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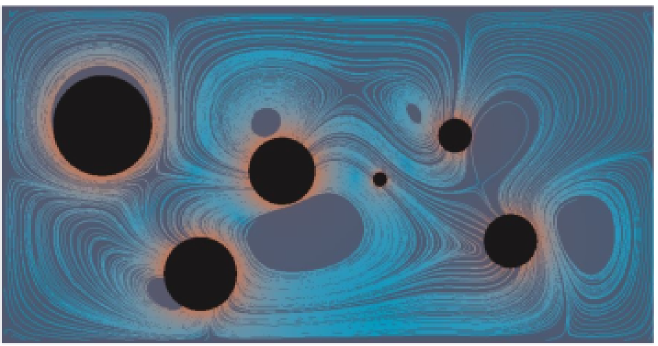

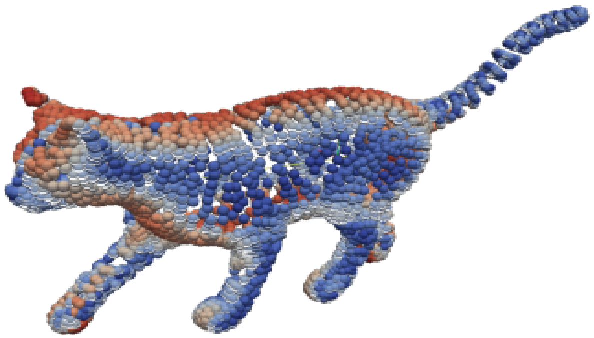

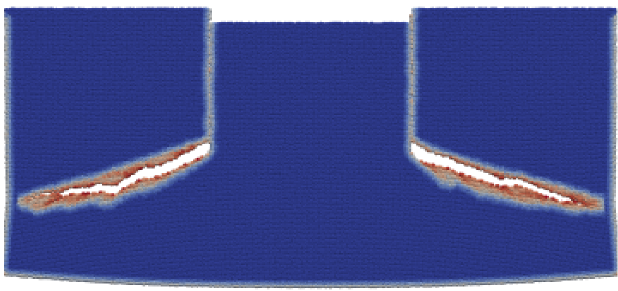

# A data-driven exterior calculus for model discovery

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# Physical biases in data-driven modeling

We extract models from data where first principles derivation is intractable, **while guaranteeing well-posed models in small data limits**

**Ex:**

- Turbulence models
- Multiscale closures
- Equations of state
- Noneq. chemistry/kinetics

$$\partial_t u = F(u, x, t)$$

Black Box ML

$$\partial_t u = \nabla \cdot F(u, x, t)$$
$$+ \text{ physics constraints}$$

Physics informed ML

$$\partial_t u + u \cdot \nabla u = -\nabla p + \nu \nabla^2 u$$

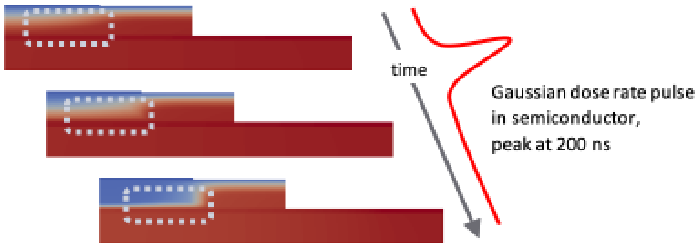
Parameter estimation

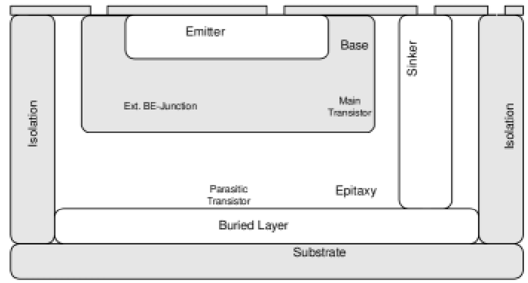
Black-box ML ⟷ Strong inductive biases

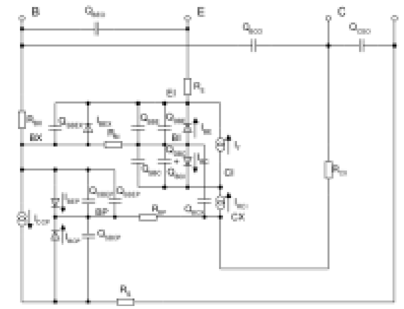
Fewer biases
More expressive

More biases
More exploitable structure

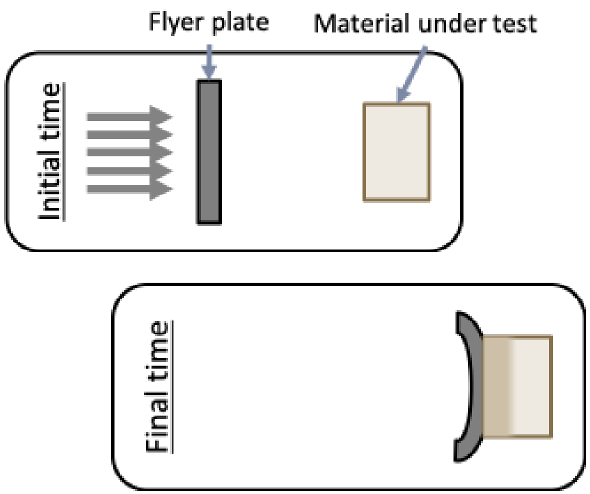
# Data-driven modeling at SNL

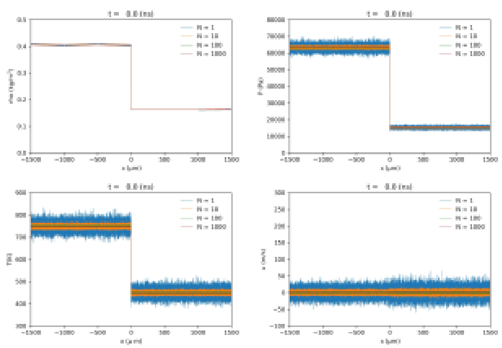


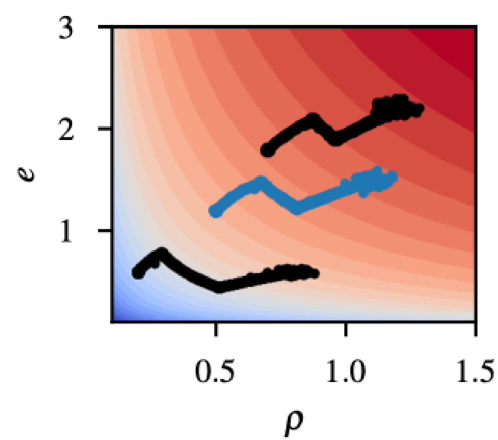




Can high-fidelity E&M simulations for semiconductors be encoded as efficient circuit models?






