JOHNS HOPKINS
WHITING SCHOOL of ENGINEERING

Accelerating Numerical Solvers with AI-based Surrogate Models

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Physics-based Models

Can represent the Processes of Nature

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

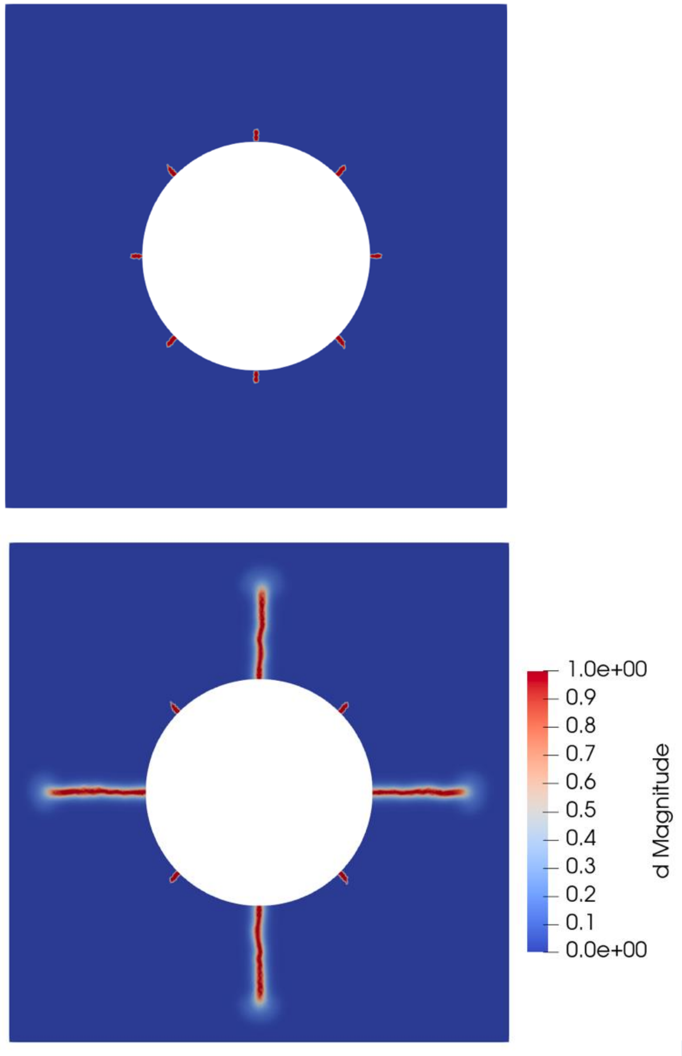
  To model earthquake: $m\frac{d^2u}{dt^2} + \mathrm{k}\frac{du}{dt} + F_0 = 0$

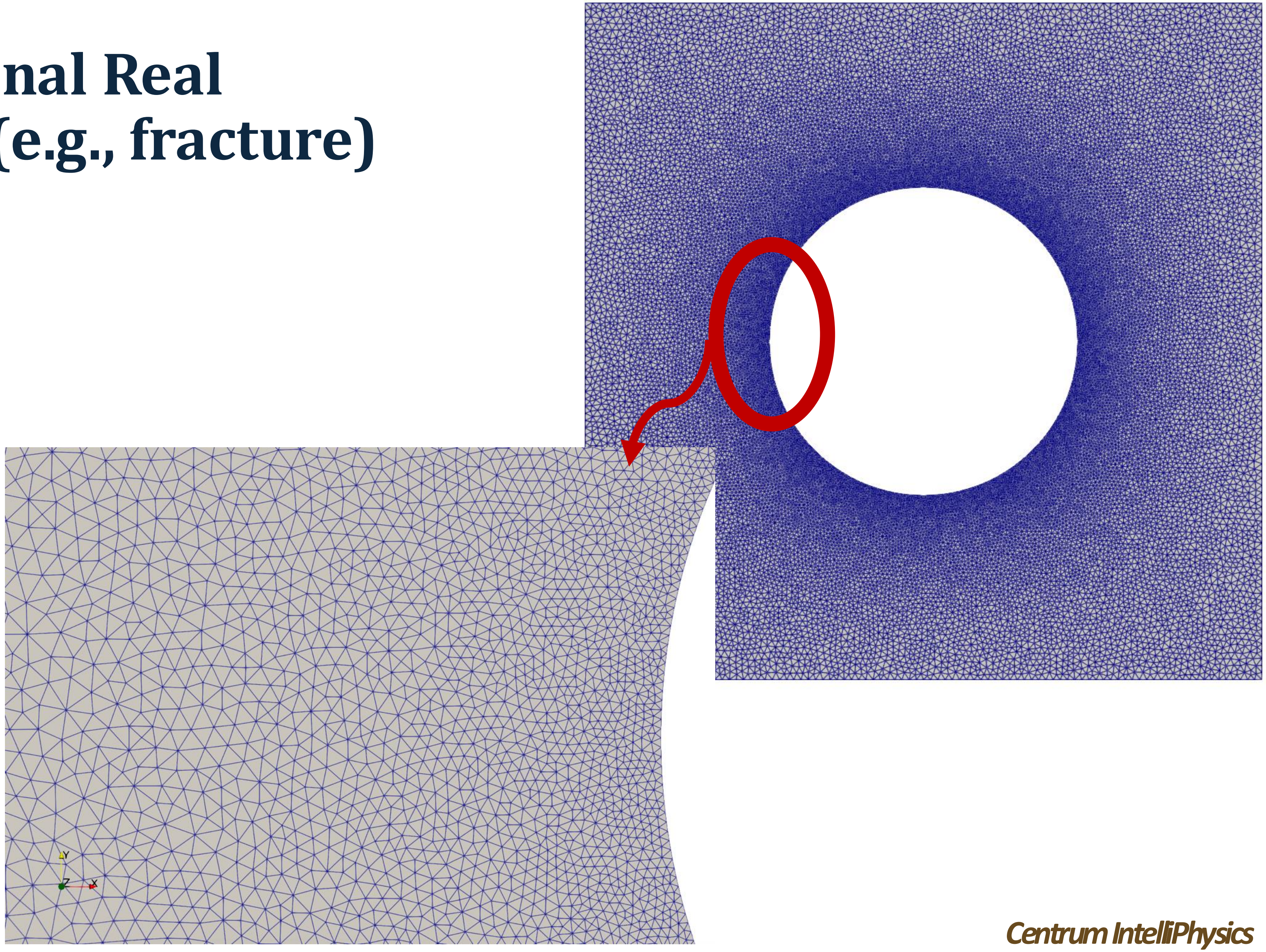
  To model waves: $\frac{\partial^2 u}{\partial t^2} - \nu^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = 0$
- Computational Mechanics helps us simulate these equations.

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.

High Dimensional Real World System (e.g., fracture)





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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

