

# **A Cross Machine and Parametric Neural Operator Surrogate Model for MHD Simulations**

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Qiyun Cheng<sup>1</sup>, Cesar Clauser<sup>1</sup>, E.d.D. Zapata-Cornejo<sup>1</sup>, Nathaniel Ferraro<sup>2</sup>, Cristina Rea<sup>1</sup>

1. Plasma Science & Fusion Center, MIT

2. Princeton Plasma Physics Laboratory, Princeton



12/12/2025

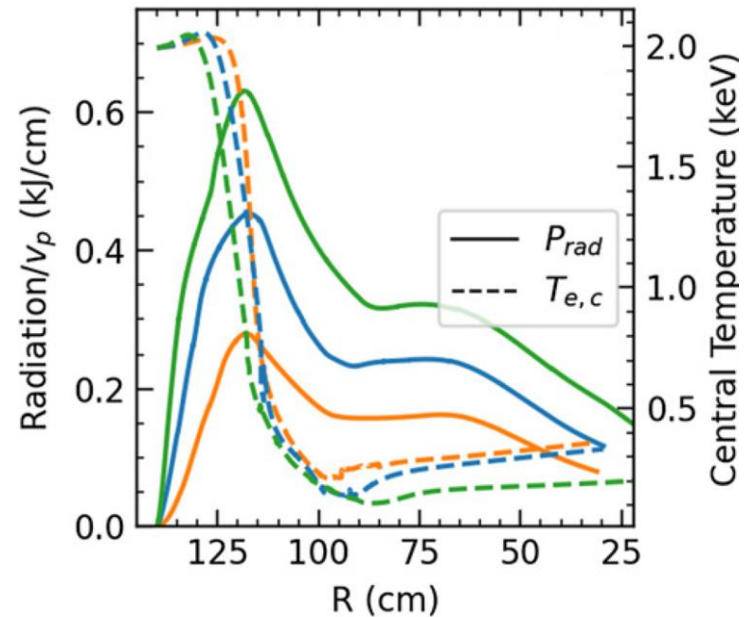
# Motivation & Research Background

- Future fusion device (e.g., ARC™) designs require large-scale **parameter optimizations** (e.g., disruption mitigation optimization)



JET runaway electrons damage.  
<https://www.iter.org/newsline/-/2234>

Unmitigated disruptions in ITER is expected to become of the order 1 in  $10^4$  discharges [1].



Different **pellet injection velocities** (three colors) lead to varying **radiated power ( $P_{rad}$ )** and the **plasma electron central temperature ( $T_{e,c}$ )** [2].

[1] E.J. Strait et al., *Nucl. Fusion* **59** 112012 (2019)

[2] C.F. Clauser et. al., *Nucl. Fusion*, **61**, 116003 (2021)

# Motivation & Research Background

- High-fidelity nonlinear MHD simulations (e.g., M3D-C1) are essential but computationally expensive
  - E.g., one 3D M3D-C1 simulation with 8 toroidal planes (Data provided by Rishabh Datta)
  - One time step  $\sim 53s$ , 20~30k time steps for several milliseconds
  - On Perlmutter with 8 nodes for  $\sim 2$  weeks
- Neural network-based surrogate models offer a potential approach to accelerate this optimization

# Outlines

- Introduction of Operator Learning
- Generalization Methods of Neural Operator Surrogates
  - Parameter generalization
  - Geometry generalization
  - Demonstration
- M3D-C1 Solver Acceleration

# Neural Operator & Operator Learning

**Neural Operator:** Neural networks for PDE surrogate modeling

PDE in operator form:  $\mathcal{O}(\mathbf{p})[u(\mathbf{x})] = S(\mathbf{x})$



Solution of the field function:

$$u(\mathbf{x}) = \underline{\mathcal{O}^{-1}(\mathbf{p})}[S(\mathbf{x})]$$

Solution Operator

Computational expensive matrix inverse

Steady state electron temperature equation:

$$\begin{aligned} n_e(T_e \nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla T_e) + \sigma_e T_e \\ = (\gamma - 1)(\nabla \cdot (\kappa_{\perp} \nabla T_e) + \nabla \cdot (\kappa_{\parallel} \mathbf{b} \mathbf{b} \cdot \nabla T_e) \\ + \eta J^2 + Q_{rad} + Q_{\dots}) \end{aligned}$$

Operator form:

$$\mathcal{O}(\nu, \sigma_e, \kappa_{\perp}, \kappa_{\parallel})[T_e(r, z)] = S(r, z)$$

**Neural operator (N.O.)** as a surrogate of the solution operator

$$u_{N.O.}(\mathbf{x}) = \mathcal{O}_{N.O.}^{-1}(\mathbf{p})[S(\mathbf{x})] \approx \mathcal{O}^{-1}(\mathbf{p})[S(\mathbf{x})]$$

