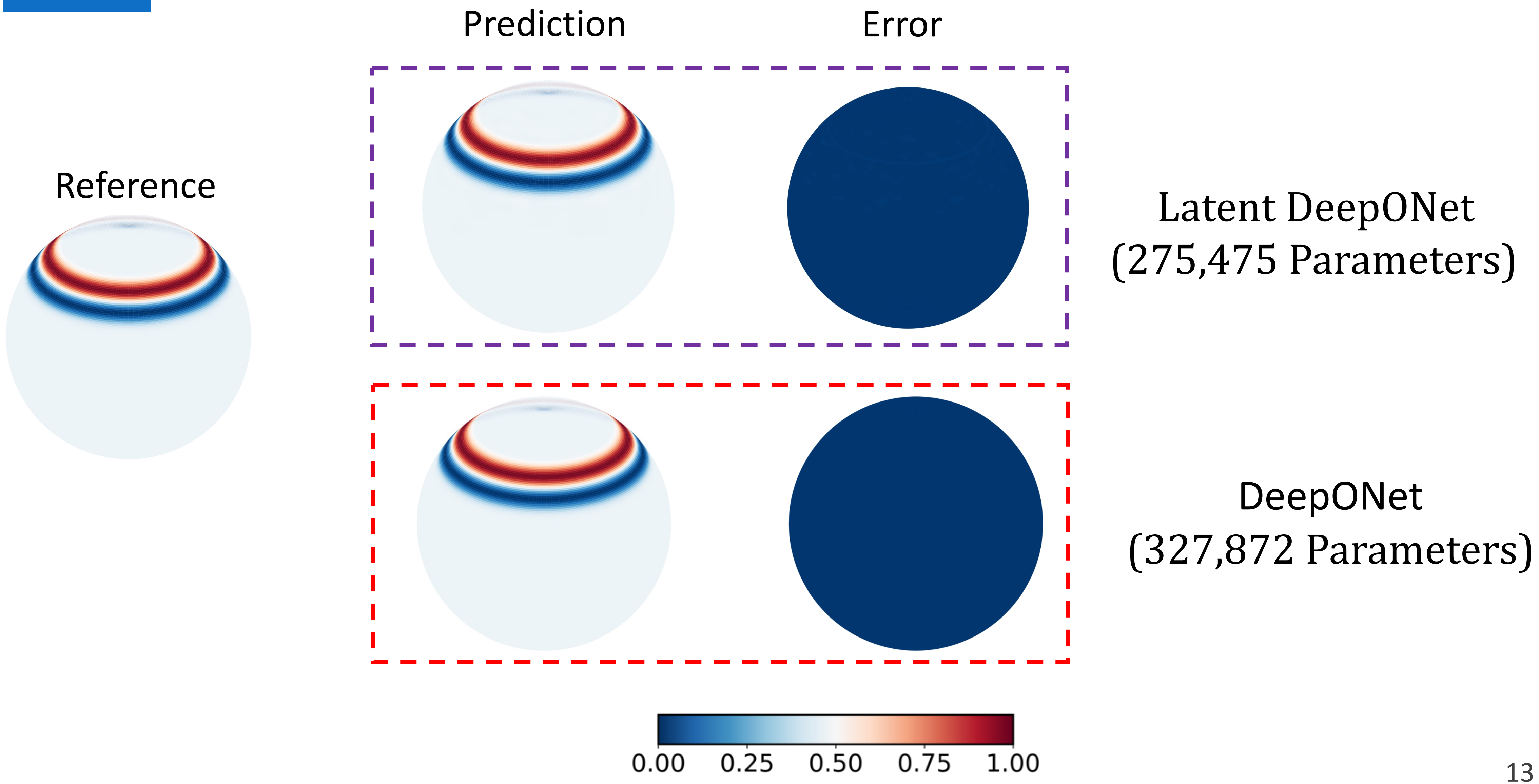
Training Time (seconds)

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



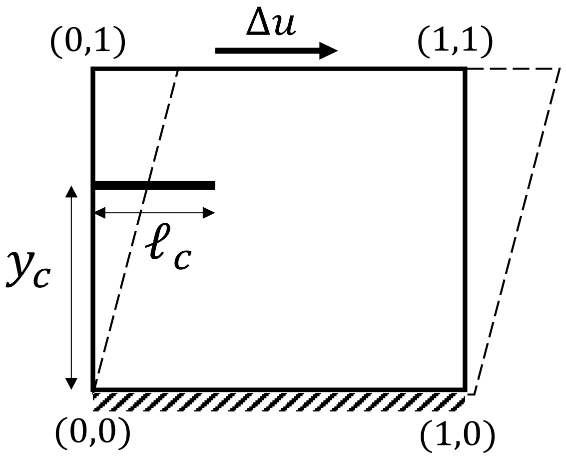



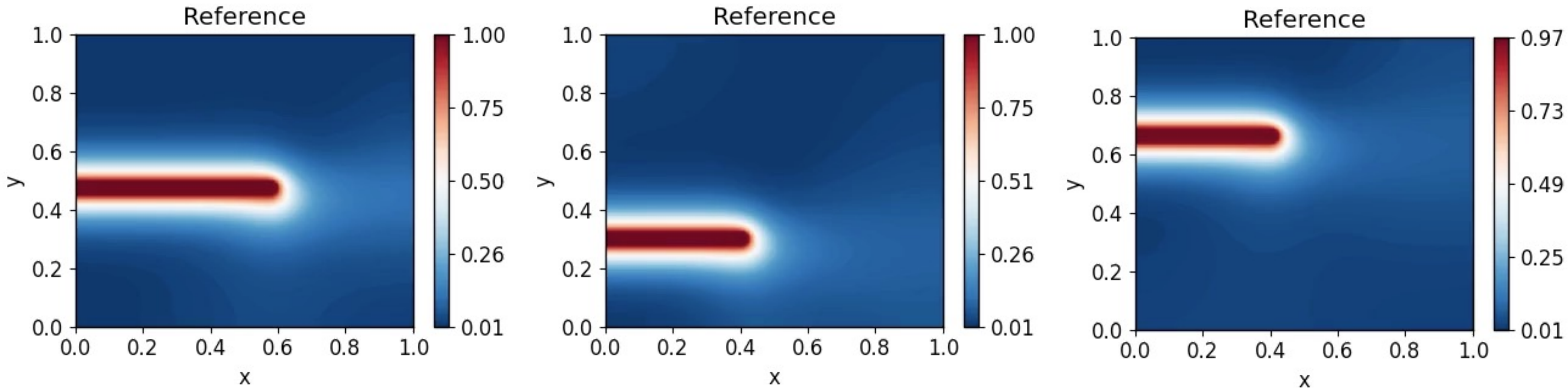
# Results


Prediction
Error
Reference
Latent DeepONet
(275,475 Parameters)
DeepONet
(327,872 Parameters)
0.00
0.25
0.50
0.75
1.00