Physics Informed

Finite Dimensional

Infinite Dimensional

PCA

Auto-encoders

K-PCA

Diffusion maps

f-PCA

DeepONet

LNO

WNO

FNO

F-RKHS

PINNs

PI-DeepONet

PINO

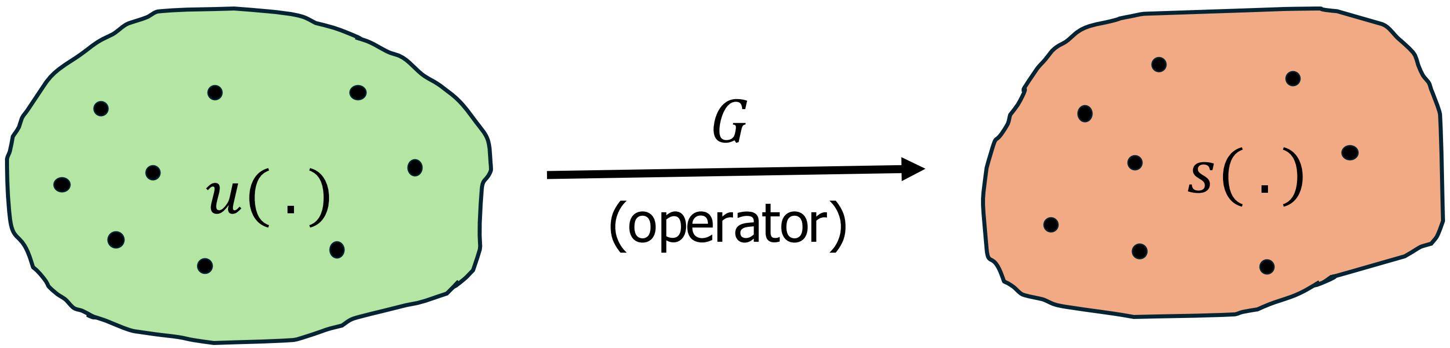
Operator Learning Framework

Input-output map

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

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

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



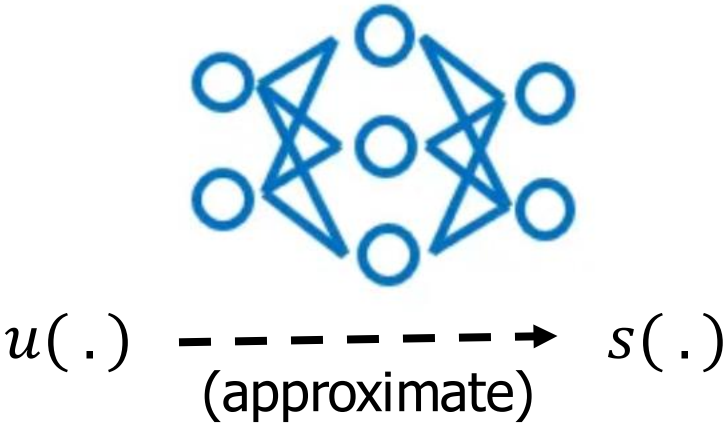
Input function space

Output function space

Operator learning

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

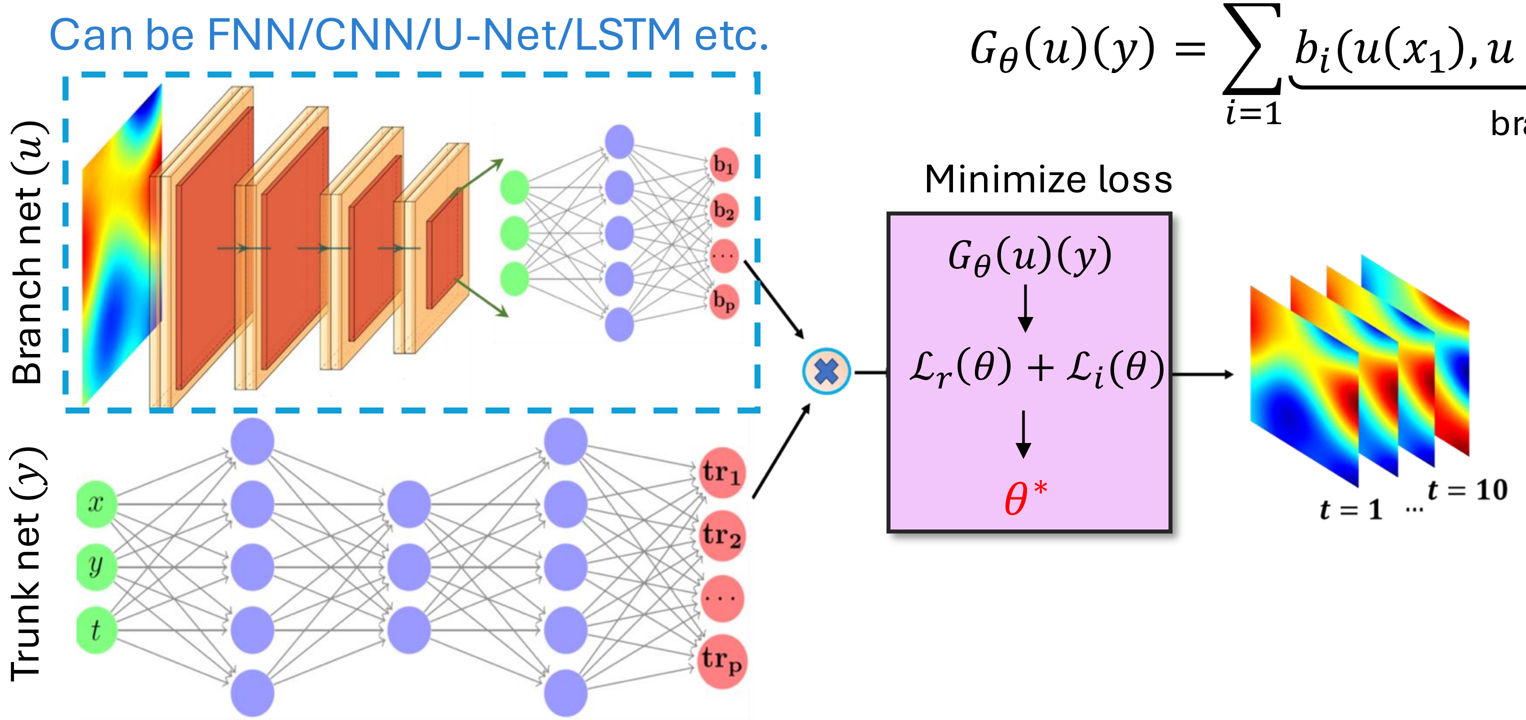
Training $\theta^* = \mathrm{argmin}_\theta l(\{\mathcal{U}_n, \Psi(\mathcal{S}_n, \theta)\})$



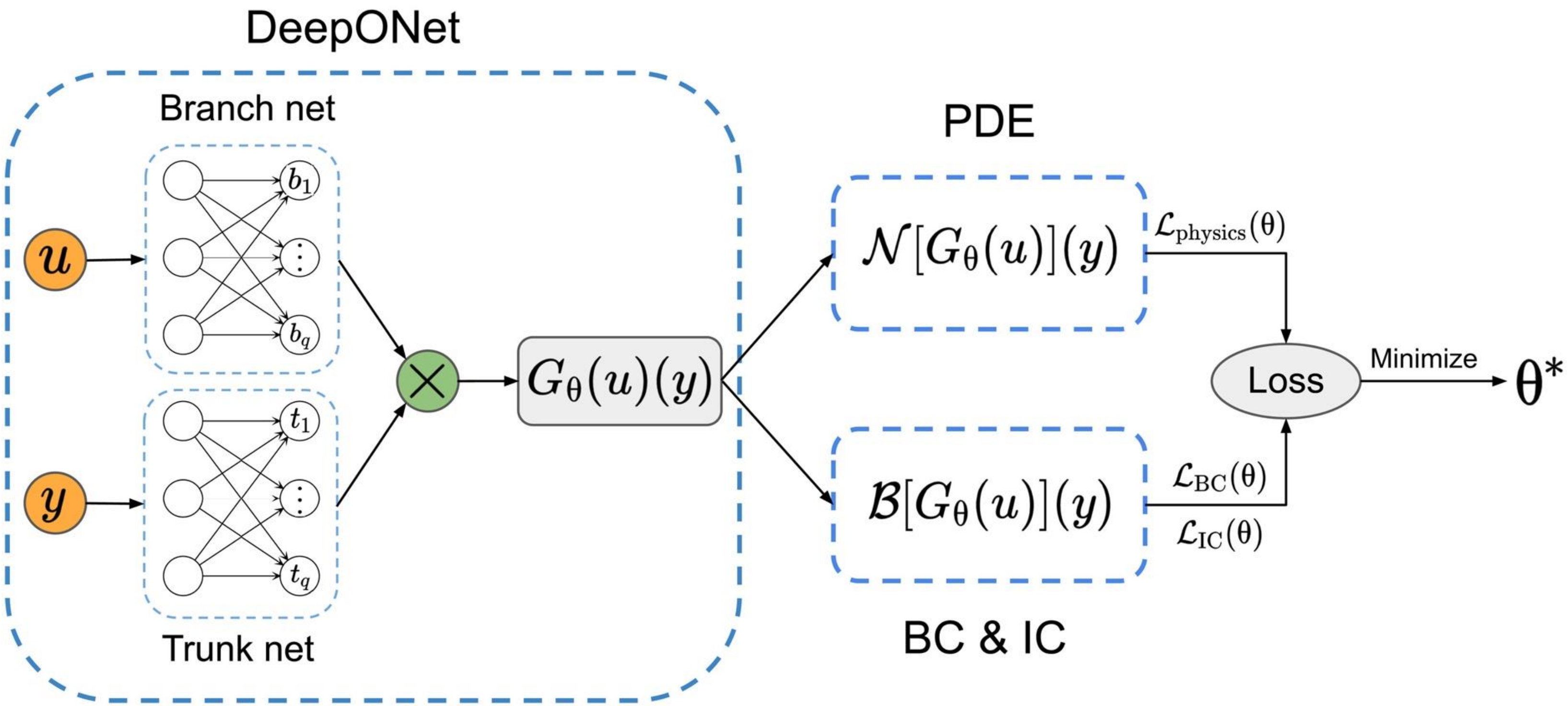
Deep Operator Network (DeepONet)

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

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



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.