Take any source and give predicted field function

# Existing Issues of Neural Operator Surrogates

$$u_{N.O.}(x) = \mathcal{O}_{N.O.}^{-1}(p)[S(x)]$$

## (1) Data acquisition

Comprehensive parameter scans are infeasible

## (2) Cross-machine generalization

Evolving device designs make it impossible to obtain sufficient data

## (3) Accuracy degradation

Extrapolation performance remains low fidelity

## (4) Limited interpretability

Safety-critical applications require transparent and explainable models

# Parameter Generalization – Equation Recast

Train a **canonical neural operator** with  $\mathbf{p}^*$

$$\mathcal{O}(\mathbf{p}^*)[u(\mathbf{x})] = S(\mathbf{x}) \quad \longrightarrow \quad \mathcal{O}_{N.O.}^{-1}(\mathbf{p}^*)$$

$$T_e \nabla \cdot \mathbf{v}^* + \mathbf{v}^* \cdot \nabla T_e - \frac{(\gamma - 1)\kappa_{\perp}^*}{n_e^*} \nabla^2 T_e = S \quad \underbrace{\left( \nabla \cdot \mathbf{v}^* + \mathbf{v}^* \cdot \nabla - \frac{(\gamma - 1)\kappa_{\perp}^*}{n_e^*} \nabla^2 \right)}_{\mathcal{O}(\mathbf{p}^*)} T_e = S$$

# Parameter Generalization – Equation Recast

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$$\mathcal{O}(\mathbf{p}^*)[u(\mathbf{x})] = S(\mathbf{x}) \quad \longrightarrow \quad \mathcal{O}_{N.O.}^{-1}(\mathbf{p}^*)$$

Given  $\mathbf{p}'$ , decompose the operator:

$$\mathcal{O}(\mathbf{p}')[u(\mathbf{x})] = \left( \mathcal{O}(\mathbf{p}') - \mathcal{O}(\mathbf{p}^*) + \mathcal{O}(\mathbf{p}^*) \right)[u(\mathbf{x})] = S(\mathbf{x})$$

Residual operator:  $\delta\mathcal{O}(\delta\mathbf{p})$

$$T_e \nabla \cdot \mathbf{v}^* + \mathbf{v}^* \cdot \nabla T_e - \frac{(\gamma - 1)\kappa_{\perp}^*}{n_e^*} \nabla^2 T_e = S \quad T_e \nabla \cdot \mathbf{v}' + \mathbf{v}' \cdot \nabla T_e - \frac{(\gamma - 1)\kappa'_{\perp}}{n'_e} \nabla^2 T_e = S$$

$$T_e (\nabla \cdot \mathbf{v}' - \nabla \cdot \mathbf{v}^*) + (\mathbf{v}' \cdot \nabla T_e - \mathbf{v}^* \cdot \nabla T_e) - \left( \frac{(\gamma - 1)\kappa'_{\perp}}{n'_e} \nabla^2 T_e - \frac{(\gamma - 1)\kappa_{\perp}^*}{n_e^*} \nabla^2 T_e \right)$$

$$\delta\mathcal{O}(\delta\mathbf{p})[u(\mathbf{x})]$$

# Parameter Generalization – Equation Recast

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Residual operator:  $\delta\mathcal{O}(\delta\mathbf{p})$

**Equation Recast:**  $\mathcal{O}(\mathbf{p}^*) [u(\mathbf{x})] = S(\mathbf{x}) - \delta\mathcal{O}(\delta\mathbf{p})[u(\mathbf{x})]$

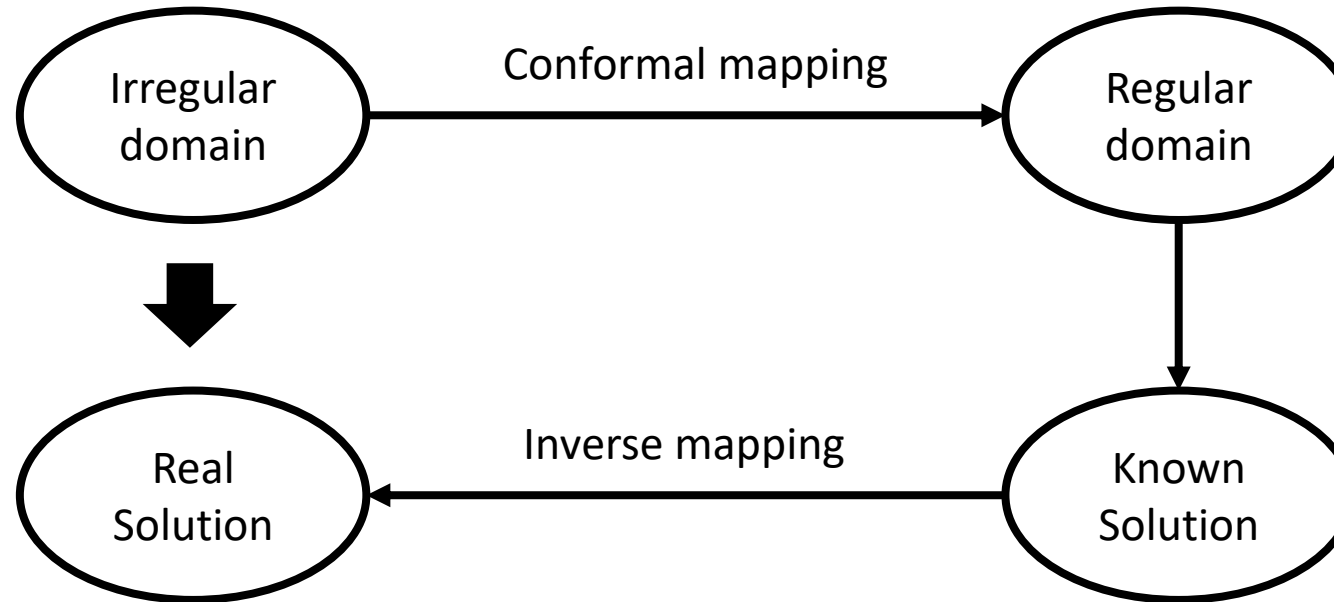
$$\longrightarrow \quad u(\mathbf{x}; \mathbf{p}') = \mathcal{O}_{N.O.}^{-1}(\mathbf{p}^*) \left[ \underline{S(\mathbf{x}) - \delta\mathcal{O}(\delta\mathbf{p})[u(\mathbf{x})]} \right]$$