Can a data-driven EOS be extracted from observations of Riemann problems at high energy states

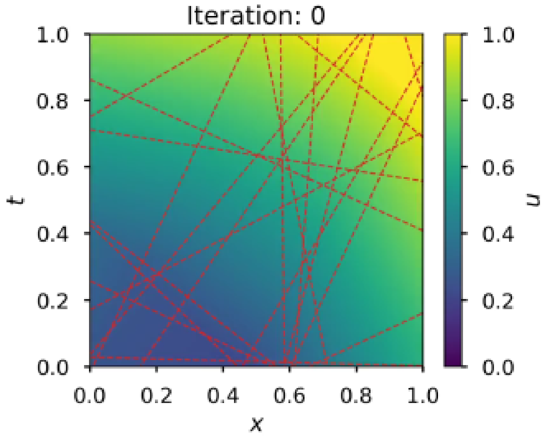
**Exact physics treatment and solvability guarantees are critical**

# The state-of-the-art in physics-informed ML

**Make list of desired features and penalize them after the fact:**
**PDE structure, BC, IC, conservation, etc.**

$$\mathbf{L} = \mathbf{L}_{data} + \epsilon \mathbf{L}_{physics}$$

$$\mathbf{L} = ||u_{data} - \mathcal{N}\mathcal{N}||_{\ell_2}^2 + \epsilon ||\mathcal{L}[u_{data}] - \mathcal{L}[\mathcal{N}\mathcal{N}]||_{\ell_2}^2$$




**<u>Key Challenges:</u>**

Our applications need physics to hold exactly – not just by penalty
e.g. electromagnetics, fluid mechanics

What happens when the governing PDE and material parameters are unknown – is it still possible to impose physical constraints?

**If physics can be imposed *exactly* then a source of uncertainty is eliminated**

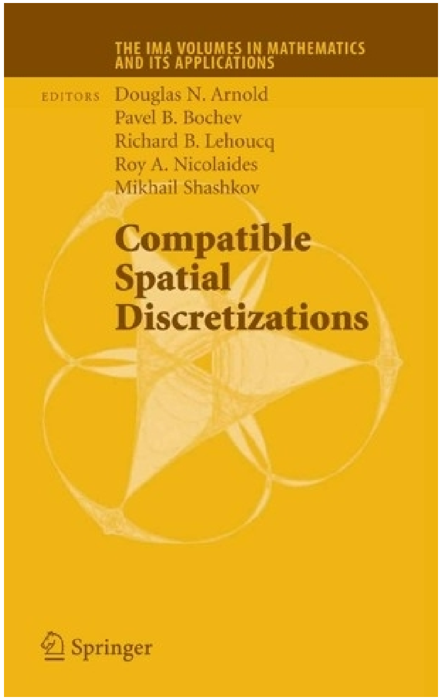
# What are physics compatible discretizations for PDEs?

**Methods for solving PDEs which:**

Use generalized Stokes theorems to approximate differential operators

Preserve topological structure in governing equations

Mimic properties of continuum operators (thus sometimes called **mimetic discretizations**)




Arnold, D. N., Bochev, P. B., Lehoucq, R. B., Nicolaides, R. A., & Shashkov, M. (Eds.). (2007). *Compatible spatial discretizations* (Vol. 142). Springer Science & Business Media.

# Two key ingredients:

**<u>1: A topological structure</u>**

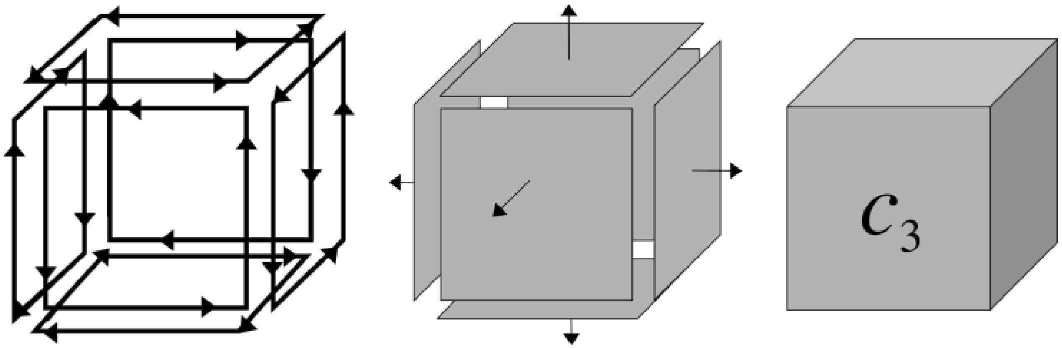
In PDE discretization this is a mesh, with boundary operators linking cells, faces, edges, and nodes

**We will use a graph as an inexpensive low-dimensional mesh surrogate**

**<u>2: Metric information</u>**

Measures associated with mesh entities, ensuring discrete exterior derivatives converge to div/grad/curl

**Graphs are purely topological with no natural metric, we will use ML to extract metric information from data**

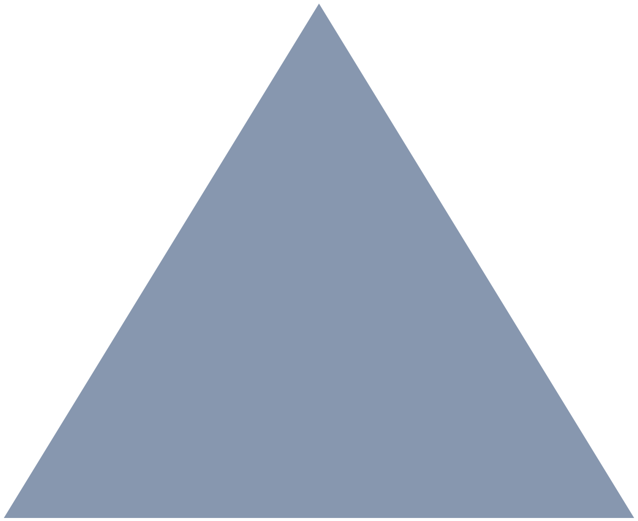


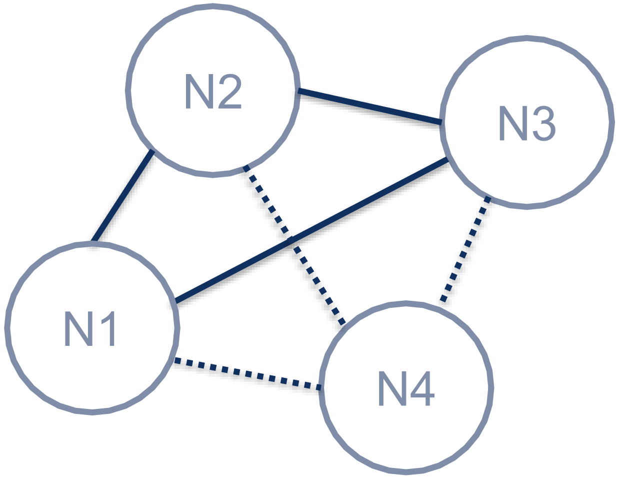

$$0 \leftarrow \partial\partial c_3 \xleftarrow{\;\partial\;} \partial c_3 \xleftarrow{\;\partial\;} c_3$$

$$\nabla \cdot \mathbf{u} = \frac{1}{\mu(C)} \sum_{f \in \partial C} \int_f \mathbf{u} \cdot d\mathbf{A}$$

