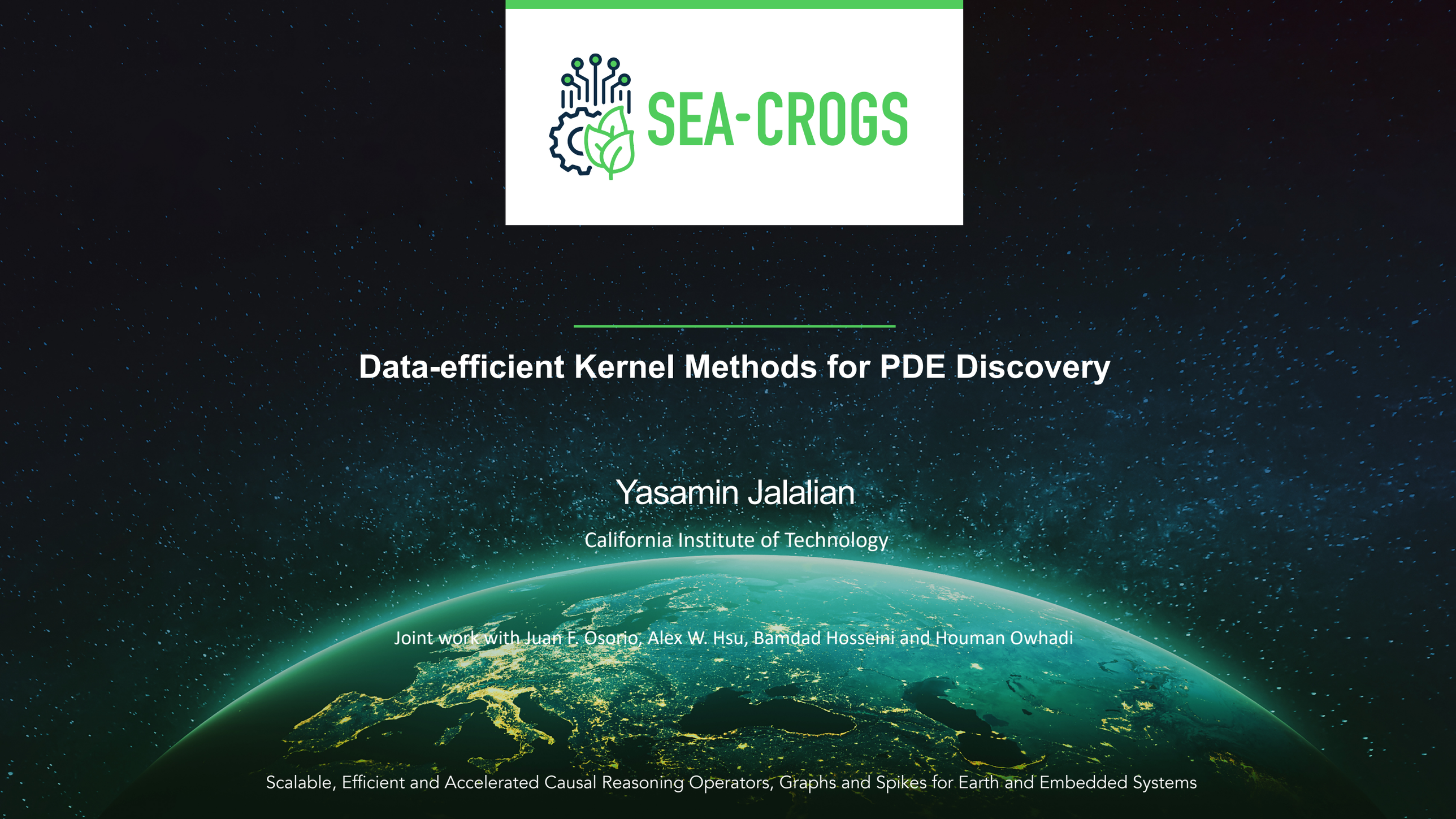

Data-efficient Kernel Methods for PDE Discovery

Yasamin Jalalian

California Institute of Technology

Joint work with Juan F. Osorio, Alex W. Hsu, Bamdad Hosseini and Houman Owhadi

Scalable, Efficient and Accelerated Causal Reasoning Operators, Graphs and Spikes for Earth and Embedded Systems