Absorb parameter variance into source term  
Form an iterative scheme using canonical N.O.

**The canonical N.O. is generalized to all parameters with preserved physics**

# Cross Machine Generalization – Domain Unification

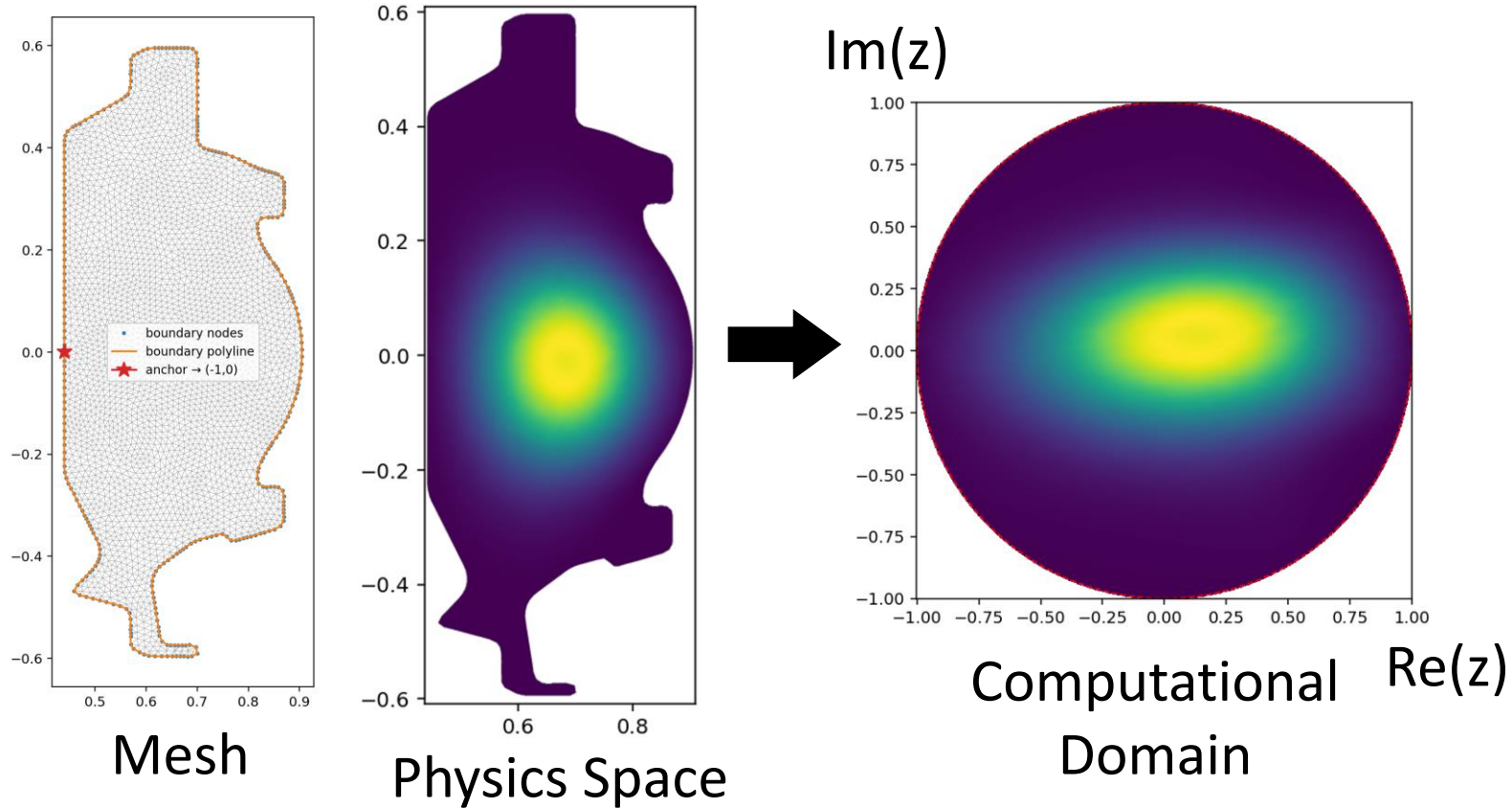
Solving a PDE analytically:



# Cross Machine Generalization – Domain Unification

Cross machine geometry unification via **Harmonic Mapping**:

## C-Mod 2D Mesh (Cross Section)



Boundary:

$$f|_{\partial\Omega} = e^{i\theta}$$

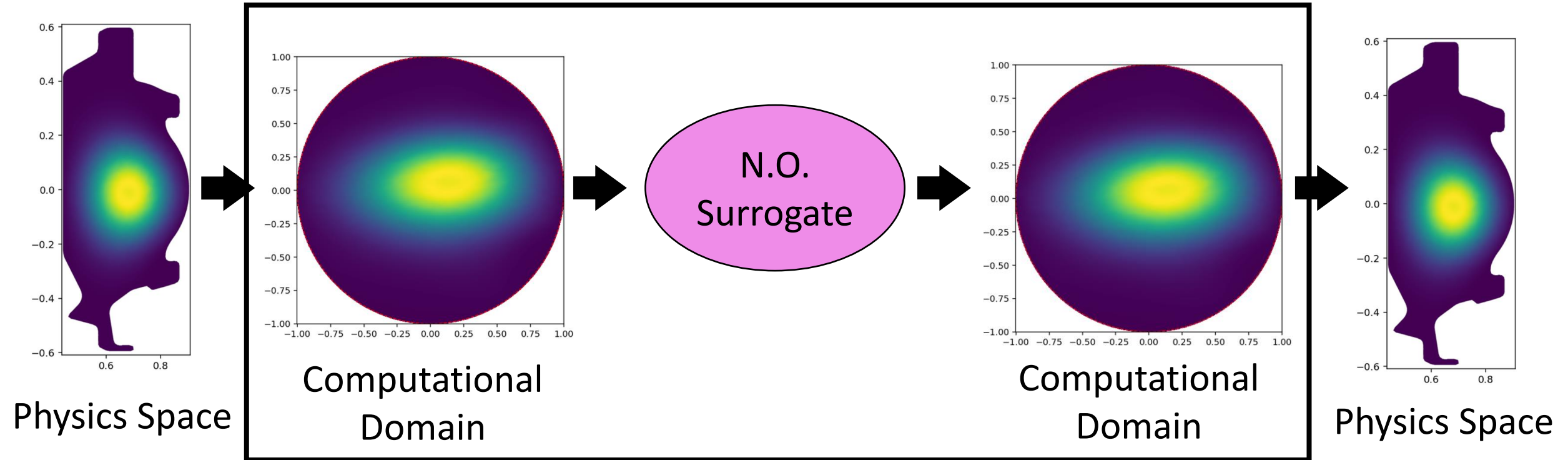
Harmonic functions:

$$\Delta u = \Delta v = 0$$

**Harmonic Mapping** is uniquely determined by the geometry

# Cross Machine Generalization – Domain Unification

Cross machine geometry unification via **Harmonic Mapping**:

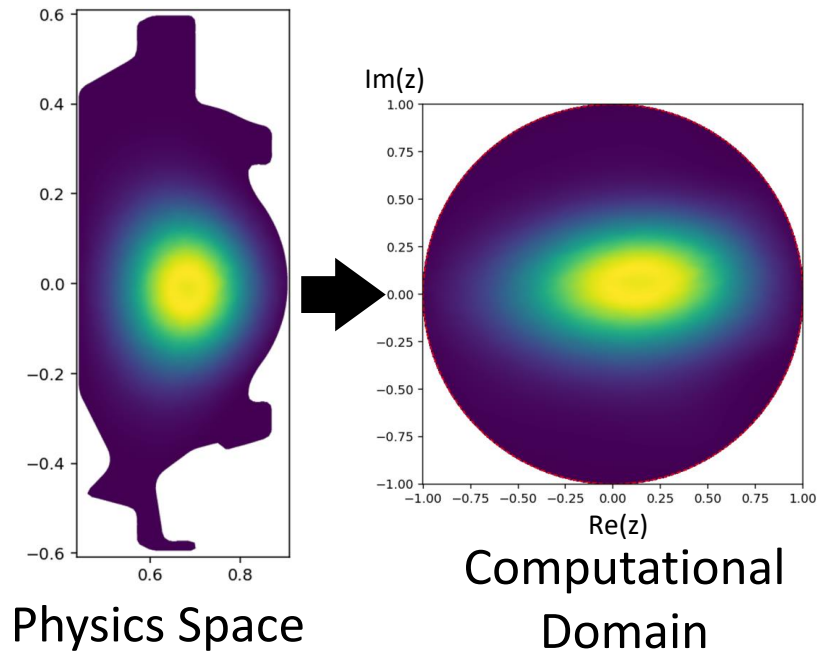


Separate the geometry analytically, achieving **geometry-agnostic** training

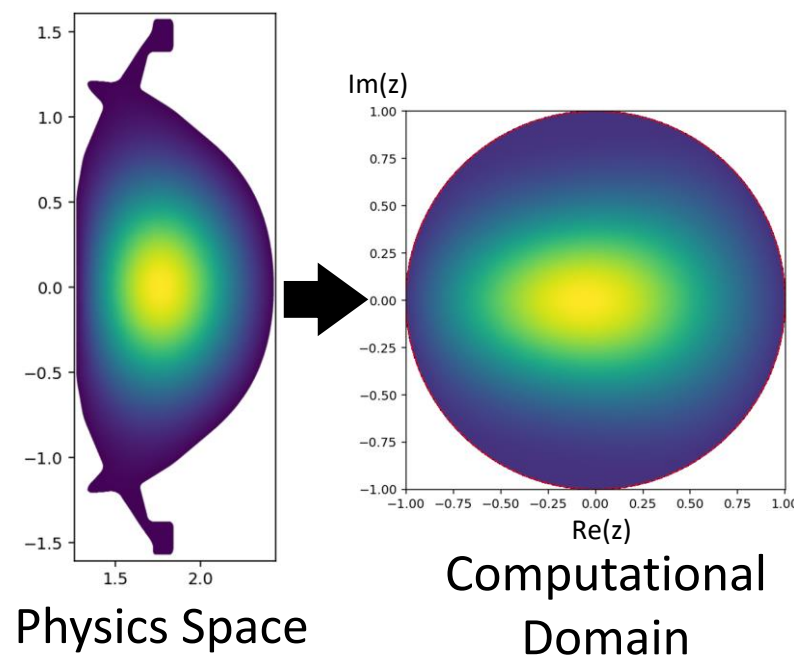
PDE is defined in the computational domain, same PDE for all machines (+ Jacobians)

# Cross Machine Generalization – Domain Unification

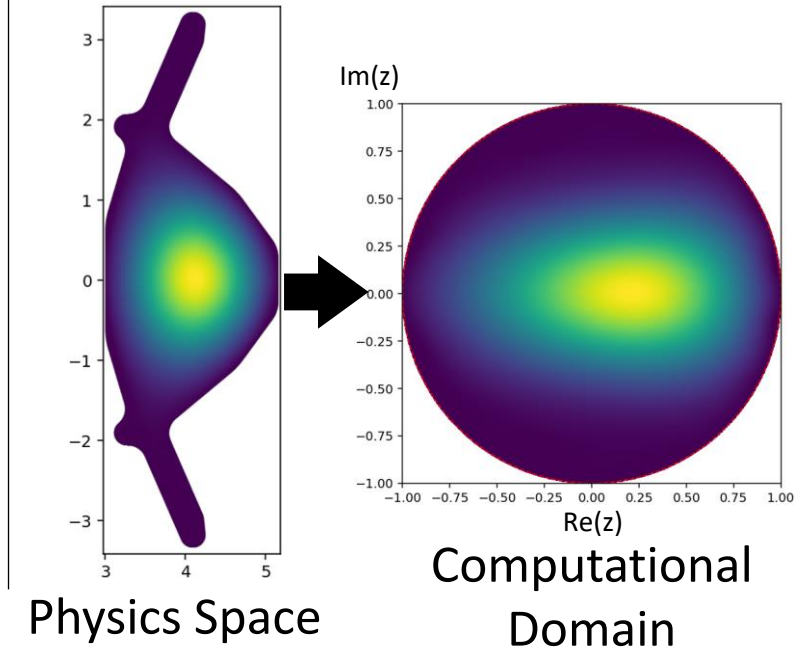
## C-Mod



## SPARC



## ARC\_V2A



Mappings and inverse mapping are **precalculated**

Different Jacobians can be **precalculated** and **absorbed** using Equation Recast

# Demo – Fourier Neural Operator (FNO) based Surrogate

Simplified thermal quenching problem (single energy equation)

$$n_e \left( \frac{\partial T_e}{\partial t} + \cancel{T_e \nabla \cdot \mathbf{v}} + \cancel{\mathbf{v} \cdot \nabla T_e} \right) \cancel{+ \sigma_e T_e}$$