# Exterior calculus preliminaries: chain complex

$$C_0 \xleftarrow{\partial_0} C_1 \xleftarrow{\partial_1} C_2 \xleftarrow{\partial_2} C_3$$

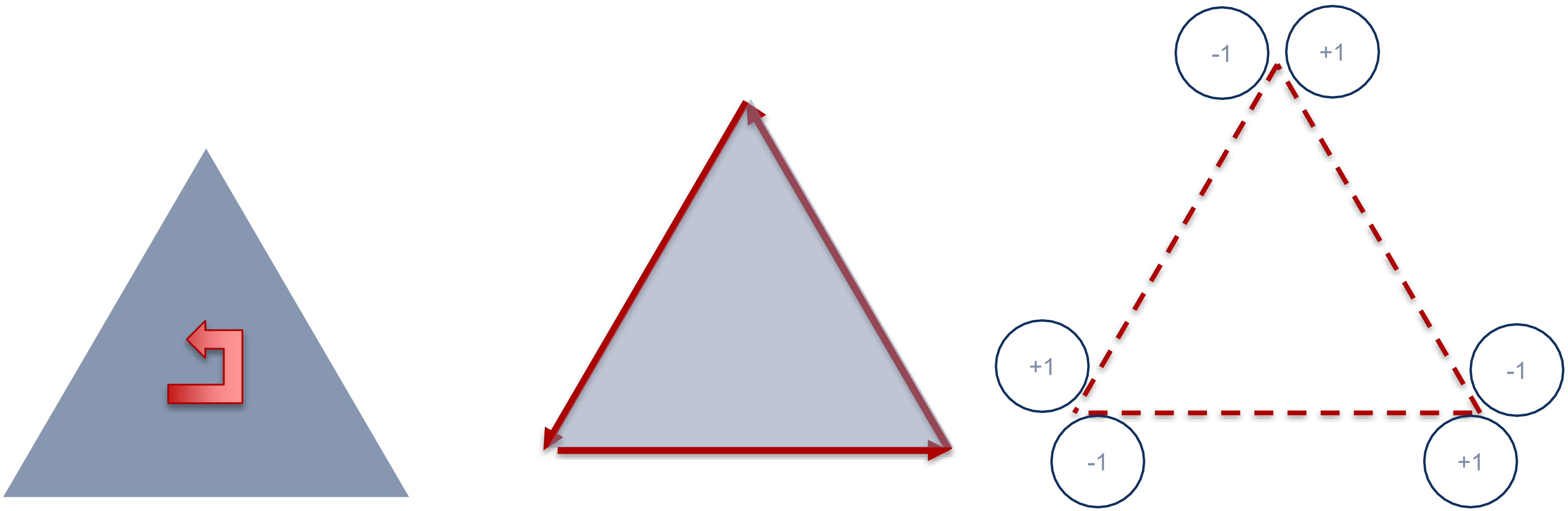





| Compat. PDE | Comb. Hodge |
|---|---|
| Mesh entities | K-cliques |

# Exterior calculus preliminaries: chain complex

$$C_0 \xleftarrow{\partial_0} C_1 \xleftarrow{\partial_1} C_2 \xleftarrow{\partial_2} C_3$$




$f \in C_2$ $\quad$ $\partial_2 f \in C_1$ $\quad$ $\partial_1 \partial_2 f \in C_0$

Exact sequence property: $\forall k, \partial_k \partial_{k+1} = 0$

# Exterior calculus preliminaries: cochain complex

$$C_0 \xleftarrow{\partial_0} C_1 \xleftarrow{\partial_1} C_2 \xleftarrow{\partial_2} C_3$$

$$C^0 \xrightarrow{d_0} C^1 \xrightarrow{d_1} C^2 \xrightarrow{d_2} C^3$$

*Coboundary operators* define maps $d_k : C^k \to C^{k+1}$ satisfying $d_{k+1} d_k = 0$

Boundary and coboundary operators satisfy the *generalized Stokes theorem*

$$\int_\omega du = \int_{\partial\omega} u$$

| Comb. Hodge | Compat. PDE |
|---|---|
| $grad[s](i,j) = \int_{e_{ij}} \nabla s \cdot d\mathbf{l} = s_j - s_i$ | $grad[s](i,j) = s_j - s_i$ |
| $curl[X](F) = \int_F \nabla \times X \cdot d\mathbf{A} = \sum_{e \in \partial F} \int_e X \cdot d\mathbf{l}$ | $curl[X](i,j,k) = X_{ij} + X_{jk} + X_{ki}$ |

# Traditional DEC

$$C_0 \xleftarrow{\partial_1} C_1 \xleftarrow{\partial_2} C_2 \xleftarrow{\partial_3} C_3$$

$$C^0 \underset{d_0^\star}{\overset{d_0}{\rightleftarrows}} C^1 \underset{d_1^\star}{\overset{d_1}{\rightleftarrows}} C^2 \underset{d_2^\star}{\overset{d_2}{\rightleftarrows}} C^3$$

Introducing inner products $(\cdot,\cdot)_k$, we define the *codifferential* operator $d_k^\star : C^{k+1} \to C^k$ as

$$(v, d_k^\star u)_k = (d_k v, u)_{k+1}$$

Again, $d_{k-1}^\star * d_k^\star = 0$

# A data-driven exterior calculus (DDEC)

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

**Idea:** Take graph calculus and introduce learnable inner products

$$(x, y)_{\mathbf{B}_k} = x^\intercal \mathbf{B}_k y$$

$$(x, y)_{\mathbf{D}_k} = x^\intercal \mathbf{D}_k y$$

to find data-driven exterior calculus operators that inherit the structure of graph exterior calculus

# What does all this give you?

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

- Differential operators which locally and globally conserve fluxes, circulations, potentials
- Invertible Hodge Laplacians $\Delta_k = d^\star_{k+1} d_{k+1} + d_k d^\star_{k+1}$
- Exact sequence properties $d_{k+1} d_k = d^\star_k d^\star_{k+1} = 0$
- Hodge decomposition $u = d^* \alpha + d\beta + \gamma$
- Corollary: treatment of nontrivial null-spaces in electromagnetism

# Theorems…

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**Theorem 3.1.** *The discrete derivatives* $\mathsf{d}_k$ *in* (11) *form an exact sequence if the simplicial complex is exact, and in particular* $\mathsf{d}_{k+1} \circ \mathsf{d}_k = 0$. *In* $\mathbb{R}^3$, *we have* $CURL_h \circ GRAD_h = DIV_h \circ CURL_h = 0$.