Challenges With Neural Operators

- For Data Driven Models: Requires voluminous amount of high-fidelity training dataset – extensive parametric sweep on the numerical solvers.

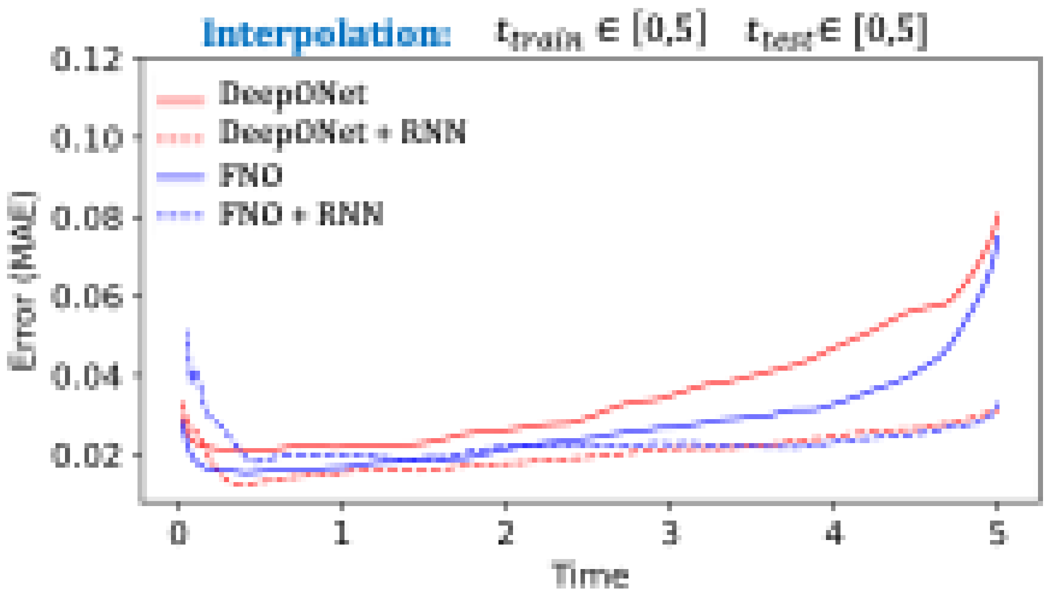
- For Physics-Informed Models : Physics-Informed Neural Operators –
  - Extremely expensive to train* due to the computation of the gradients for large number of function used to represent the function space.
  - No proofs on error boundedness for generalization accuracy.

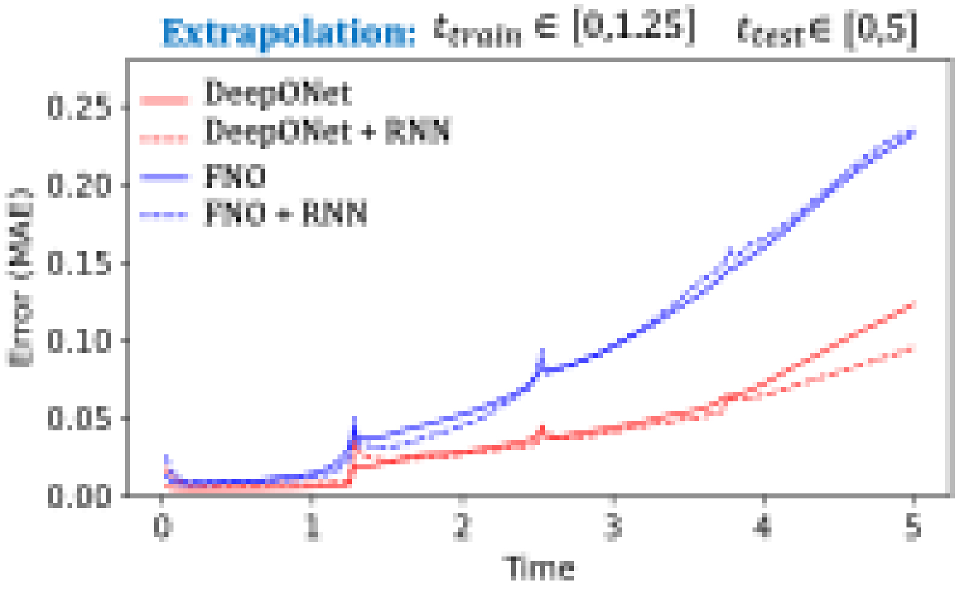
* Mandl, Luis, Somdatta Goswami, Lena Lambers, and Tim Ricken. "Separable physics-informed DeepONet: Breaking the curse of dimensionality in physics-informed machine learning." *Computer Methods in Applied Mechanics and Engineering* 434 (2025): 117586.

Data-driven ML Models for Dynamical Systems

KdV equation: $u_t - \eta u u_x + \gamma u_{xxx} = 0$

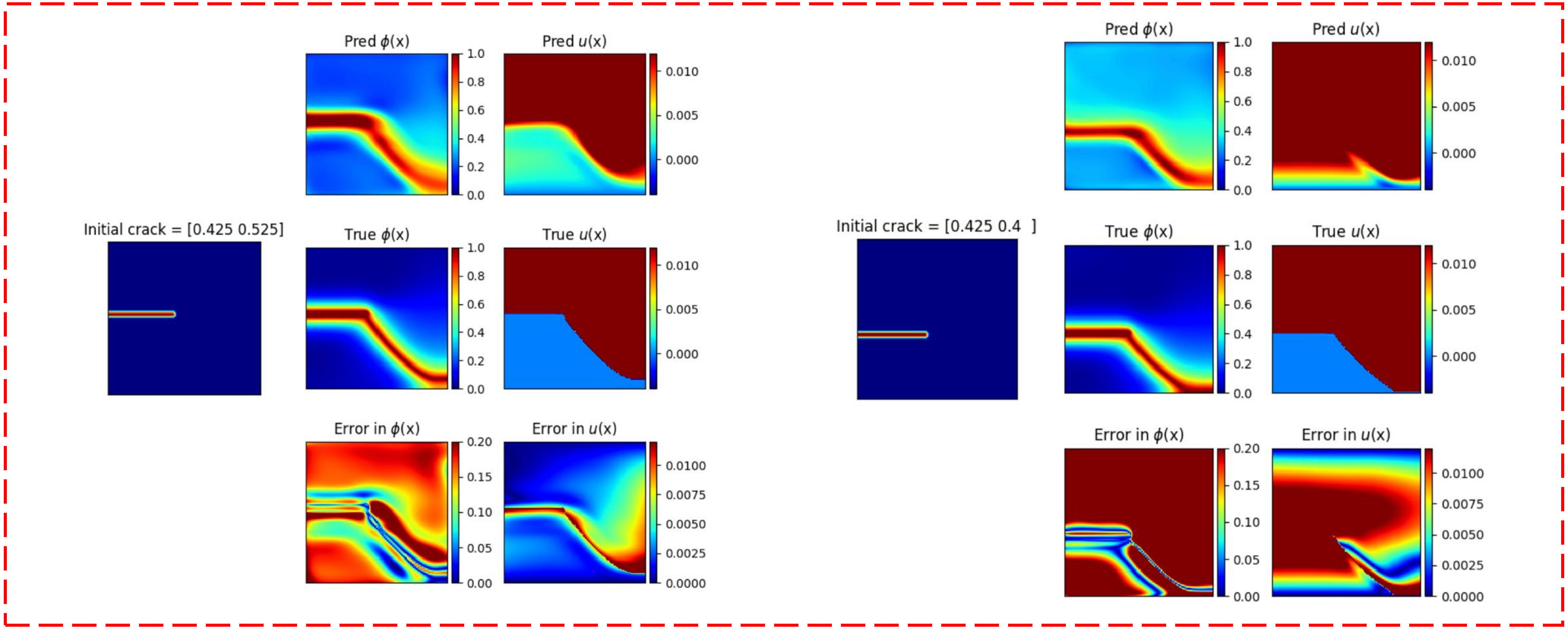
Learning Task: $u(x, t = 0) \rightarrow u(x, t)$,
$\Omega_x = [0,10]$ $\Delta t = 0.025$ $\Delta x = 0.2$





Michałowska, K., Goswami, S., Karniadakis, G. E., & Riemer-Sørensen, S. (2024, June). Neural operator learning for long-time integration in dynamical systems with recurrent neural networks. In *2024 International Joint Conference on Neural Networks (IJCNN)* (pp. 1-8). IEEE.