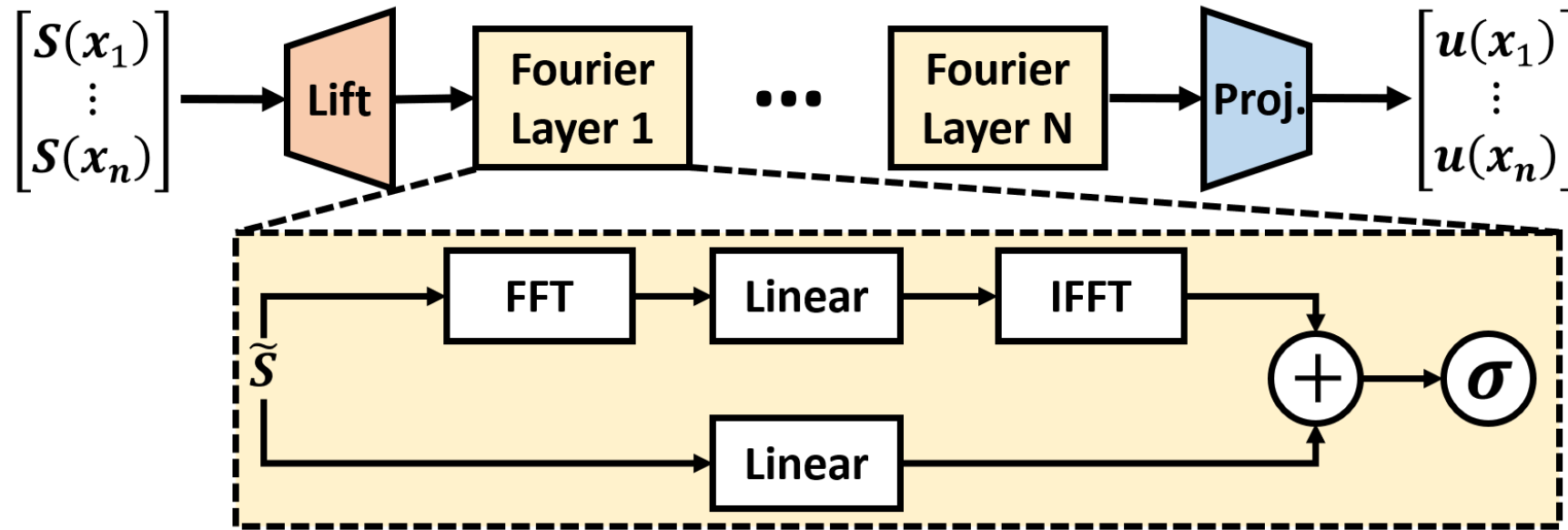
$$= (\gamma - 1)(\nabla \cdot (\kappa_{\perp} \nabla T_e) + \nabla \cdot (\kappa_{\parallel} \cancel{\mathbf{b}\mathbf{b}} \cdot \nabla T_e) + \eta J^2 \cancel{+ Q_{rad}} + Q_{ext})$$

$$\Rightarrow T_e^{i+1} = \underbrace{\left( \frac{1}{\delta t} - \frac{(\gamma - 1)}{n_e} \kappa_{\perp}^* \nabla^2 \right)^{-1}}_{\text{Neural Operator}} \left[ \underbrace{\frac{\gamma - 1}{n_e} (\eta J^2 + Q_{ext})}_{\text{I. C.}} + \underbrace{\frac{1}{\delta t} T_e^i + \frac{\gamma - 1}{n_e} (\kappa_{\perp}^{test} - \kappa_{\perp}^*) \nabla^2 T_e^{i+1}}_{\text{Additional Source}} \right]$$