**Theorem 3.2.** *The discrete derivatives* $\mathsf{d}_k^*$ *in* (11) *form an exact sequence of the simplicial complex is exact, and in particular* $\mathsf{d}_k^* \circ \mathsf{d}_{k+1}^* = 0$. *In* $\mathbb{R}^3$, $DIV_h^* \circ CURL_h^* = CURL_h^* \circ GRAD_h^* = 0$.

**Theorem 3.3** (Hodge Decomposition). *For* $C^k$, *the following decomposition holds*

$$C^k = \mathrm{im}(\mathsf{d}_{k-1}) \bigoplus_k \ker(\Delta_k) \bigoplus_k \mathrm{im}(\mathsf{d}_k^*), \tag{17}$$

*where* $\bigoplus_k$ *means the orthogonality with respect to the* $(\cdot,\cdot)_{\mathbf{D}_k\mathbf{B}_k^{-1}}$*-inner product.*

**Theorem 3.4** (Poincaré inequality). *For each* $k$, *there exists a constant* $c_{P,k}$ *such that*

$$\|\mathbf{z}_k\|_{\mathbf{D}_k\mathbf{B}_k^{-1}} \le c_{P,k} \|\mathsf{d}_k \mathbf{z}_k\|_{\mathbf{D}_{k+1}\mathbf{B}_{k-1}^{-1}}, \quad \mathbf{z}_k \in \mathrm{im}(\mathsf{d}_k^*),$$

*and another constant* $c_{P,k}^*$ *such that*

$$\|\mathbf{z}_k\|_{\mathbf{D}_k\mathbf{B}_k^{-1}} \le c_{P,k}^* \|\mathsf{d}_{k-1}^* \mathbf{z}_k\|_{\mathbf{D}_{k-1}\mathbf{B}_{k-1}^{-1}}, \quad \mathbf{z}_k \in \mathrm{im}(\mathsf{d}_{k-1}).$$

*Thus, for* $\mathbf{u}_k \in C^k$, *we have*

$$\inf_{\mathbf{h}_k \in \ker(\Delta_k)} \|\mathbf{u}_k - \mathbf{h}_k\|_{\mathbf{D}_k\mathbf{B}_k^{-1}} \le C \left( \|\mathsf{d}_k \mathbf{u}_k\|_{\mathbf{D}_{k+1}\mathbf{B}_{k+1}^{-1}} + \|\mathsf{d}_{k-1}^* \mathbf{u}_k\|_{\mathbf{D}_{k-1}\mathbf{B}_{k-1}^{-1}} \right),$$

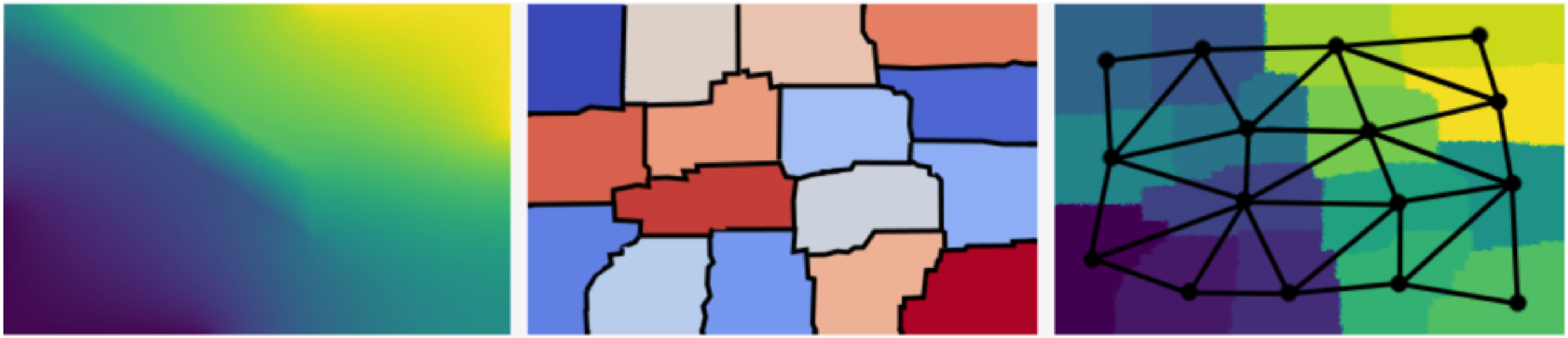
*where constant* $C > 0$ *only depends on* $c_{P,k}$ *and* $c_{P,k}^*$.

**Theorem 3.5** (Invertibility of Hodge Laplacian). *The* $k^{th}$*-order Hodge Laplacian* $\Delta_k$ *is positive-semidefinite, with the dimension of its null-space equal to the dimension of the corresponding homology* $H^k = \ker(\mathsf{d}_k)/\,\mathrm{im}(\mathsf{d}_{k-1})$.

# Using DDEC to discover structure preserving surrogates

$$\nabla \cdot \mathbf{F} = f \qquad d_0^{\star}\mathbf{F} = f$$

$$\mathbf{F} + \kappa \nabla \phi = 0 \qquad \mathbf{F} + \xi d_0 \phi + \mathcal{N}_\eta(\phi) = 0$$



High-fidelity PDE solution

Apply graph-cut to coarse-grain chain complex

Average over partitions to obtain training data

# General optimization problem

Fluxes: $$\mathbf{w}_{k+1} = \mathsf{d}_k \mathbf{u}_k + \epsilon \mathcal{N}\mathcal{N}(\mathsf{d}_k \mathbf{u}_k; \xi),$$

Conservation: $$\mathsf{d}_{k-1}\ \mathsf{d}^*_{k-1} \mathbf{u}_k + \mathsf{d}^*_k \mathbf{w}_{k+1} = \mathbf{f}_k\,.$$

$$\Rightarrow \quad a(\mathbf{v}, \mathbf{u}; \mathbf{B}, \mathbf{D}) + N_{\mathbf{v}}[\mathbf{u}; \xi] = b(\mathbf{v})$$

Invertible bilinear form

Nonlinear perturbation

If we can fit the model to data while imposing equality constraint, then during training we restrict to manifold of solvable models preserving physics

$$\underset{\mathbf{B},\mathbf{D},\xi}{\text{argmin},} \,||\mathbf{w} - \mathbf{w}_{\text{data}}||^2$$

$$\text{such that } \mathcal{L}[\mathbf{w}, \mathbf{u}; \mathbf{B}, \mathbf{D}, \xi] = 0$$

# Is PDE constraint well posed?

$$a(\mathbf{v}, \mathbf{u}; \mathbf{B}, \mathbf{D}) + N_{\mathbf{v}}[\mathbf{u}; \xi] = b(\mathbf{v})$$