# Fracture: Shear failure of plate with notch

- Unit square plate with horizontal crack
- Both location $y_c$ and length $\ell_c$ of the crack are considered random
- Boundary conditions: $u(x,0) = v(x,0) = 0$, $u(x,1) = \Delta u$
- Data: $N = 261$, $y_c \in [0.2, 0.675]$, $\ell_c \in [0.3, 0.65]$
- Input dimension: 162x162 Output dimension: 8x162x162



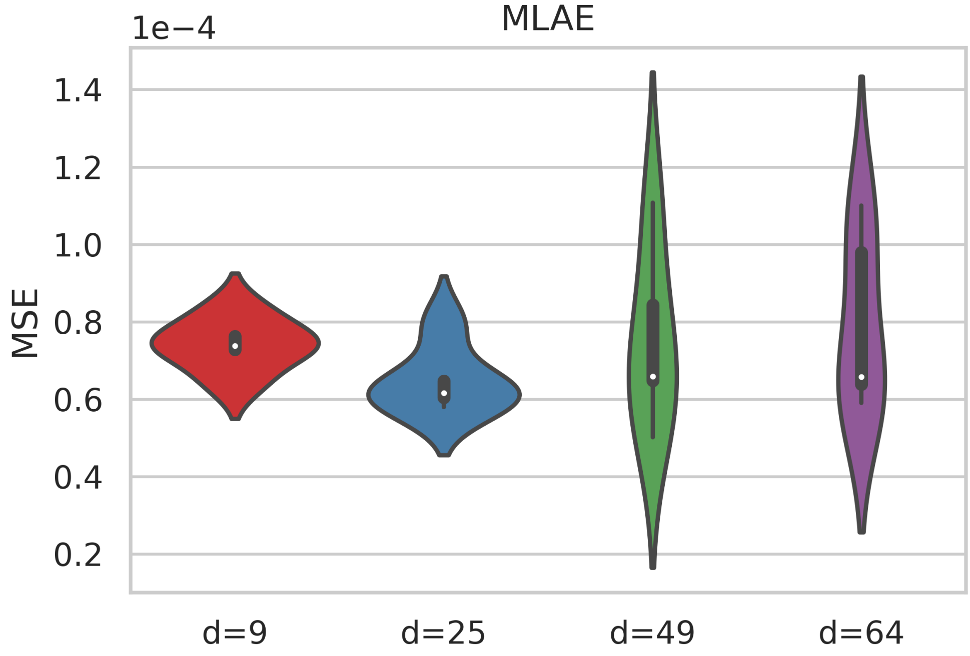



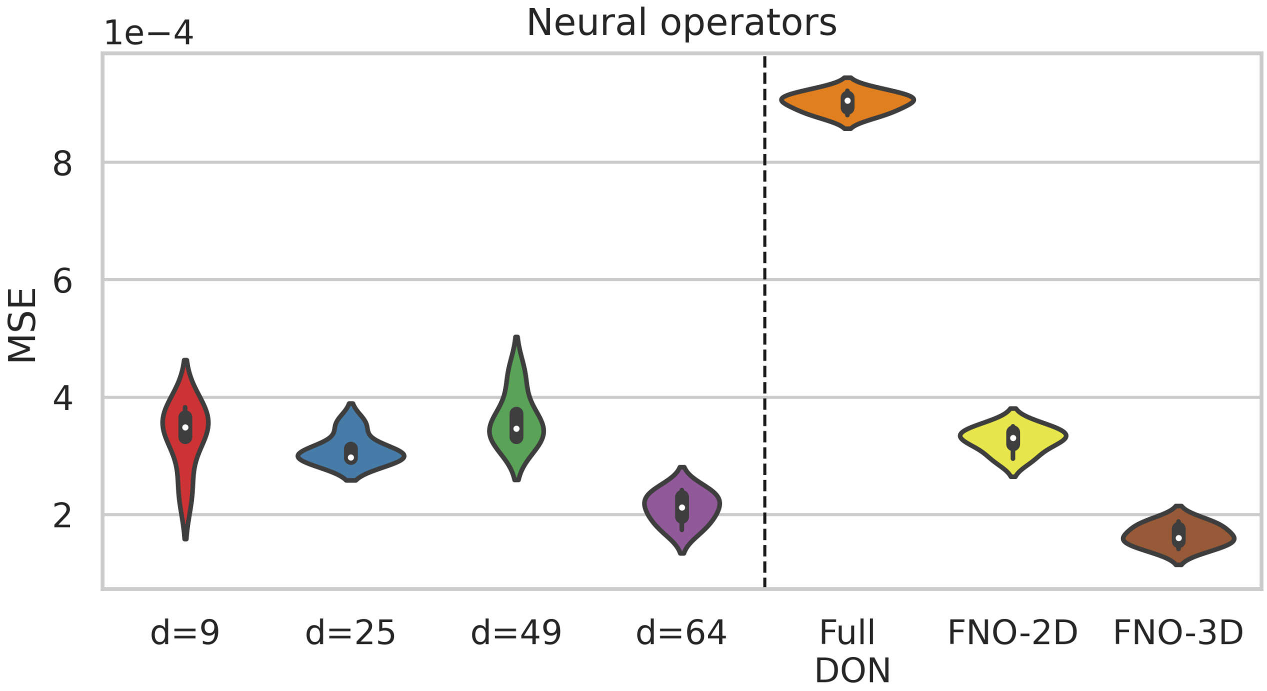



Goswami et al. (2021) A physics-informed variational DeepONet for predicting the crack path in brittle materials

