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Data-Driven Compatible Schemes for Structure-Preserving Surrogate Models

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Given:
high-fidelity data that obeys physics laws

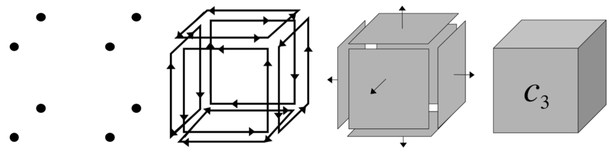
Goal:
recover surrogate model preserving physics structure

Challenges

1. How to **enforce structure preservation** from sampled point data?
2. How to extract a generalizable **parameterized model** from small amounts of data?
3. How to guarantee **stability** and **convergence** properties?

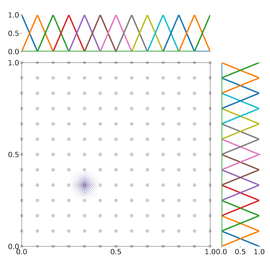
Chain Complexes as Surrogate Models?

- Guarantee Exact Sequence property
- Enforce Stokes' Theorem
- Ensure compatibility between spaces

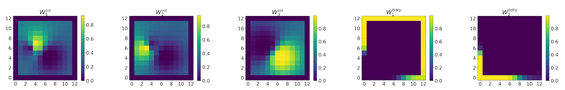


Chain Complex Model Parameterization

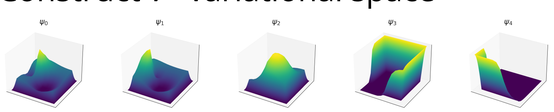
1. Fit free-knot splines



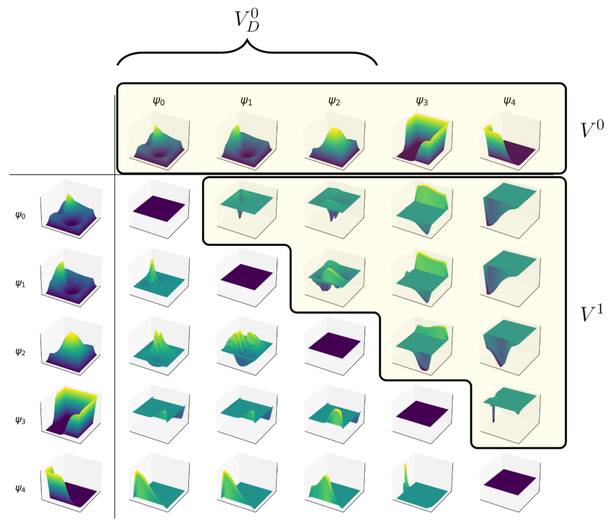
2. Coarsen to POUs



3. Construct V^0 variational space



4. Construct V^1 variational space



5. Introduce learnable (co)boundary metrics

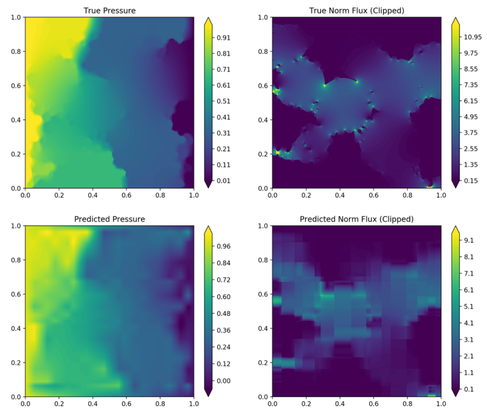
$$\begin{array}{ccccccccccc}
C^0 & \xleftarrow{\mathrm{d}_0^*} & C^1 & \xleftarrow{\mathrm{d}_1^*} & C^2 & \xleftarrow{\mathrm{d}_2^*} & C^3 & \xleftarrow{\mathrm{d}_3^*} & \cdots & \xleftarrow{\mathrm{d}_{d-1}^*} & C^d \\
\downarrow{\scriptstyle \mathbf{D}_0^{-1}} & & \downarrow{\scriptstyle \mathbf{D}_1^{-1}} & & \downarrow{\scriptstyle \mathbf{D}_2^{-1}} & & \downarrow{\scriptstyle \mathbf{D}_3^{-1}} & & & & \downarrow{\scriptstyle \mathbf{D}_d^{-1}} \\
C^0 & \xleftarrow[\delta_0]{\delta_0^*} & C^1 & \xleftarrow[\delta_1]{\delta_1^*} & C^2 & \xleftarrow[\delta_2]{\delta_2^*} & C^3 & \xleftarrow[\delta_3]{\delta_3^*} & \cdots & \xleftarrow[\delta_{d-1}]{\delta_0^*} & C^d \\
\downarrow{\scriptstyle \mathbf{B}_0} & & \downarrow{\scriptstyle \mathbf{B}_1} & & \downarrow{\scriptstyle \mathbf{B}_2} & & \downarrow{\scriptstyle \mathbf{B}_3} & & & & \downarrow{\scriptstyle \mathbf{B}_d} \\
C^0 & \xrightarrow{\mathrm{d}_0} & C^1 & \xrightarrow{\mathrm{d}_1} & C^2 & \xrightarrow{\mathrm{d}_2} & C^3 & \xrightarrow{\mathrm{d}_3} & \cdots & \xrightarrow{\mathrm{d}_{d-1}} & C^d
\end{array}$$

6. Minimize model residual against data

$$\min_{\substack{\text{POU parameters } \theta \\ \text{metrics } \mathbf{D_0}, \mathbf{D_1}, \mathbf{B_0}, \mathbf{B_1}}} \left\| p_{\text{data}} - \sum_i \hat{p}_i \psi_i \right\|_2^2 + \left\| \mathbf{F}_{\text{data}} - \sum_{ij} \hat{F}_{ij} \psi_{ij} \right\|_2^2$$

$$\text{such that } \begin{bmatrix} M_1 & M_1 D_1^{-1} \delta_0 D_0 \\ B_0^{-1} \delta_0^* B_1 M_1 & 0 \end{bmatrix} \begin{bmatrix} \hat{F} \\ \hat{p} \end{bmatrix} = \begin{bmatrix} g \\ f \end{bmatrix}$$

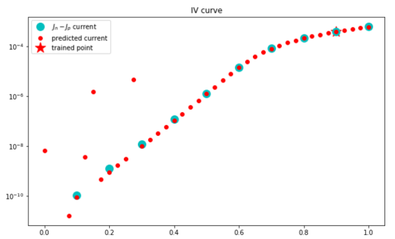
Darcy Flow



- 5.89 M nodes
- 11.8 M elements
- 5.89 M DoF solve

- 8 interior POUs
- 8 boundary POUs
- 264 DoF solve

Drift-Diffusion



- Train to fit an applied voltage of $f_\theta = 0.9$
- Solution changes nonlineary from linear to exponential regime
- Measure current $I = (\mathbf{J}_n - \mathbf{J}_p) \cdot \vec{n}$ at boundary

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