Physics-Informed Surrogate Models



A physics-informed variational DeepONet for predicting crack path in quasi-brittle materials – Goswami et. al, CMAME, 2022

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Hybrid Solvers: Physics-Informed ML-Integrated Numerical Simulators

The Hybrid Solver

1. Employ Domain Decomposition Framework:

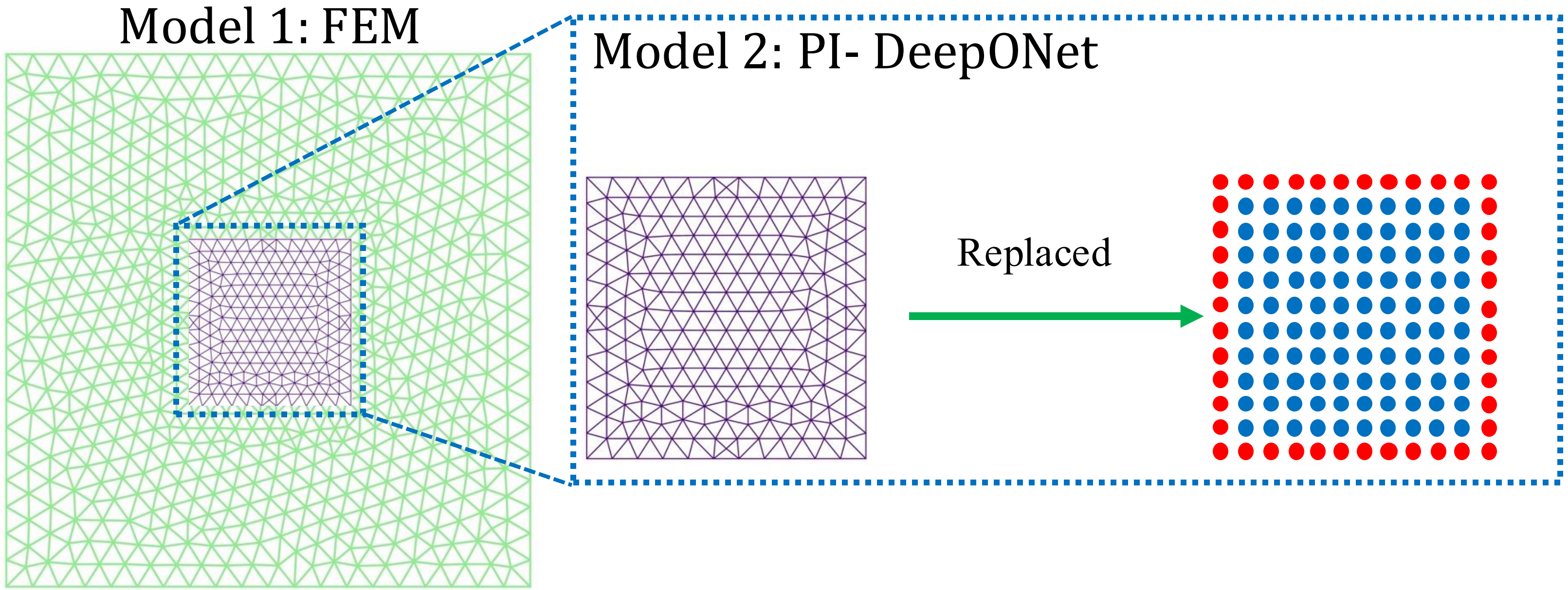
    Location requiring finer discretization –approximated using **physics informed neural operators**

    Locations 'ok' with coarser discretization – approximated using numerical solvers.