# Fracture: Shear failure of plate with notch

Error metric: $$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$$



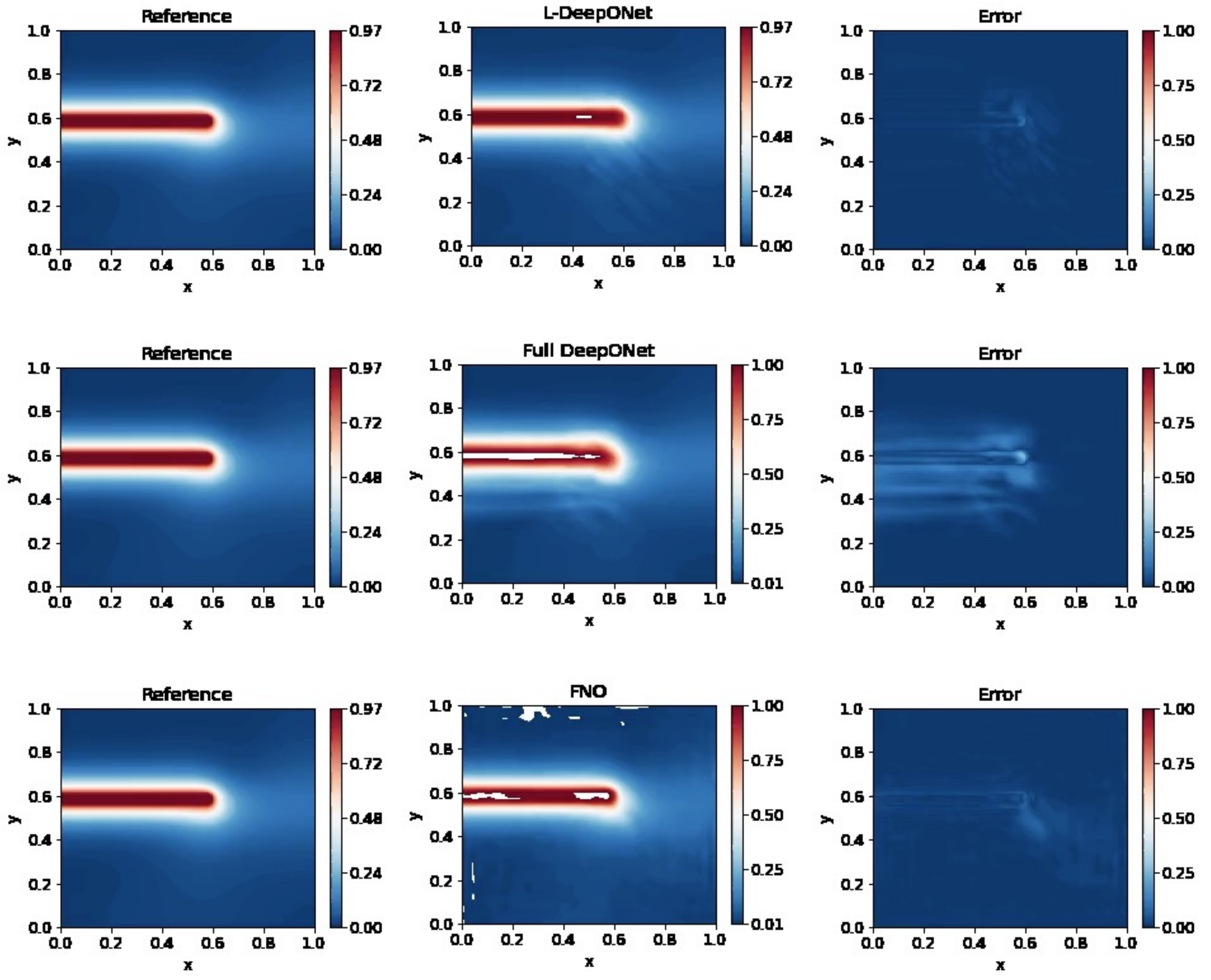



# Comparison with Benchmark DeepONet

L-DeepONet

Full DeepONet

FNO



# Consolidated results

*MLAE: multi-layer autoencoders*
*PCA: principal component analysis*

Accuracy of *L-DeepONet for MLAE and PCA*

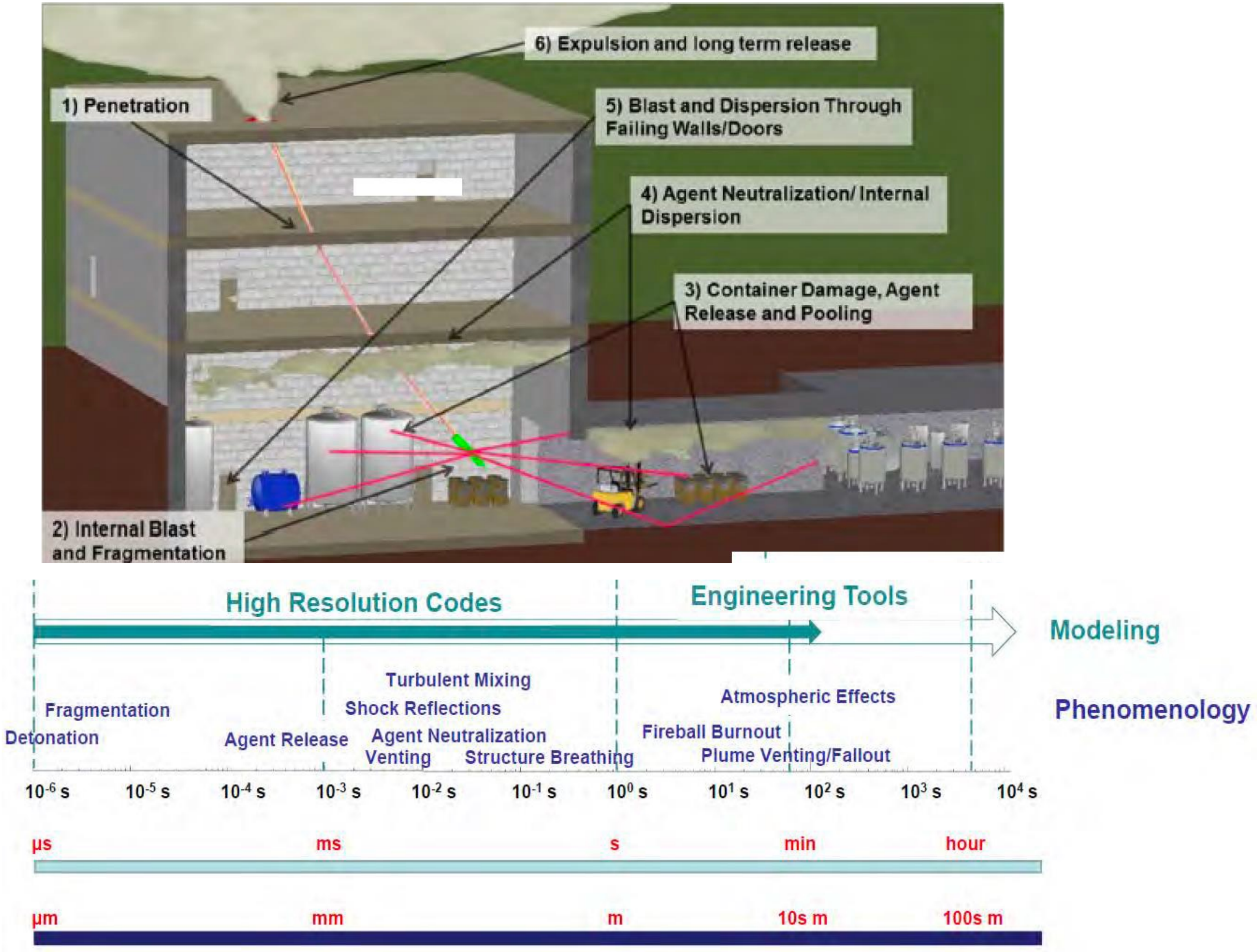
| Application | $d$ | with MLAE | with PCA |
|---|---|---|---|
| Brittle material fracture | 9 | $3.33 \cdot 10^{-4} \pm 4.99 \cdot 10^{-5}$ | $2.71 \cdot 10^{-3} \pm 6.62 \cdot 10^{-6}$ |
| | 64 | $2.02 \cdot 10^{-4} \pm 1.88 \cdot 10^{-5}$ | $3.13 \cdot 10^{-4} \pm 4.62 \cdot 10^{-6}$ |
| Rayleigh-Bénard 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 | – |

# Stiff Chemical Kinetics

- DTRA needs high-fidelity CFD modeling to enhance hazard predictions for countering weapons of mass destruction.
- Complexities involve long timeframes, unpredictable phenomena, and resource intensive chemical kinetics models.
- Stiff chemical kinetics models are the primary computational bottleneck.



