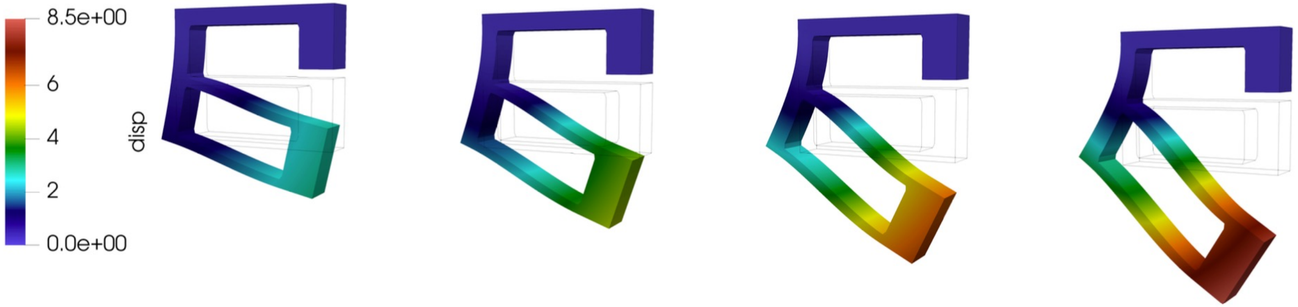
Hybridization of large-scale numerical simulations with SciML

PRÉSENTATION
2024

ANITI Parametric partial differential equations (PDEs)



- Example of application areas:
  - Uncertainty quantification
  - Design optimization
  - Inverse problems

Let $\Omega \in R^d, B \in R^p$, and $V = V(\Omega)$ be a Hilbert space. The parametric problem is given in abstract strong form as:

For a given $\beta \in B$, find the solution $u(\beta) \in V$, s.t.

$$P(\beta)\, u(\beta) = f(\beta), \text{ in } V',$$

where $P(\beta): V \rightarrow V'$ is a differential operator and $f(\beta)$ is a linear continous form.

- Example of parametrizations:
  - Material parameters
  - Source terms
  - Boundary conditions
  - Geometry

Zhang, Kahana, Kopaničáková, Turkel, Ranade, Pathak, Karniadakis. Blending neural operators and relaxation methods in PDE numerical solvers. Nature Machine Intelligence. 2024
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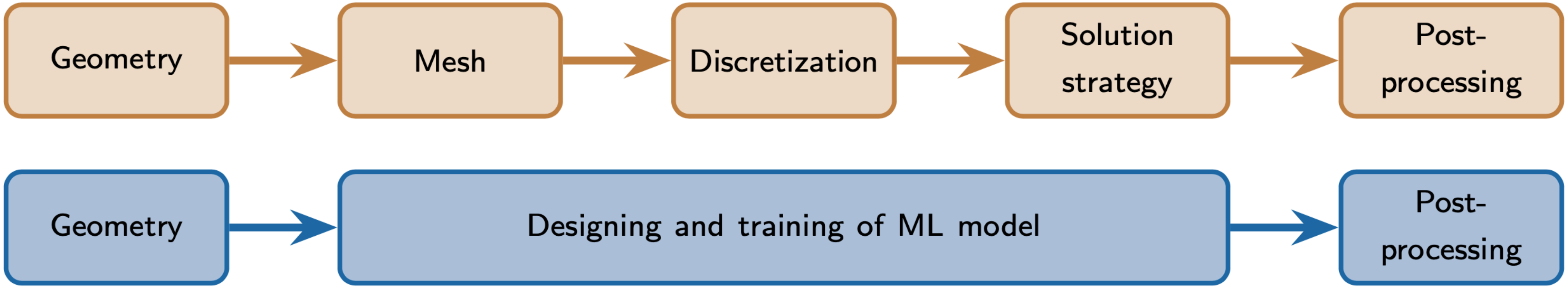
Numerical solution of parametric PDEs



Classical numerical methods:

- High-fidelity solution using advanced numerical methods, such as FEM, FDM, …
- High-computational cost, especially as problem size grows
- Capture physics on multiple scales
- Encounter challanges in data integration

Scientific machine-learning:

- Exceptionally cheap low-fidelity surrogates
- Requires expensive training phase
- Allows to discover unknown systems dynamics
- Seamless integration of data