2. The two solvers handing over an overlapping domain and are coupled using the Alternating Schwartz coupling framework.

3. For time dependent systems, the time marching employs a Newmark-Beta method, instead of the neural operators

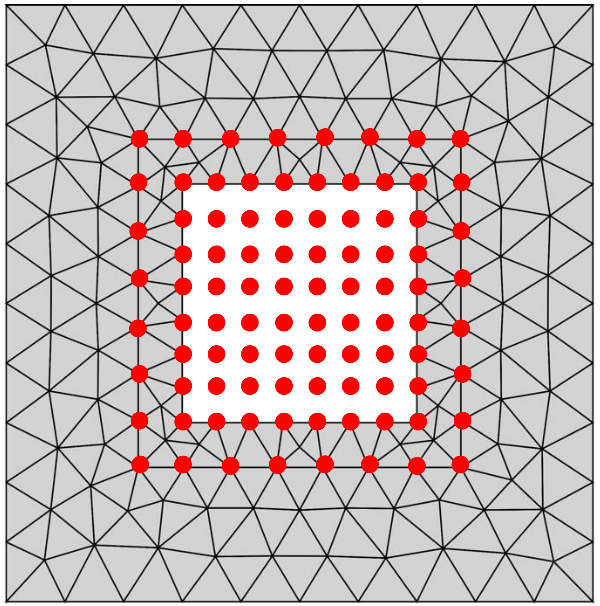
Domain Decomposition Framework



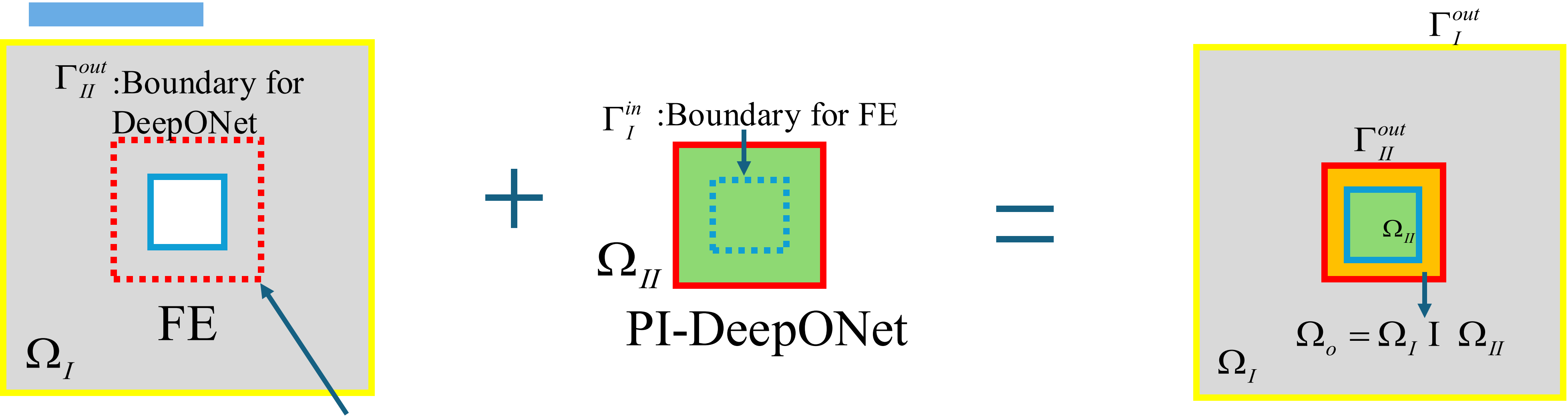
Can suffice with coarse mesh

Requires fine mesh

Overlapping Decomposed Domains



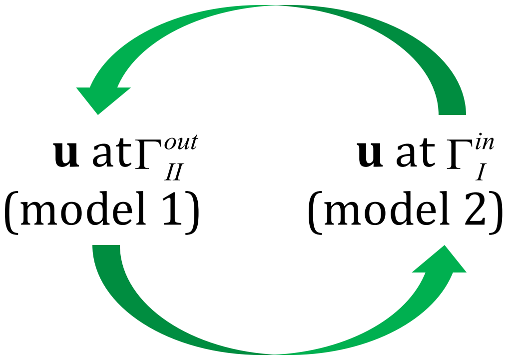
Spatial Domain Coupling



Inner iteration

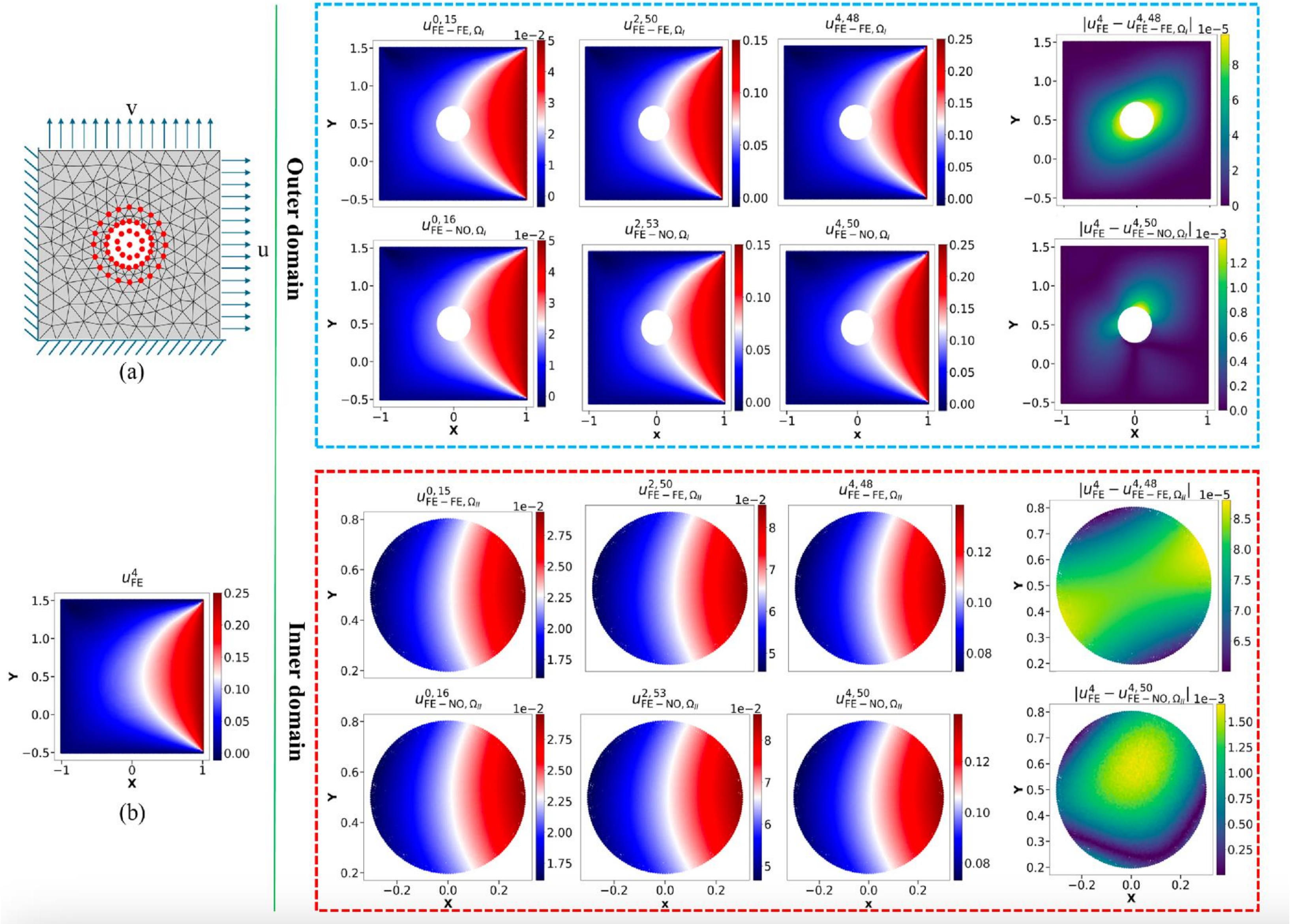
Schwartz alternating method at overlapping boundary:

Information Exchange

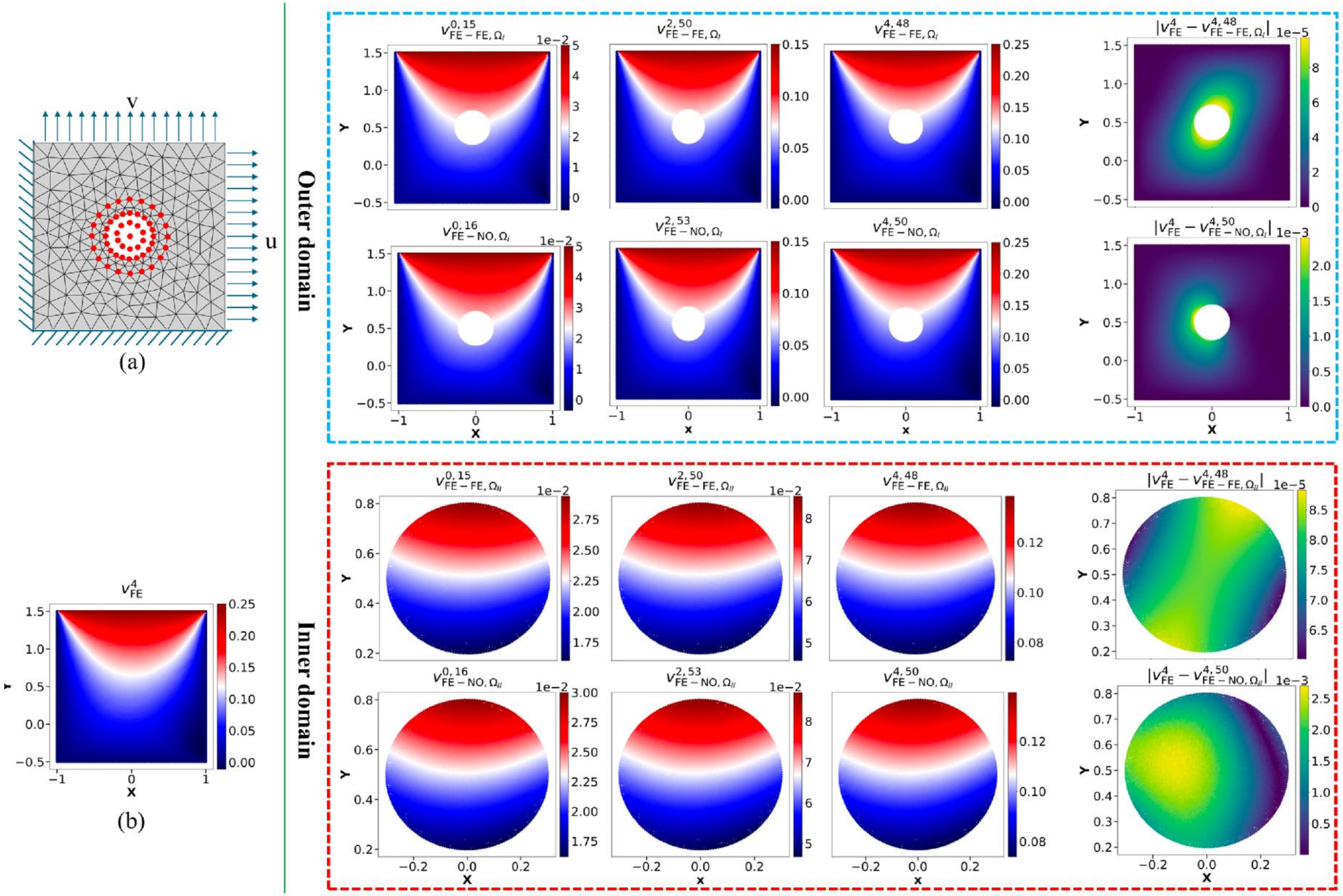


1. Receive the boundary conditions of Ω_I and obtain the displacement **u** at Γ_{II}^{out}, pass it to model 2 in Ω_{II}.
2. Receive the boundary conditions of Ω_{II} and obtain the displacement **u** at Γ_I^{in}, pass it to model 1 in Ω_I.
3. Obtain the results when the **u** difference from two successive iterations is smaller than the critical value.