# Chemical Kinetics Solution Propagator

$$\frac{\partial \Phi}{\partial t} = \underbrace{-(\nu \cdot \nabla)\Phi + \frac{1}{p}\nabla \cdot (\nabla \Phi \Gamma)}_{\text{Hydrodynamic}} + \underbrace{S(\rho, \Phi)}_{\text{Chemical Kinetics}}$$

$\Delta t_{NS} \gg \Delta t_{chem}$

- $\Phi$ : Species mass fraction and temperature
- $\Gamma$ : Diffusivities at each spatial point
- S : Chemical source term
- $\rho$ : Fluid density, $\nu$ : Velocity, $p$ : Pressure

**Aim: Learn a solution propagator for $\Delta t_{NS}$ time advancement**

$$\frac{\partial \Phi}{\partial t} = S(\rho, \Phi)$$

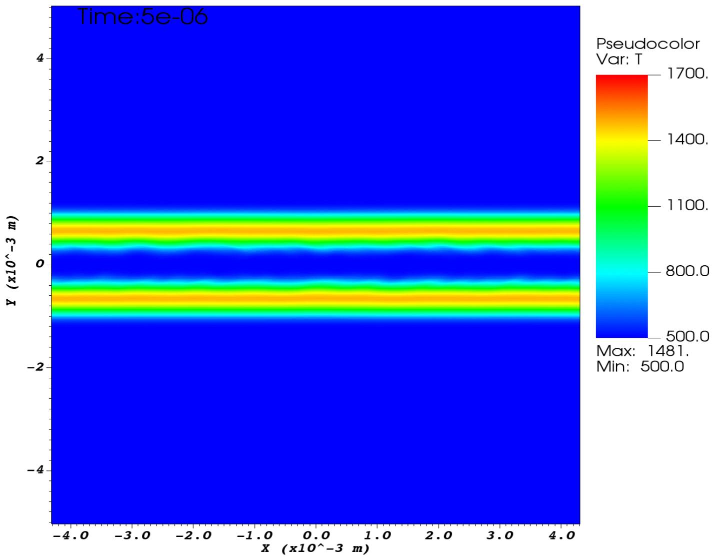
$$F_t^{t+\Delta t}: \mathbb{R}^{n+1} \rightarrow \mathbb{R}^{n+1}$$

$$\Phi(t + \Delta t) = F_t^{t+\Delta t}(\Phi(\mathrm{t}))$$

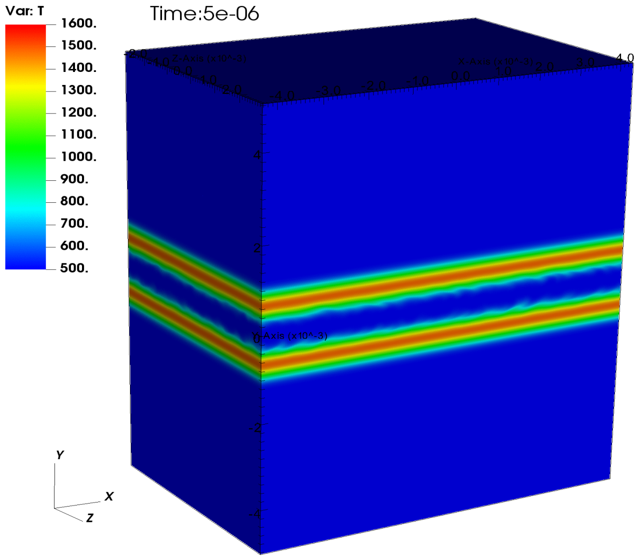
# Combustion Chemistry of Syngas

- 11 Species ($H_2, O_2, O, OH, H_2O, H, HO_2, CO, CO_2, HCO, N_2$)
- 21 Reactions
- The fuel is comprised of 50% $CO$, 10% $H_2$, and 40% $N_2$ by volume.
- The oxidizer streams comprised of 25% $O_2$ and 75% $N_2$ by volume.