Other equation evolutions are disabled in M3D-C1 simulations

# Demo – Fourier Neural Operator (FNO) based Surrogate

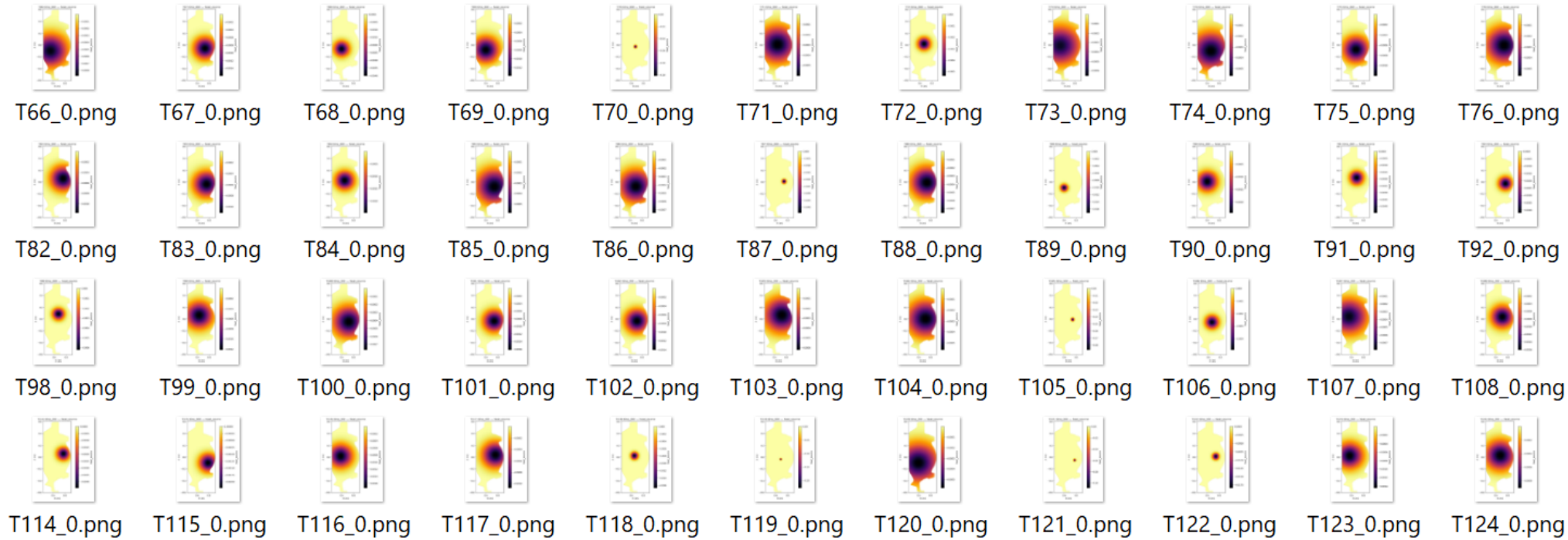
$$S(r, z) = \frac{\gamma - 1}{n_e} (\eta J^2 + Q_{ext}) + \frac{1}{\delta t} T_e^i + \frac{\gamma - 1}{n_e} (\kappa_{\perp}^{test} - \kappa_{\perp}^*) \nabla^2 T_e^{i+1} \quad u(r, z) = T_e^{i+1}(r, z)$$



Fourier neural operator [1]

[1] Z. Li, et al., Fourier Neural Operator for Parametric Partial Differential Equations, International Conference on Learning Representations, 2021.

# Demo – Fourier Neural Operator (FNO) based Surrogate



C-MOD Mesh  
256 Gaussian sources  
Random Var  
Random Center

256 Sources  $\times$  5 time steps

$$N_{train} = 256 \times 5 = 1280$$

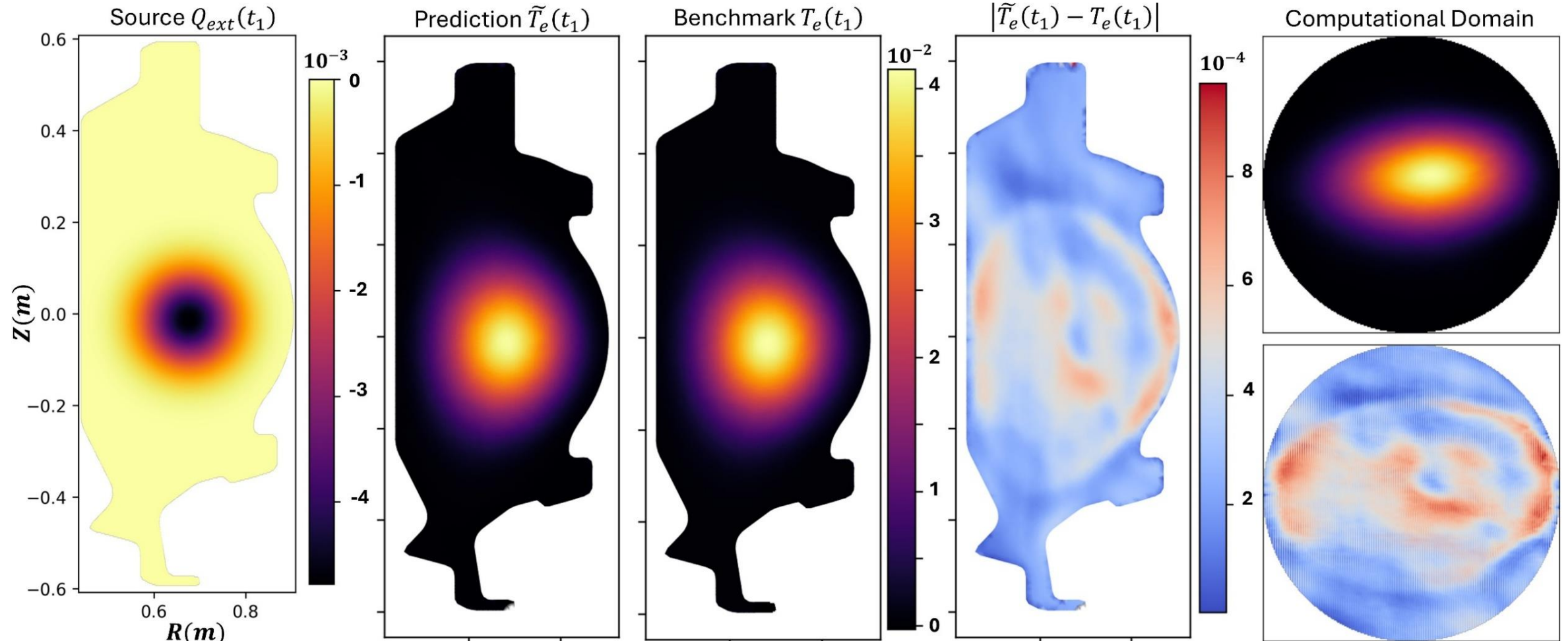
2 Nodes with  $8 \times$  A100 GPUs (MIT Engaging Cluster)