Hyper-elasticity under quasi-static loading conditions



Hyper-elasticity under quasi-static loading conditions



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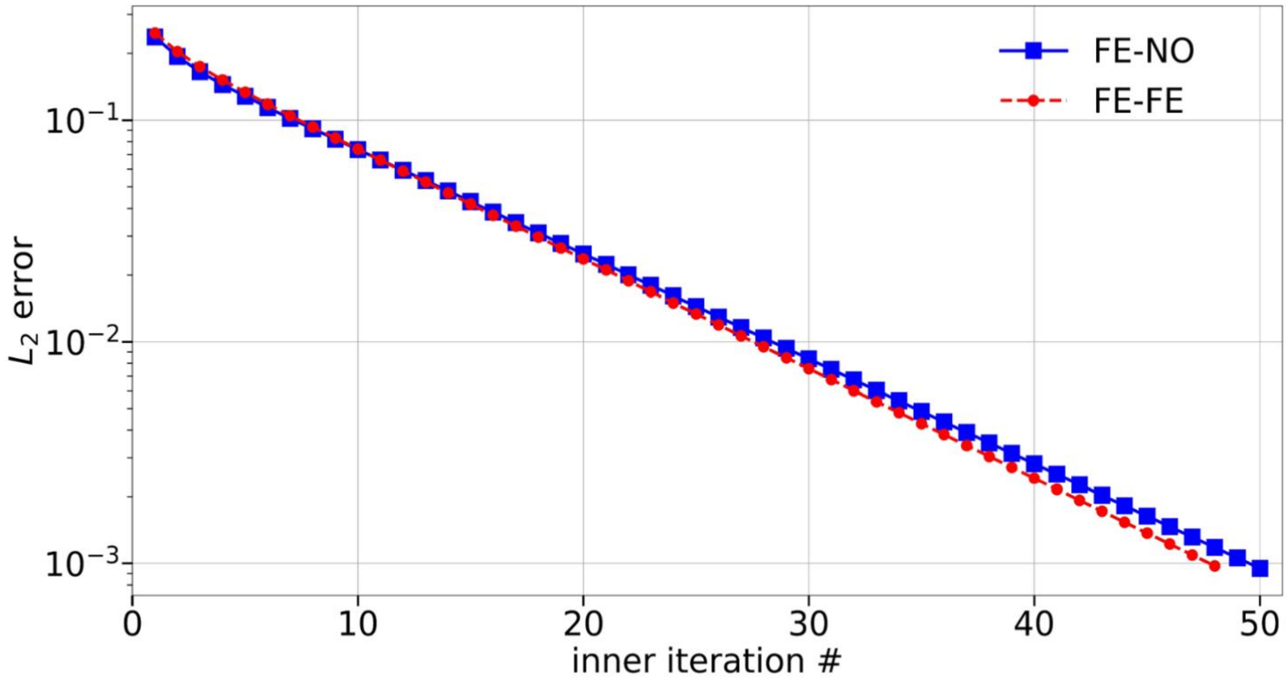
Performance of FE-NO



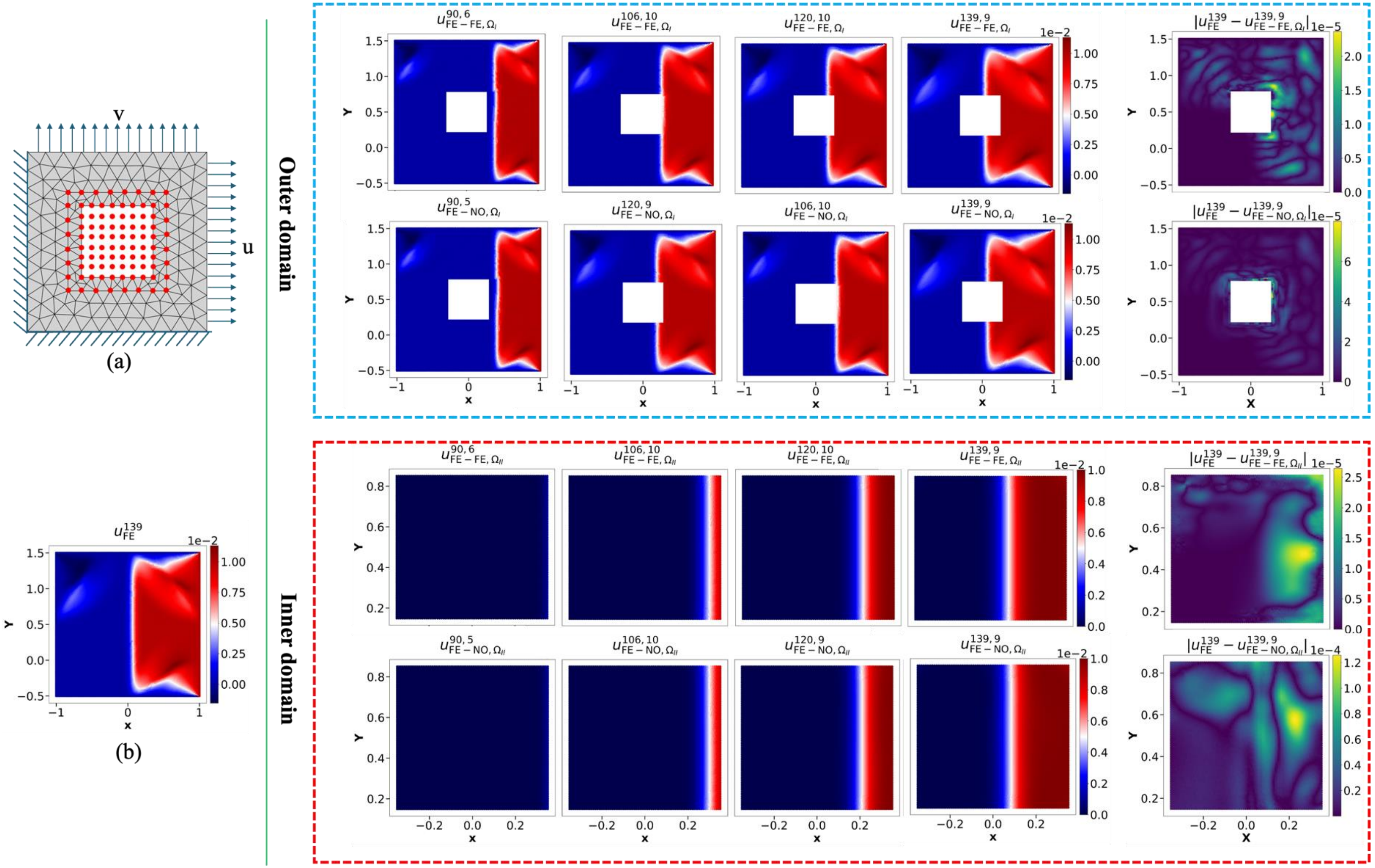
At t=4, the neural operators (NO) coupling needs more inner iterations.

No need Newton's solver for additional root-finding iterations at each inner iterations.