**DNS: Temperature (2D)**

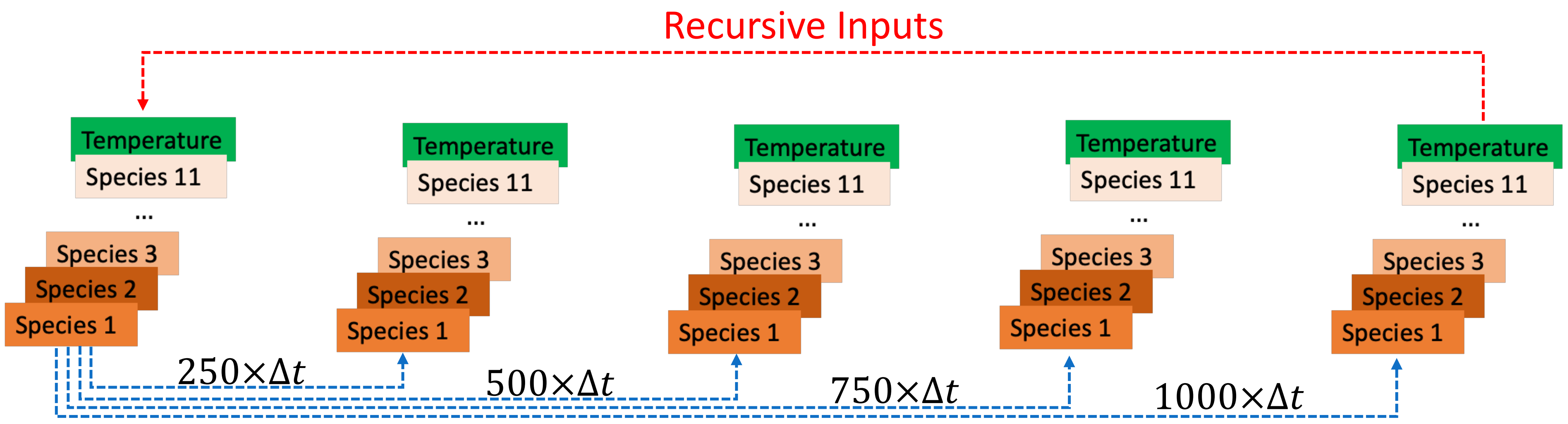



**DNS: Temperature (3D)**




**Simulation/Implementation**
**Pele-LM (AMReX)**

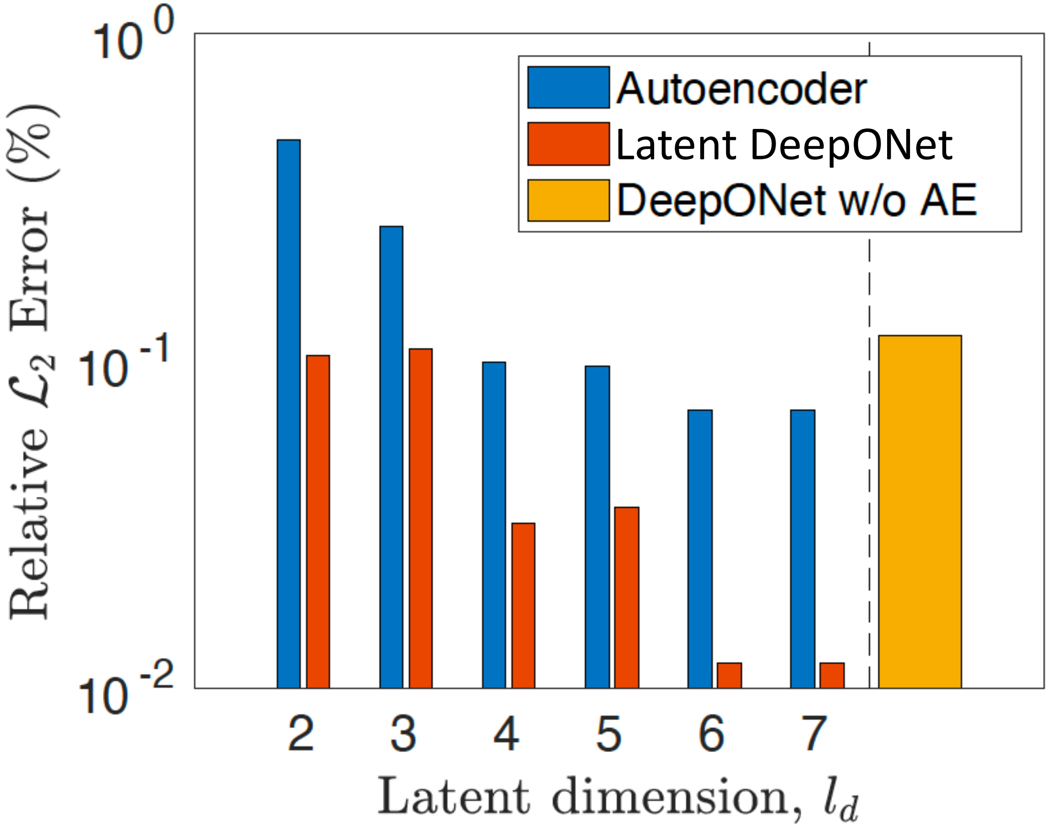
# Training and Testing

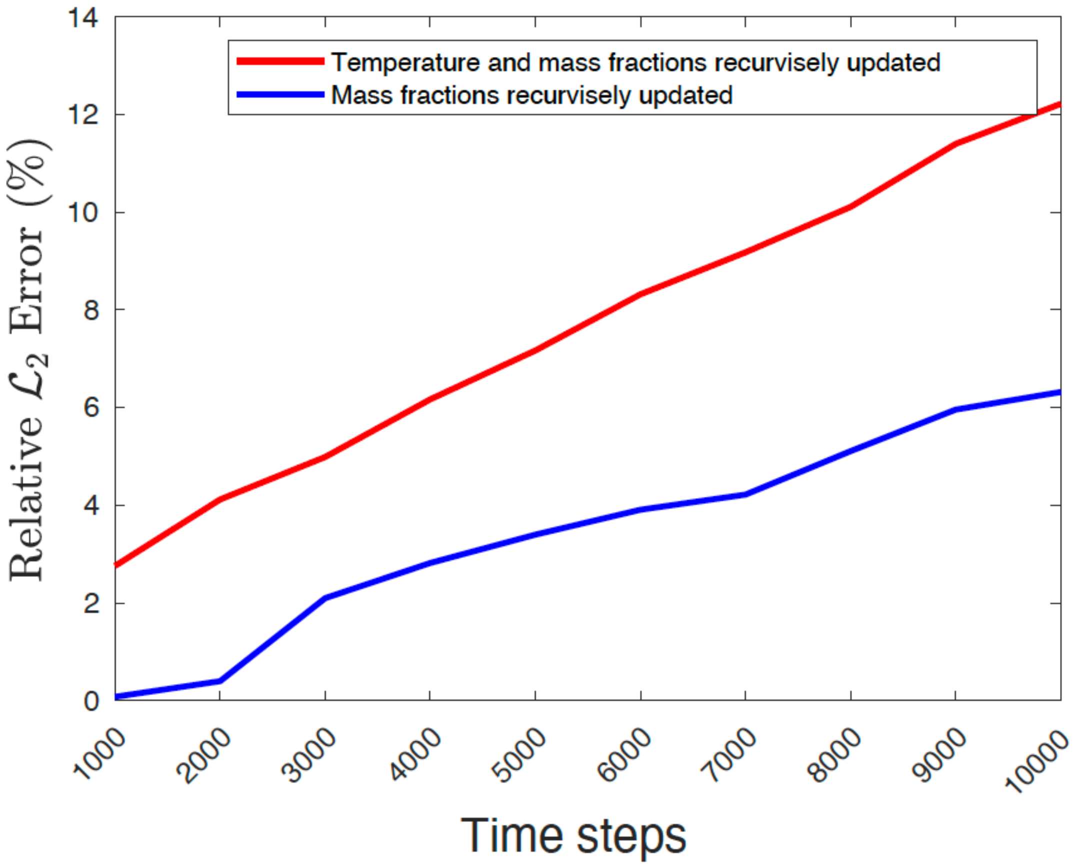



| | | | | |
|---|---|---|---|---|
| $T = t_0$ | $T_1 = t_0 + 250$ | $T_2 = t_0 + 500$ | $T_3 = t_0 + 750$ | $T_4 = t_0 + 1000$ |
| $T = 1000$ | $T_1 = 1000 + 250$ | $T_2 = 1000 + 500$ | $T_3 = 1000 + 750$ | $T_4 = 1000 + 1000$ |
| $T = 2000$ | $T_1 = 2000 + 250$ | $T_2 = 2000 + 500$ | $T_3 = 2000 + 750$ | $T_4 = 2000 + 1000$ |
| $\vdots$ | | | | |
| $T = 9000$ | $T_1 = 9000 + 250$ | $T_2 = 9000 + 500$ | $T_3 = 9000 + 750$ | $T_4 = 9000 + 1000$ |