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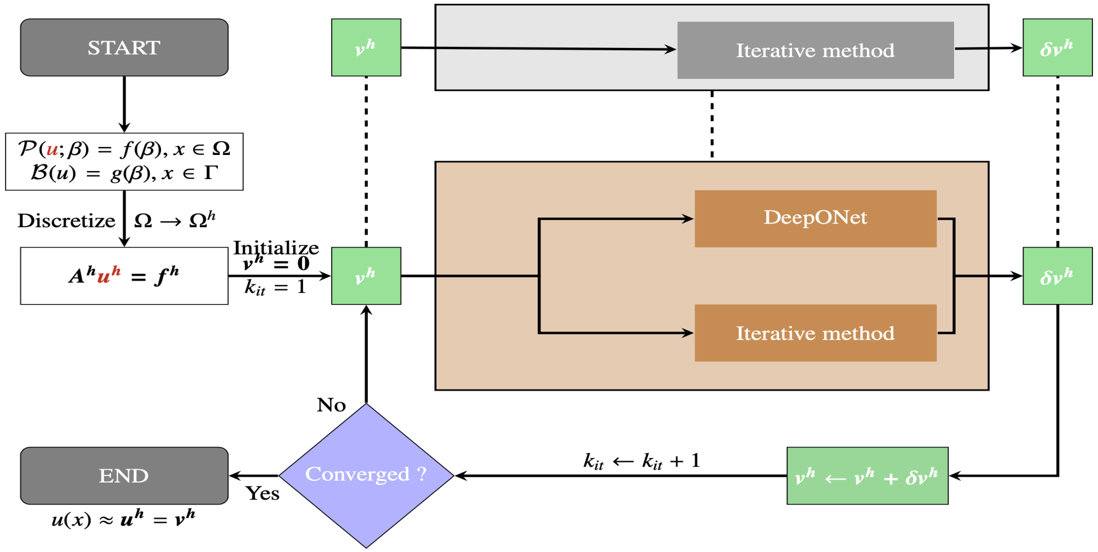
Hybridization of iterative methods with SciML

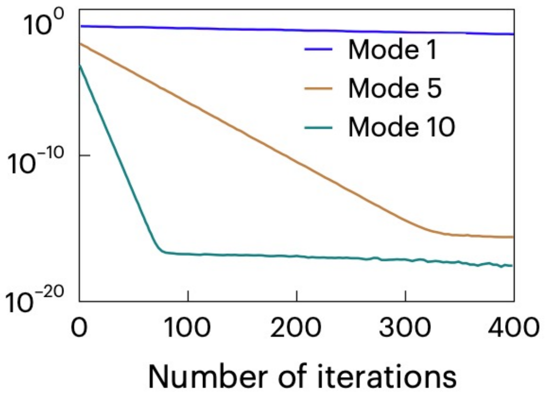
Goal:

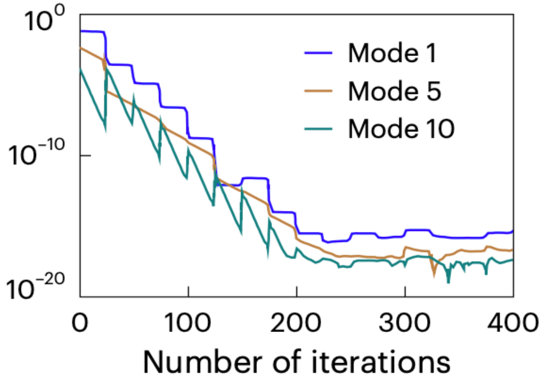
- High accuracy
- Low computational cost
- Algorithmic scalability

Observations:

- « Classical » iterative methods eliminate the high-frequency components of the error
- Operator learning approaches suffer from the spectral bias, i.e., eliminate the low-frequency components of the error quickly, while not capable to remove high-frequency components of the error