$$T_{train} \sim 2.2 \text{ hours}$$

$$\kappa_{\perp}^* = 1 \times 10^{-3}$$

# Demo – Parameter Generalization

$$\kappa_{\perp}^{test} = 5 \times 10^{-4}$$



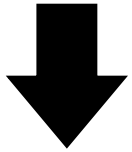
Neural Operator Infer\_time = 14ms

M3D-C1 Run\_time = 2.4s

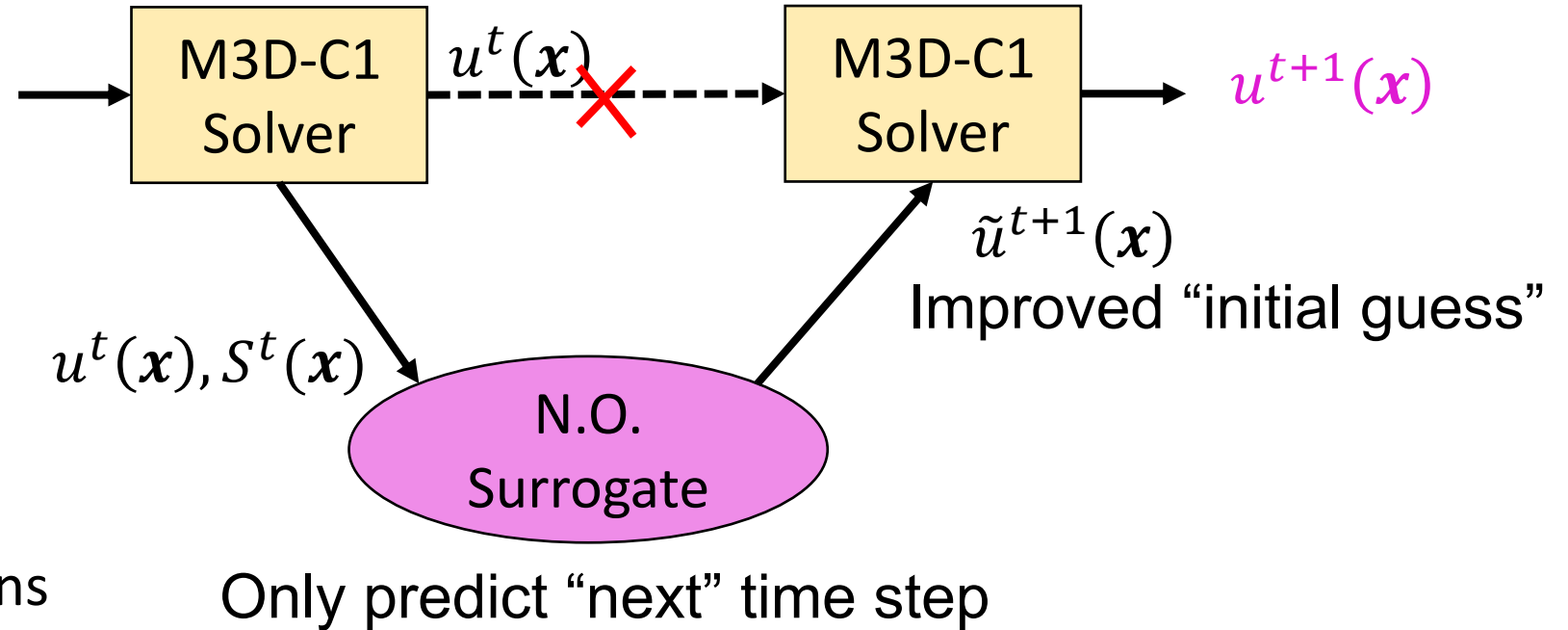
# Fidelity Preservation – Preconditioner & Hybrid Solver

Hybrid solver - use neural operator surrogate as **Preconditioner**:

- Interpretable solutions
- Preserve full fidelity
- Reduce iterations
- Jump time steps



Accelerate M3D-C1 simulations



# Conclusions and Discussions

- The neural operator surrogate successfully predicts temperature evolution across different parameters
- Its inference time is negligible compared to high-fidelity MHD solvers

## On-going work:

- Extending to complete MHD equations and more complex plasma events
- Coupling the neural operator surrogate into the M3D-C1 solver

## Potential of neural operator surrogates:

- Accelerate high-fidelity simulations
- Enable rapid prototyping for new system designs

chengq@psfc.mit.edu  
MIT Disruption Group

This work is supported by Commonwealth Fusion System.