Recursive Inputs

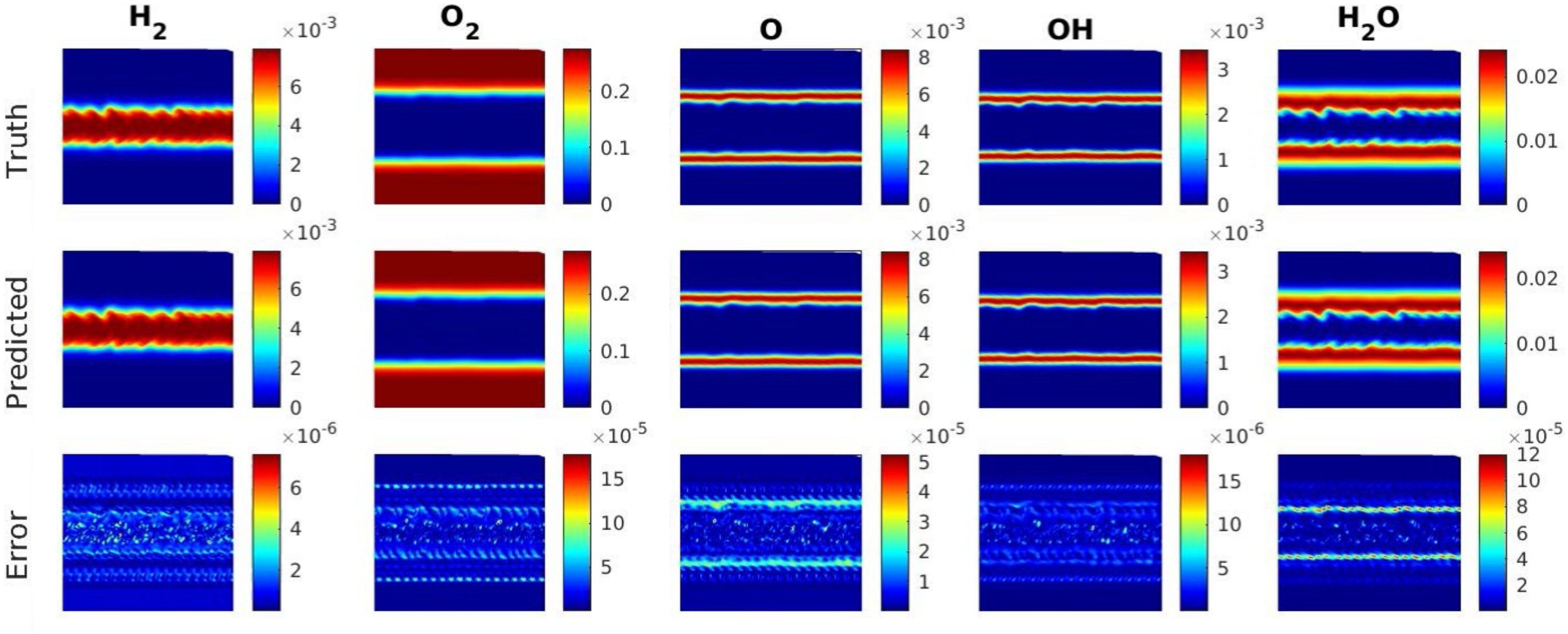
# Accuracy Comparison




Goswami, S., Jagtap, A.D., Babaee, H., Susi, B.T. and Karniadakis, G.E., 2024. Learning stiff chemical kinetics using extended deep neural operators. *Computer Methods in Applied Mechanics and Engineering*, *419*, p.116674.

# Representative Plots



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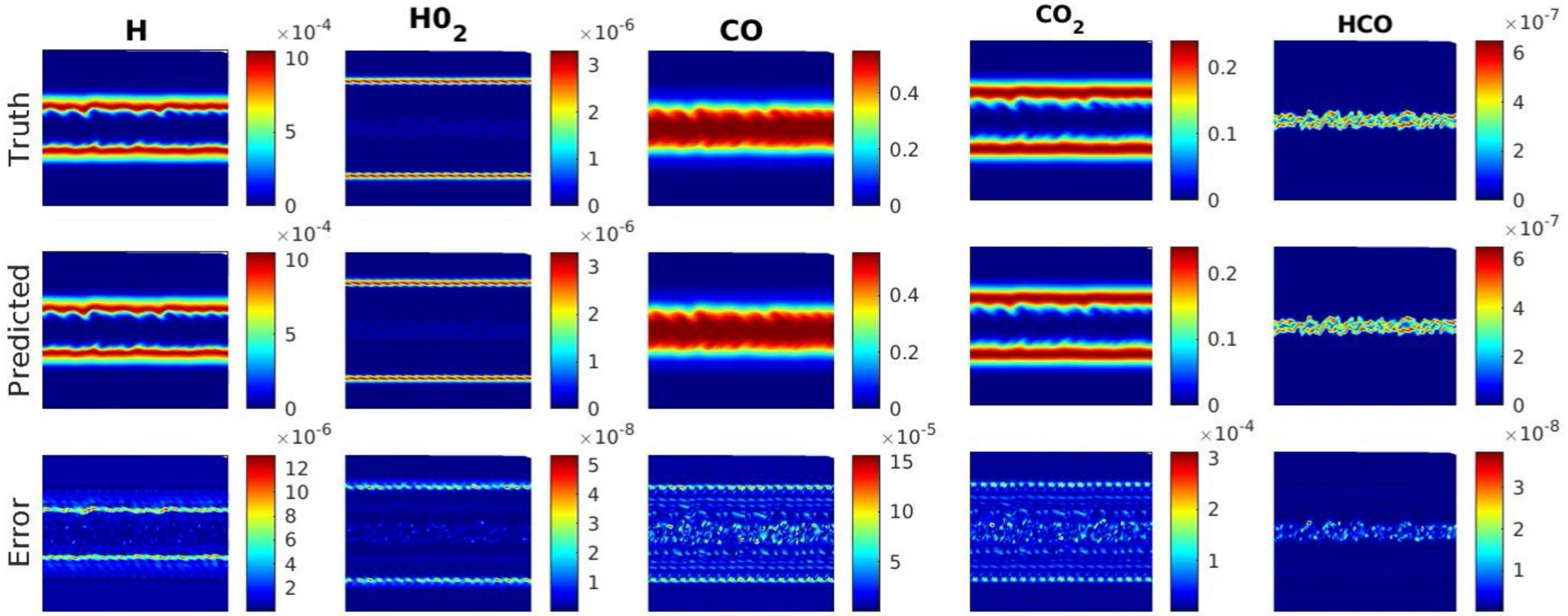
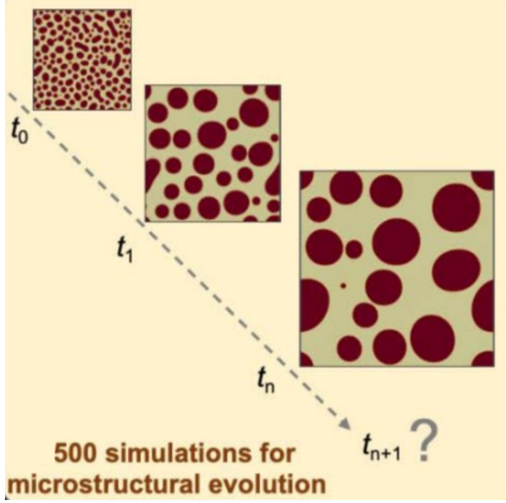