**Theorem 3.6.** *The equation (24) has at least one solution $\mathbf{u}_k \in \mathbb{V}$ satisfies*

$$\|\mathbf{u}_k\| \leq \frac{\|\mathbf{f}\|}{(C_p - C_N)}. \tag{26}$$

**Theorem 3.7.** *If $\frac{C_{\nabla N}\|\mathbf{f}\|}{C_p(C_p - C_N)} < 1$, then the equation (24) has at most one solution in $\mathbb{V}$.*

A unique solution exists if the Hodge-Laplacian is sufficiently large relative to the nonlinear part, following standard elliptic PDE arguments

- Poincare constant easily estimated from matrix eigenvalues
- Lipschitz constant on nonlinearity straightforward for DNNs

Solvability constraint could be enforced during training if desired

# “PDE”-constrained optimization

$$\mathbf{L}_{\mathbf{u},\lambda,\mathbf{B},\mathbf{D},\xi} = ||\mathbf{w} - \mathbf{w}_{\text{data}}||^2 + \lambda^\intercal \mathcal{L}[\mathbf{w}, \mathbf{u}; \mathbf{B}, \mathbf{D}, \xi]$$

$$\mathcal{L}[\mathbf{w}, \mathbf{u}; \mathbf{B}, \mathbf{D}, \xi] = 0$$

An iterative algorithm guaranteeing exact enforcement of physics at each iteration:

- Solve forward problem with current model parameters

$$\mathbf{w}, \mathbf{u} \leftarrow \nabla_\lambda \mathbf{L}_{\mathbf{u},\lambda,\mathbf{B},\mathbf{D},\xi} = 0$$

- Solve adjoint problem with current forward solution

$$\lambda \leftarrow \nabla_\mathbf{u} \mathbf{L}_{\mathbf{u},\lambda,\mathbf{B},\mathbf{D},\xi} = 0$$

- Apply gradient descent to update model

$$\mathbf{B}, \mathbf{D}, \xi \leftarrow \nabla_{\mathbf{B},\mathbf{D},\xi} \mathbf{L}_{\mathbf{u},\lambda,\mathbf{B},\mathbf{D},\xi} = 0$$

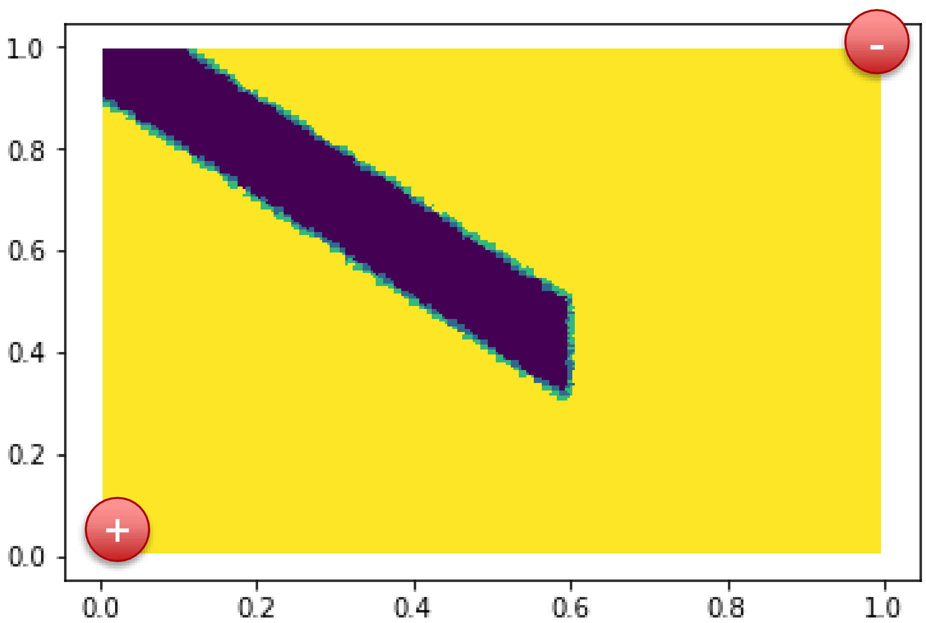
# Back to Darcy...