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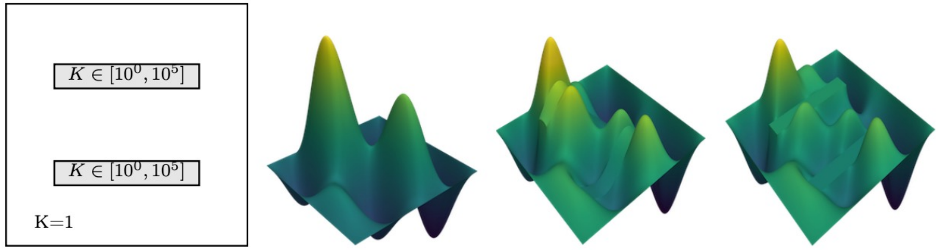
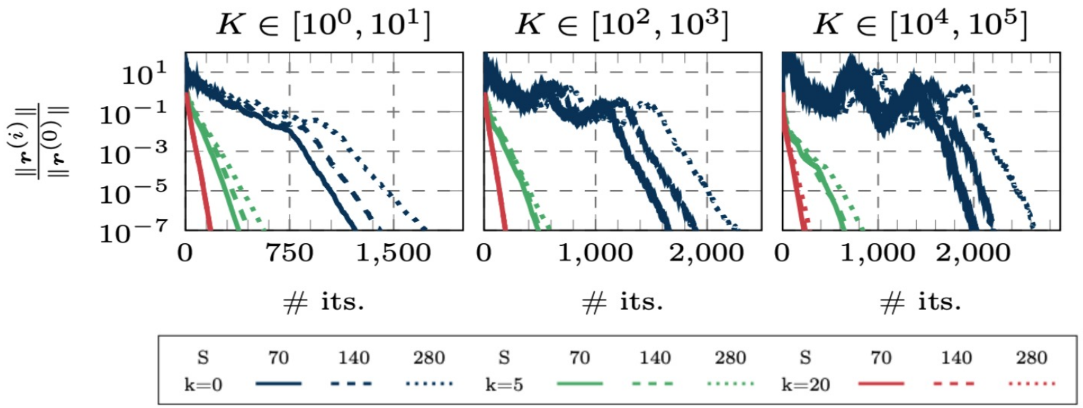
Numerical results (DeepONet augmented ASM)

Diffusion with jumping coefficients:

$$-\nabla \cdot (K(\boldsymbol{x}, \boldsymbol{\theta}) \nabla u(\boldsymbol{x})) = f(\boldsymbol{x}, \boldsymbol{\theta}), \forall \boldsymbol{x} \in \Omega,$$
$$u(\boldsymbol{x}) = 0, \text{ on } \partial\Omega,$$

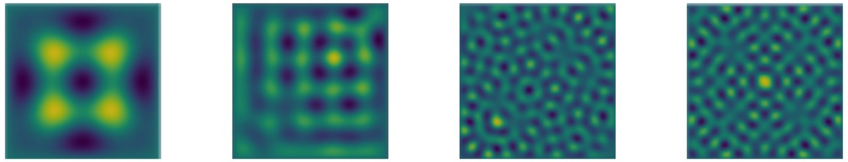


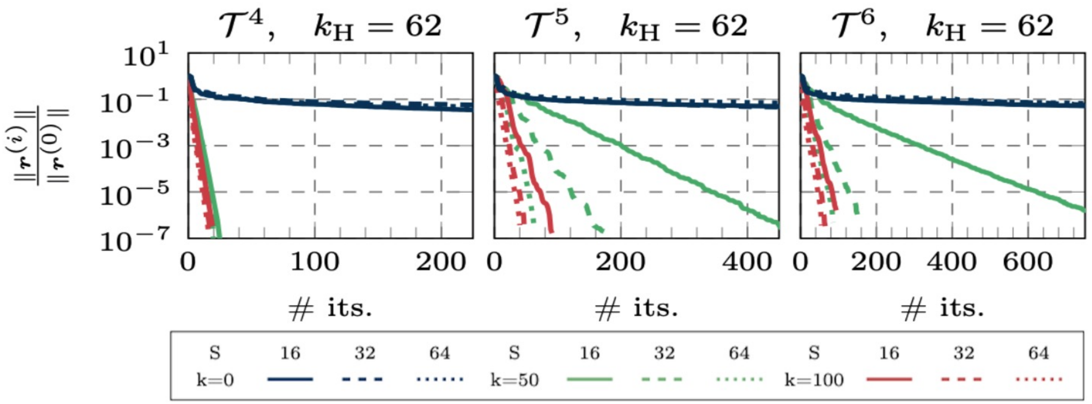
Convergence of GMRES (50) preconditioned with two-level ASM (S subdomains). Symbol k denotes a number of TB functions.



Helmholtz equation:

$$-\Delta u(\boldsymbol{x}) - k_H^2 u(\boldsymbol{x}) = f(\boldsymbol{x}, \boldsymbol{\theta}), \forall \boldsymbol{x} \in \Omega,$$
$$u(\boldsymbol{x}) = 0, \text{ on } \partial\Omega,$$





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