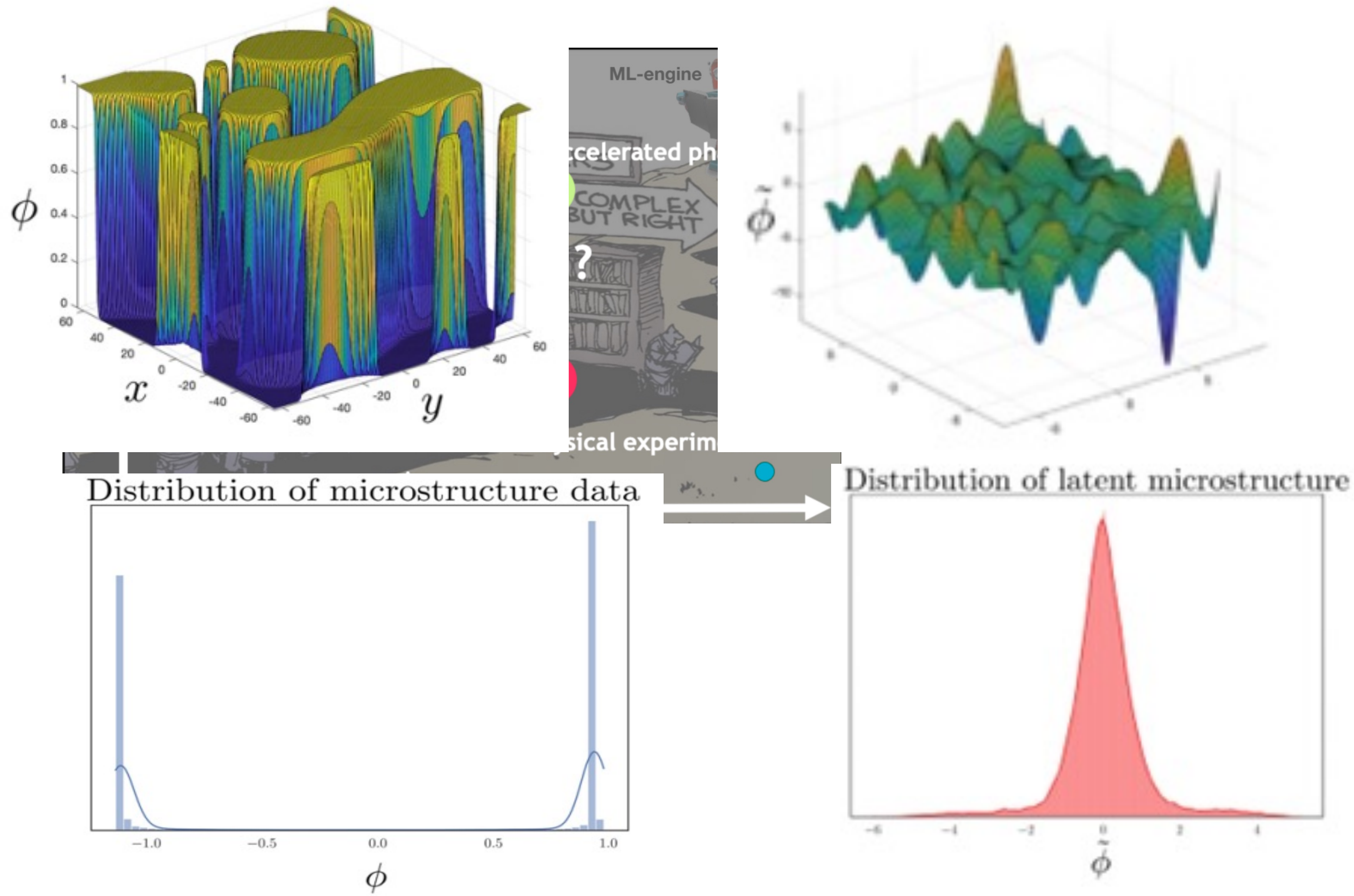
# Accelerating traditional methods

**Non-linear microstructure evolution of a two-phase mixture during Spinodal decomposition**

$$\frac{\partial \phi_i}{\partial t} = \nabla \cdot \left(M_{ij} \nabla \frac{\delta F}{\delta \phi_j}\right)$$

**High-Fidelity Simulations**




Sandia National Laboratories

Oommen, V., Shukla, K., Goswami, S., Dingreville, R. and Karniadakis, G.E., 2022. Learning two-phase microstructure evolution using neural operators and autoencoder architectures. *npj Computational Materials*, *8*(1), p.190.

# Accelerating traditional methods

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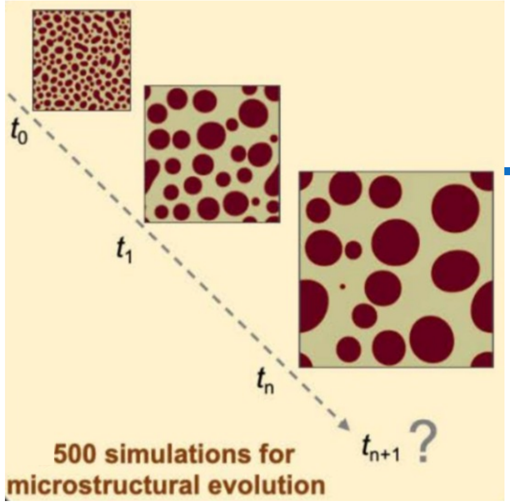
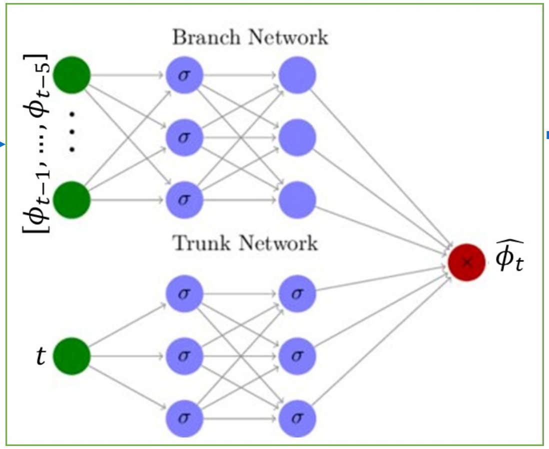
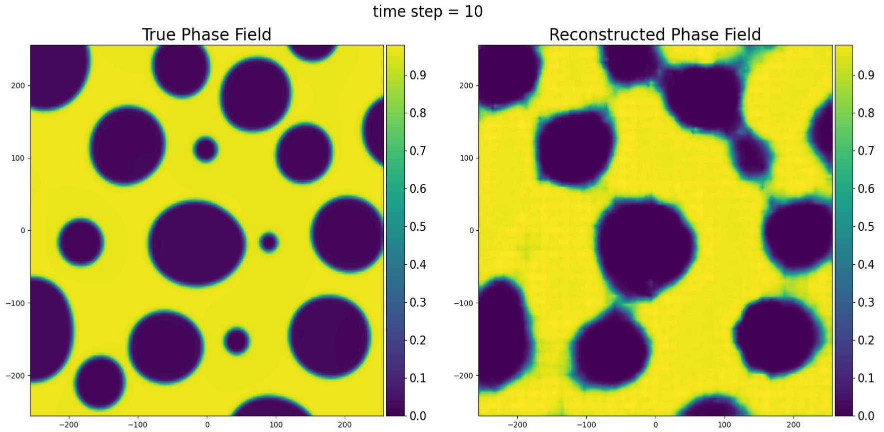
**High-Fidelity Simulations**