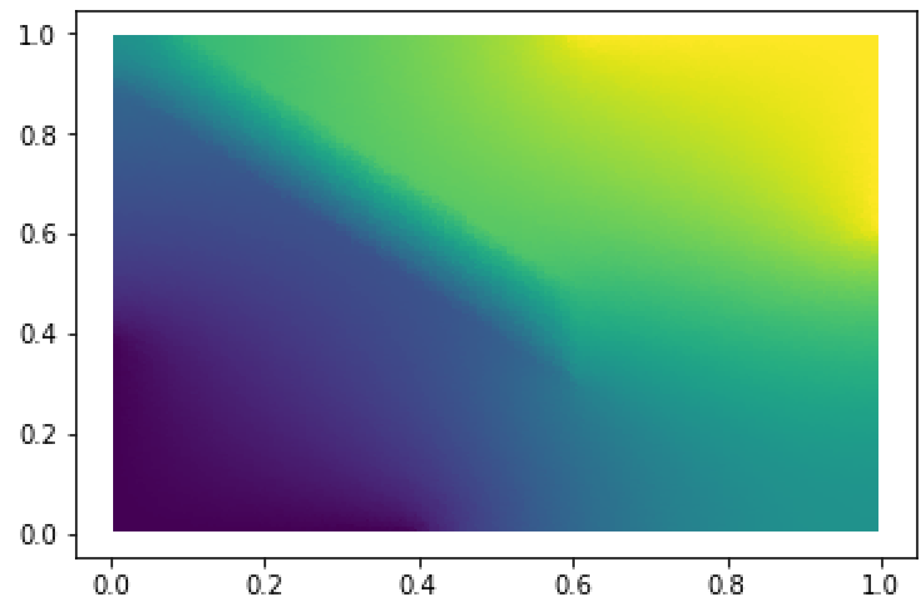
$$\nabla \cdot \mathbf{F} = f$$

$$\mathbf{F} + \kappa \nabla \phi = 0$$

$$d_0^\star \mathbf{F} = f$$

$$\mathbf{F} + \xi d_0 \phi + \mathcal{N}_\eta(\phi) = 0$$



# Comparison to traditional covolume: improved accuracy at low resolution

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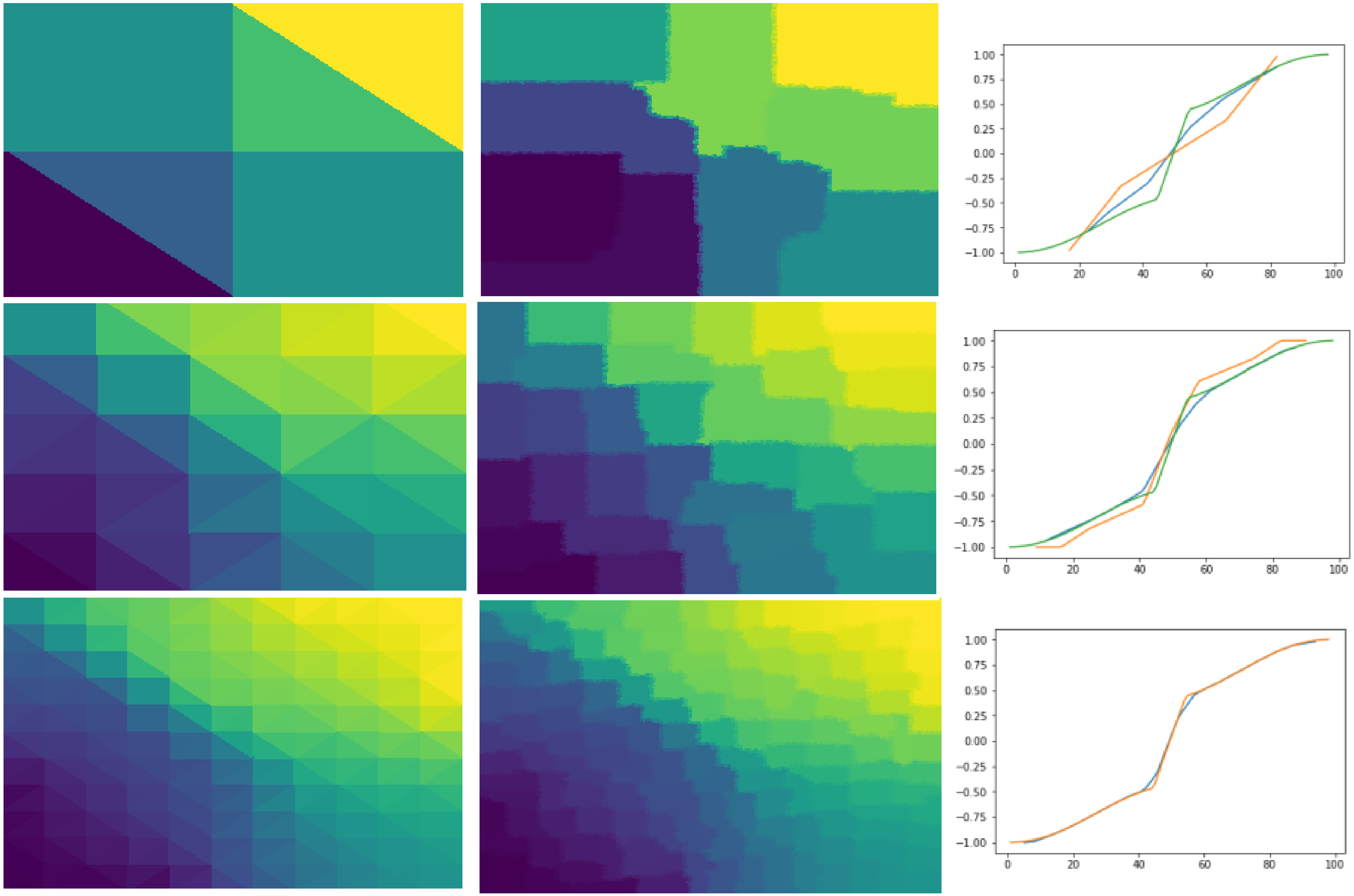
N = $2^2$