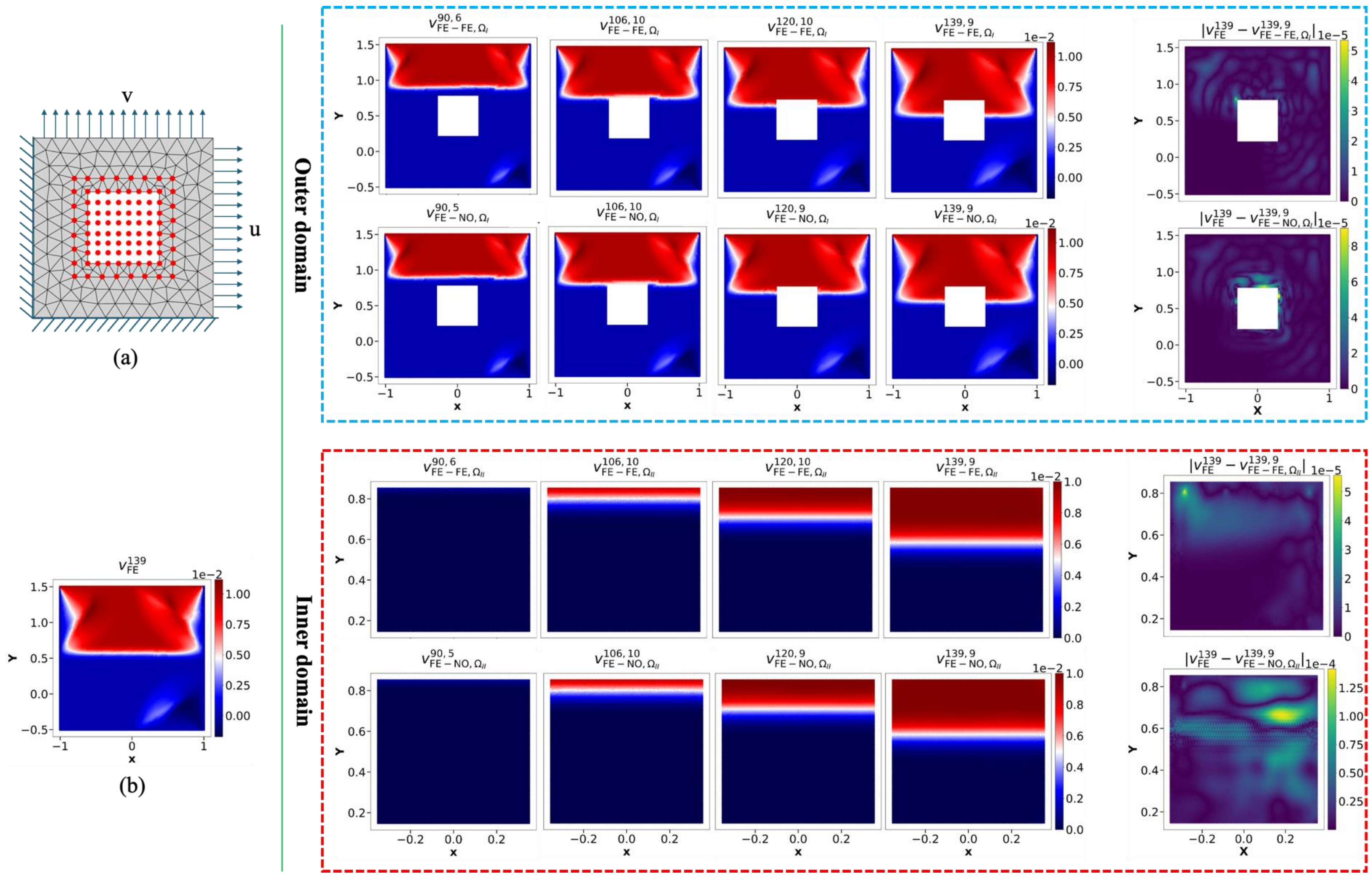
FE-NO coupling is 20% faster than FE-FE coupling.

Also, FE-NO is more stable under large loadings.