→ Convolutional Autoencoders (Reduced dimension = 100) →




→ Pre-trained Transposed Convolutional decoder → $\phi_t$



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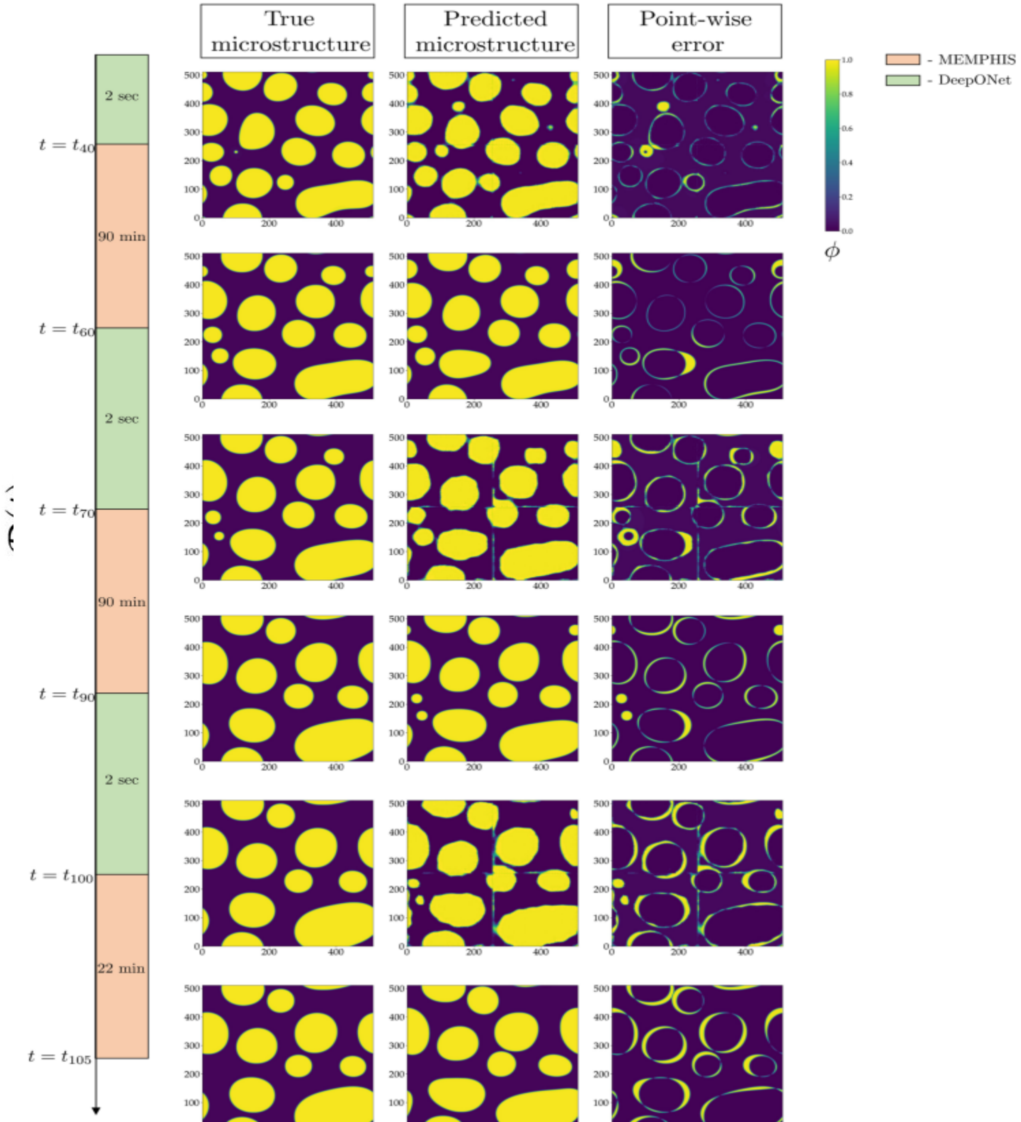
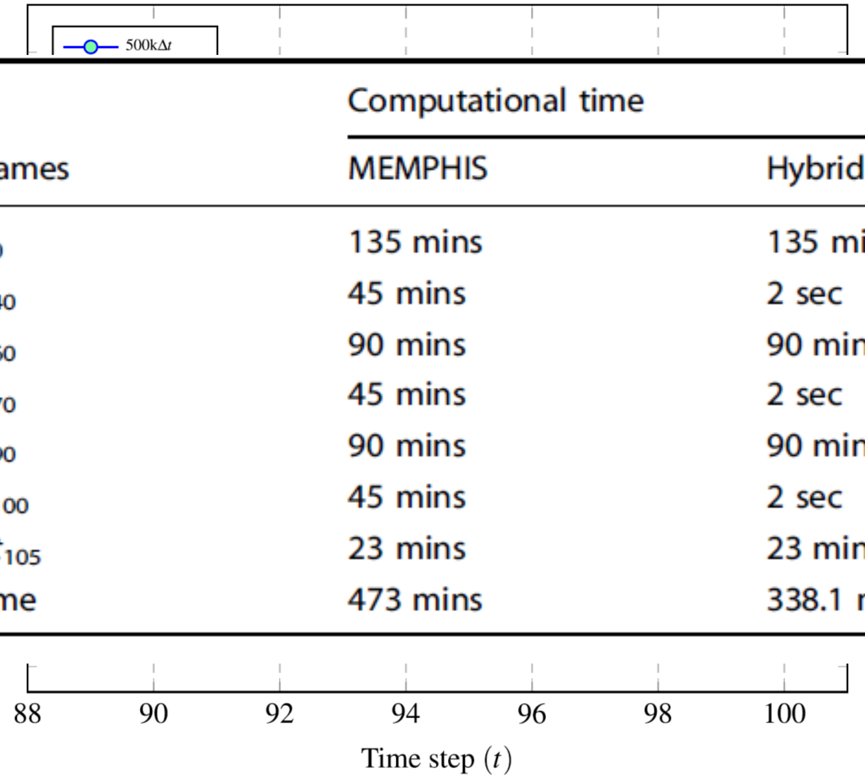



Extrapolation Error




| | Computational time | |
|---|---|---|
| Time frames | MEMPHIS | Hybrid |
| $t_1$ to $t_{30}$ | 135 mins | 135 mins |
| $t_{30}$ to $t_{40}$ | 45 mins | 2 sec |
| $t_{40}$ to $t_{60}$ | 90 mins | 90 mins |
| $t_{60}$ to $t_{70}$ | 45 mins | 2 sec |
| $t_{70}$ to $t_{90}$ | 90 mins | 90 mins |
| $t_{90}$ to $t_{100}$ | 45 mins | 2 sec |
| $t_{100}$ to $t_{105}$ | 23 mins | 23 mins |
| Total time | 473 mins | 338.1 mins |

# Key Takeaways

- Latent DeepONet is beneficial for time dependent problems that can be represented in lower-order manifold.
- The training time of the autoencoder and the latent DeepONet is less than the training time of DeepONet on high-dimensional data.
- Standalone deep learning frameworks are not enough. Integrating with numerical methods expands the application horizon of SciML.
- Future work: Integrating Physics with the L-DeepONet architecture

# *Acknowledgements*

- Prof. George Karniadakis, Brown University
- Dr. Ameya Jagtap, Brown University
- Dr. Khemraj Shukla, Brown University
- Vivek Oommen, Brown University
- Prof. Michael Shields, Johns Hopkins University
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# Thank you!