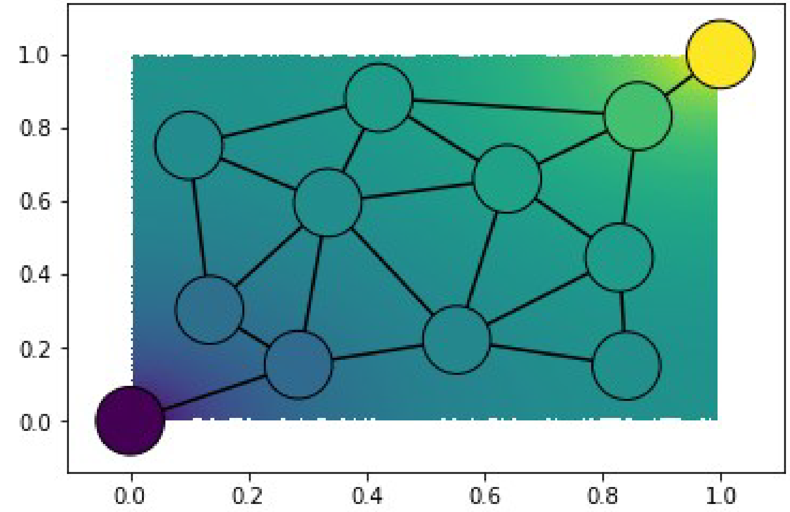
N = $5^2$

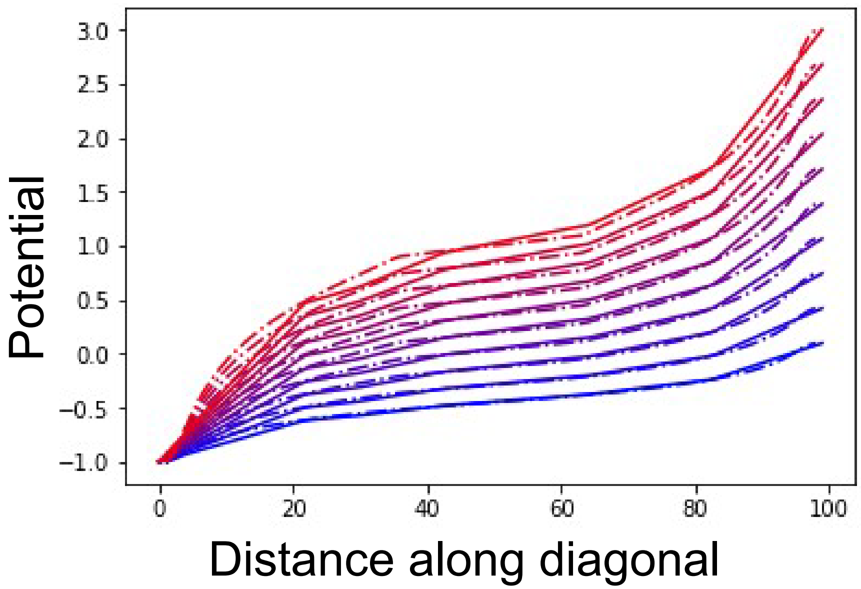
N = $10^2$

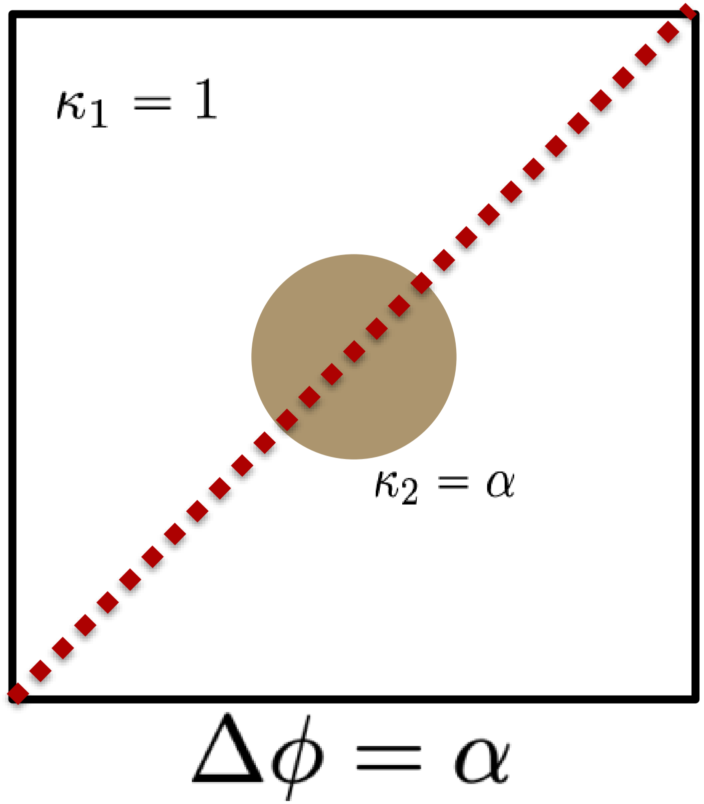



Comparison of pressure for same # DOF for FVM (left) and DDEC (center)
Right: profile along diagonal shows better fit to solution (green) by DDEC (blue) vs FVM (orange)

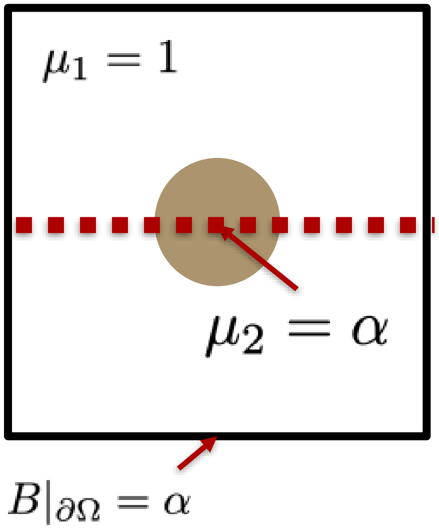
# Nonlinear Darcy: potential profile across diagonal

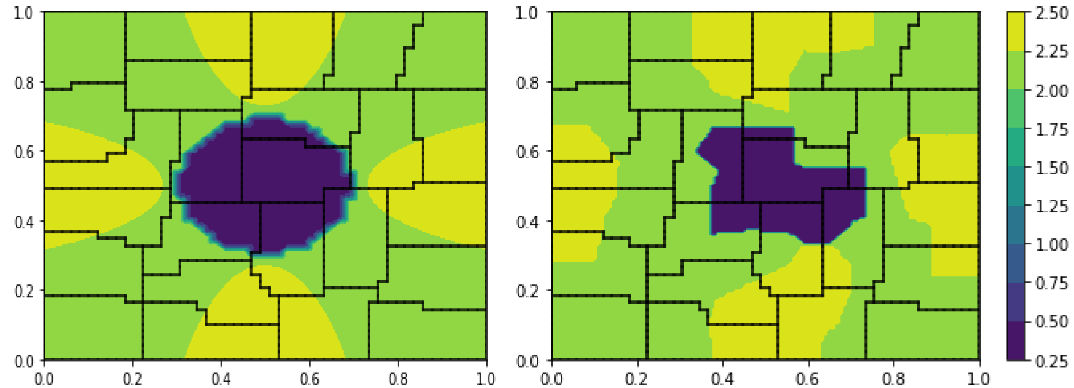


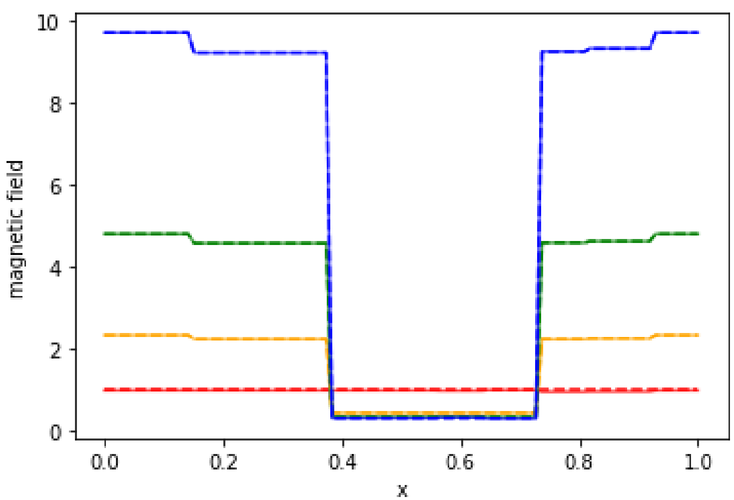



# Magnetostatics



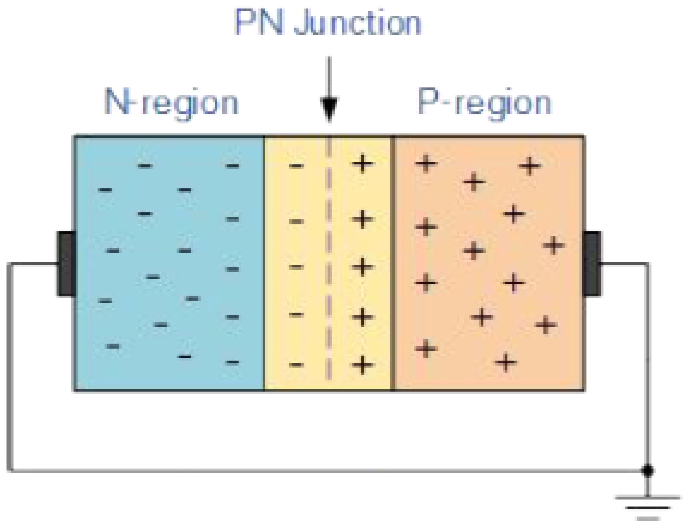






**Extracted surrogate:**
Is exactly div free
Provides sharp interfaces
Conserves circulation
Guaranteed solvable
Generalizes to other BCs

# Compact models for semiconductors: PN-diode

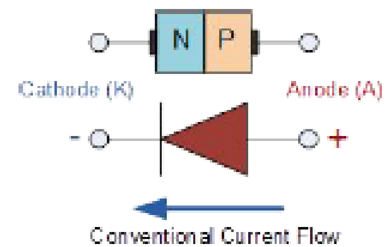
https://www.electronics-tutorials.ws/diode/diode_3.html




$$\nabla \cdot \epsilon \nabla \phi = -(p - n + N_D^+ - N_A^-)$$

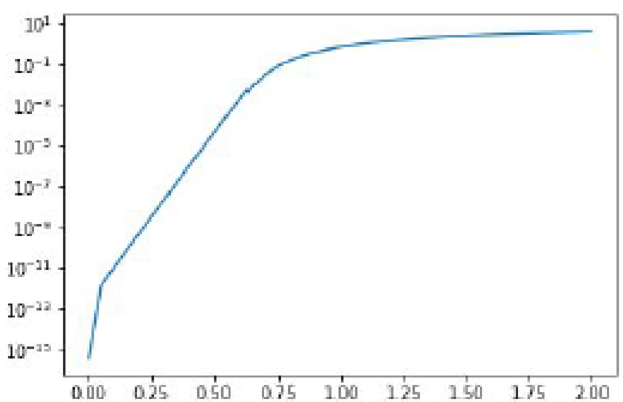
$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot (-\mu_n n E - D_n \nabla n) - R_n(n,p)$$