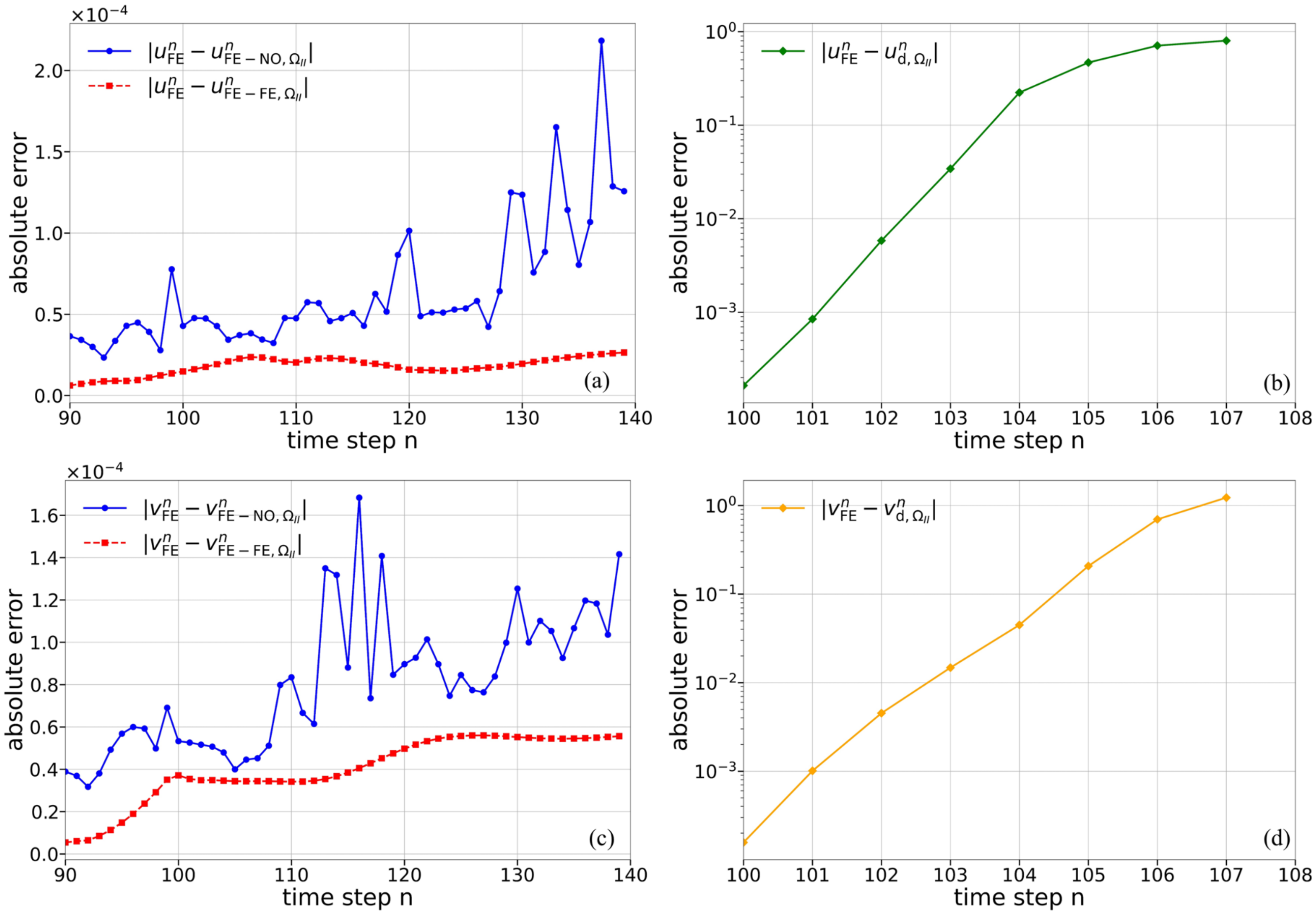
Linear Elastic Model in Dynamic Regime



Linear Elastic Model in Dynamic Regime



Improvement in Error Accumulation



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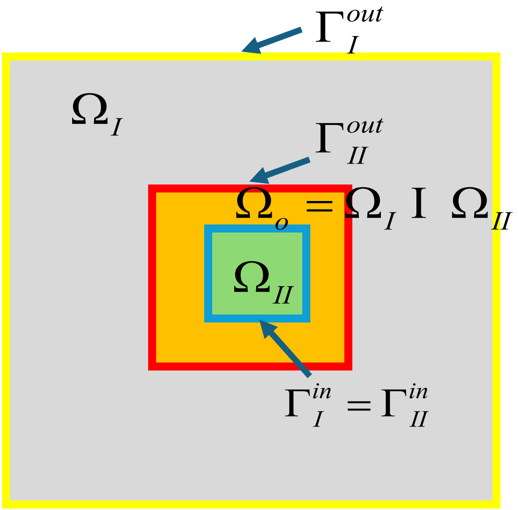
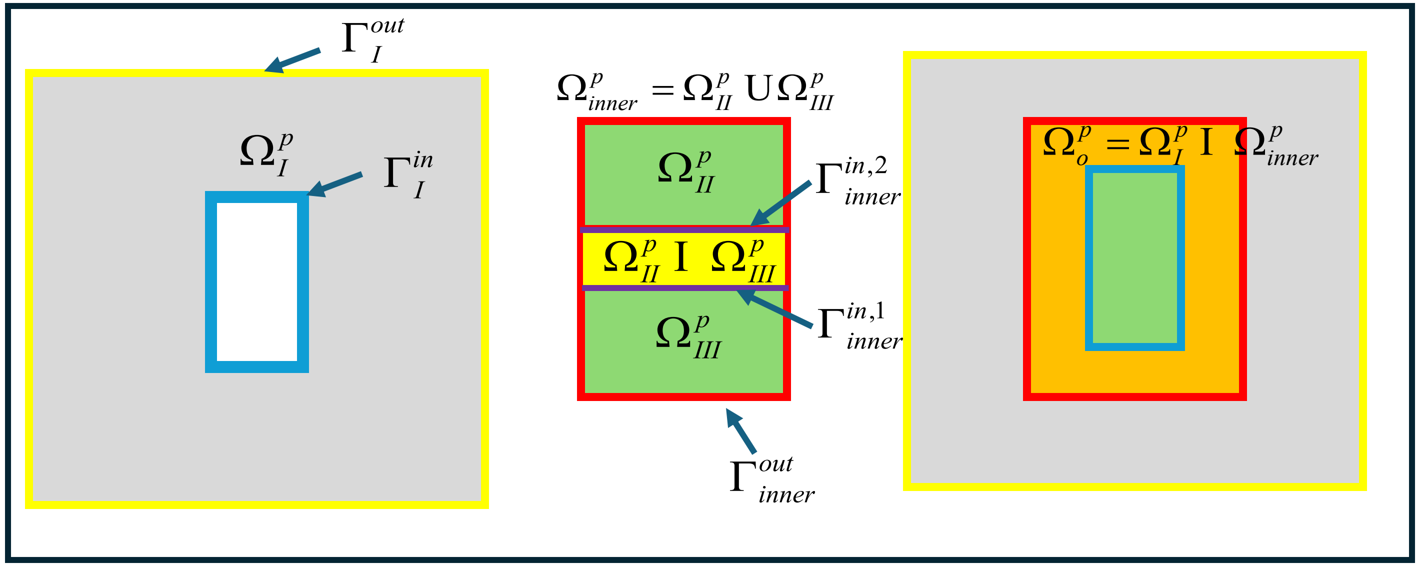
Future work: Adaptive extension of the ML –simulated subdomain

Initial decomposed domains



Decomposed domain after a few timesteps



Key Points

- We successfully employed domain decomposition using FE-NO coupling.

- We significantly reduced error accumulation for time dependent systems using Newmark-Beta time marching method.

- We are implementing adaptive extension of ML-simulated subdomains.

Thank you for your attention!

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2. Temporal dimension coupling: new physic-informed DeepONet architecture

Newmark-beta time discretization method:

$$\dot{u}(t+dt) = \dot{u} + dt\left[(1-\gamma)\ddot{u} + \gamma\ddot{u}(t+dt)\right]$$

$$\ddot{u}(t+dt) = \frac{1}{(dt)^2 \beta}\left[-u - \dot{u}\,dt + u(t+dt)\right] - \frac{(1-2\beta)}{2\beta}\ddot{u}$$

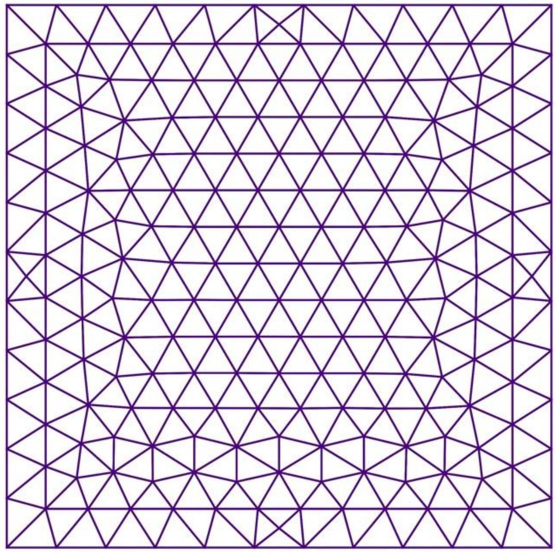
$$[M]\ddot{u}(t+dt) = [K]u(t+dt) + [F(t+dt)]$$

Time-advancing Physic-informed DeepONet:
predict the current time step values based on the displacement, velocity, acceleration from previous time step and current boundary conditions

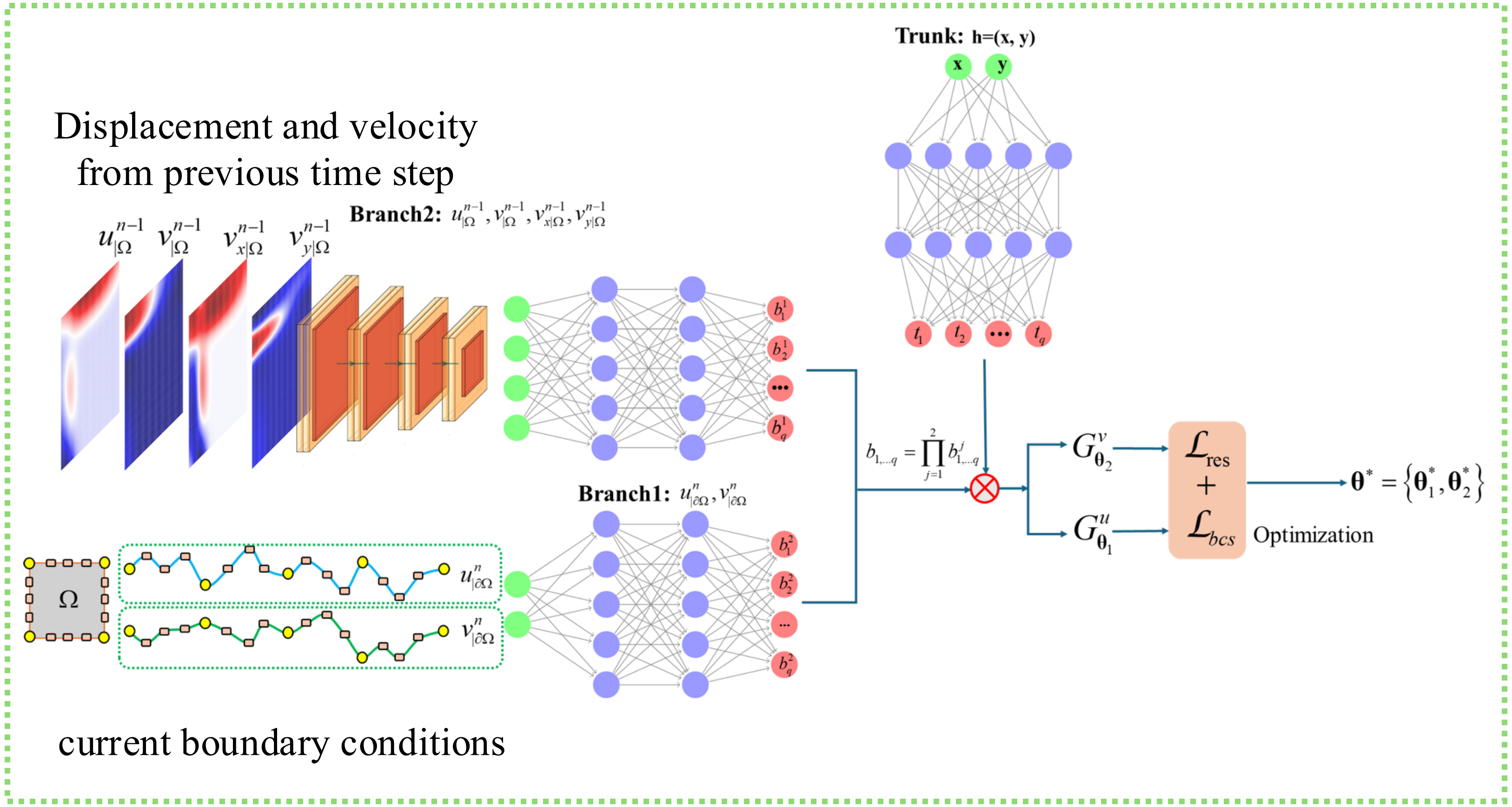
Covert into strong form in phyiscs-informed DeepONet

New DeepONet architecture

Numerical solver: FEM



equivalent



2. Temporal dimension coupling: Working Flowchart of time advancing NOs