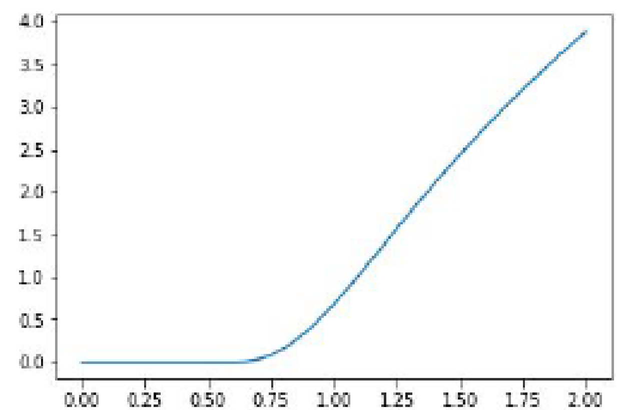
$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \left(\mu_n p E - D_p \nabla p\right) - R_p(n,p)$$




**Traditional compact models fit ideal diode + resistor, and can be tuned to match either small or large voltage regimes**

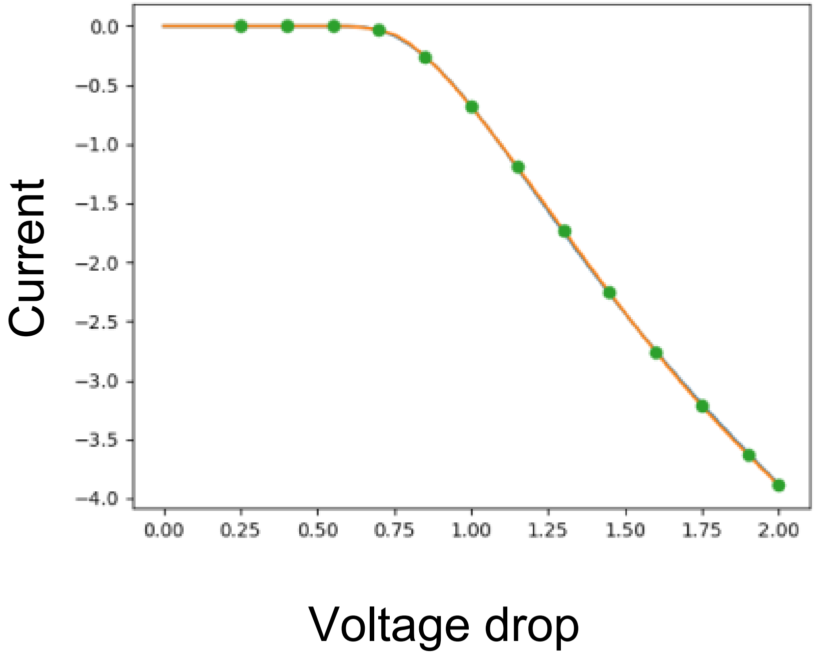
Locally exponential: I.D. model

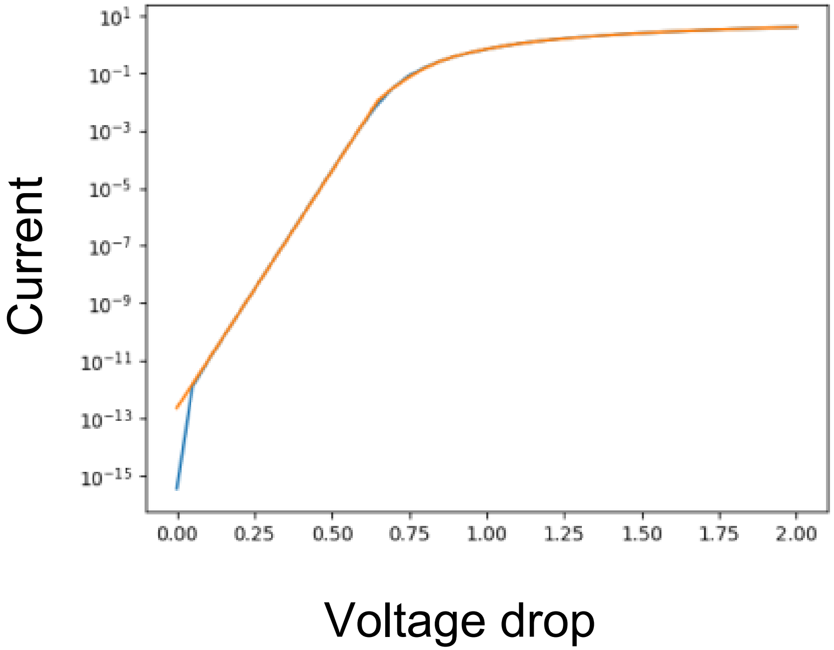



Locally linear: resistor model

# Matching IV-curve – linear scale




Extract a conservative surrogate accurate over
**fifteen orders of magnitude**

May be embedded in a circuit simulator (e.g. Xyce) to couple coarse-grained high-fidelity PDE model in multiscale model w/ millions of components

# Acknowledgements


- **PHILMs** – **Ph**ysics **I**nformed **L**earning **M**achine**s** for multiscale/multiphysics problems
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  - PI: George Karniadakis
  - SNL team: Mike Parks (PI), Pavel Bochev, Marta D'Elia, Mamikon Gulian, Ravi Patel, Mauro Perego, Nathaniel Trask
- **PIRAMID** – **P**hysics **I**nformed **R**apid and **A**utomated **M**L for compact model development
  - SNL LDRD to extract efficient compact circuit models from high-fidelity PDE simulation
  - Team: Andy Huang (PI), Xujiao Gao, Shahed Reza, Nathaniel Trask
- **DOE Early Career –** Physics informed graph neural networks for multiscale physics


## Applications

Non-equilibrium closures for autoignition in turbulent combustion

Pulse shaping for pulsed power fusion applications on Z-machine

Development of surrogate models for radiation modeling of circuits

Fracture mechanics closures for ice sheet models

Multiscale modeling of lithium-ion batteries during failure

Multiscale closure for subsurface flow through fracture networks

Multiscale data-driven closures for kinetic effects and turbulence in plasmas

**Several new projects – please contact for postdoc/collaboration opportunities**

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