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Problem Statement

$$P(x, u(x), Du(x), D^2u(x)) = f(x), \qquad \forall x \in \Omega \subset \mathbb{R}^d$$

Problem:

- $P : \mathbb{R}^{d+q} \to \mathbb{R}$ **unknown** possibly nonlinear function of known order 2
- $f : \Omega \to \mathbb{R}$ **partially observed** source term (continuous function)
- $u : \Omega \to \mathbb{R}$ **partially observed** function describing the state of the physical system (strong solution to the PDE with source term f)

Data:

data points $X \subset \Omega$

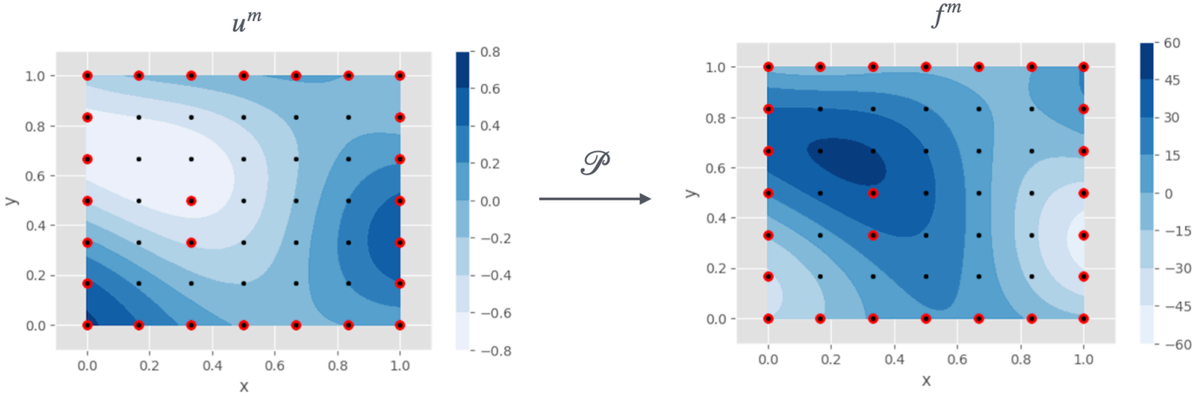
M pairs of functions (u^m, f^m)

N observation points $X_N^m = \{x_1^m, \ldots, x_N^m\} \subset X$

Objective:

- learn the function P and the functions u^m on the continuum from data

$u^m(X), u^m(X_N^m)$ $\qquad$ $f^m(X), f^m(X_N^m)$



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Example: Darcy Flow

Problem:

$$P(x, u(x), Du(x), D^2u(x)) = \nabla \cdot \big(a(x)\nabla u(x)\big) = f(x), \quad \forall x \in (0,1)^2$$

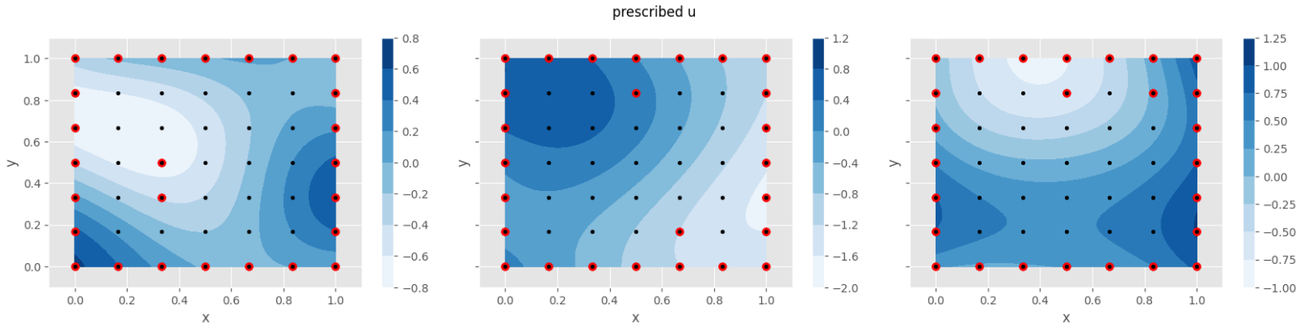
Data:

- $M = 3$ pairs of (u^m, f^m), for $m \in \{1,2,3\}$ prescribe functions $u^m \sim GP(0,K)$
- 7×7 data points X, $N = 26$ observation points X_N^m

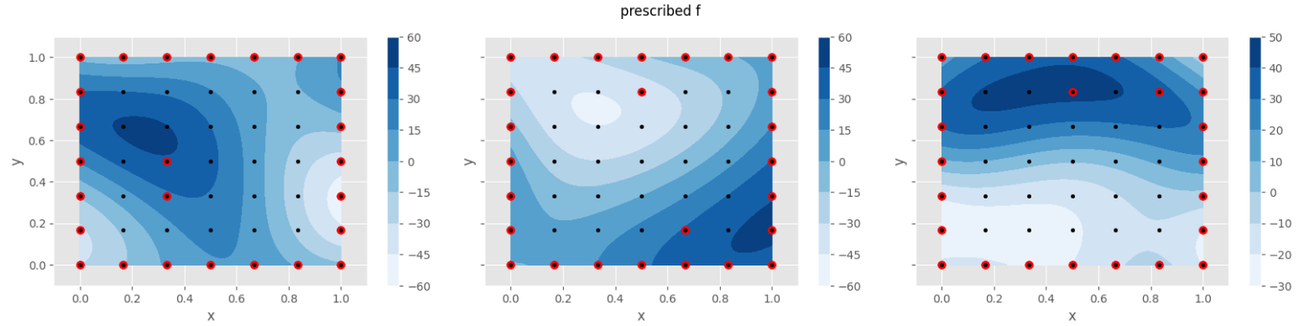
Objective:

- learn the function P and the functions u^m on the continuum from data

$u^m(X), u^m(X_N^m)$



$f^m(X), f^m(X_N^m)$



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Data-driven Methods for Solving & Learning PDEs

Current Approaches:

1. **ANN-based methods**
   - **Solving high-dimensional PDEs using deep learning**. Han, Jentzen, E, 2018
   - **Deep Hidden Physics Models: Deep Learning of Nonlinear Partial Differential Equations,** Maziar Raissi, 2018
   - **Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations.** M. Raissi, P. Perdikaris, G.E. Karniadakis, JCP 2019
   - **Model reduction and neural networks for parametric PDEs**. K. Bhattacharya, B. Hosseini, N. Kovachki, A. Stuart. 2020.
   - **Competitive Physics Informed Networks**. Q. Zeng, Y. Kothari, S. Bryngelson, F. Schäfer., 2022
   - **Self-adaptive physics-informed neural networks**. L. McClenny, U. M Braga-Neto. 2023

2. **Kernel-based methods**
   - **Bayesian Numerical Homogenization**. Houman Owhadi. 2015
   - **Gamblets for opening the complexity-bottleneck of implicit schemes for hyperbolic and parabolic ODEs/PDEs with rough coefficients.** Houman Owhadi, Lei Zhang, JCP 2016
   - **Machine learning of linear differential equations using Gaussian processes**. Maziar Raissi, Paris Perdikaris, George Em Karniadaki, 2017
   - **Numerical Gaussian Processes for Time-dependent and Non-linear Partial Differential Equations.** Maziar Raissi, Paris Perdikaris, and George Em Karniadakis, 2017
   - **Inferring solutions of differential equations using noisy multi-fidelity data.** Maziar Raissi, Paris Perdikaris, George Em Karniadakis, SISC 2018
   - **Solving and Learning Nonlinear PDEs with Gaussian Processes**. Yifan Chen, Bamdad Hosseini, Houman Owhadi, and Andrew M Stuart, 2021

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Data-driven Methods for Solving & Learning PDEs

Current Approaches:

1. ANN-based methods
2. Kernel-based methods

Advantages of kernel-based method:

- Theoretically more well-founded
- Interpretable and amenable to numerical analysis
- Number of kernel parameters to learn is smaller
- Come with rigorous a priori error estimates

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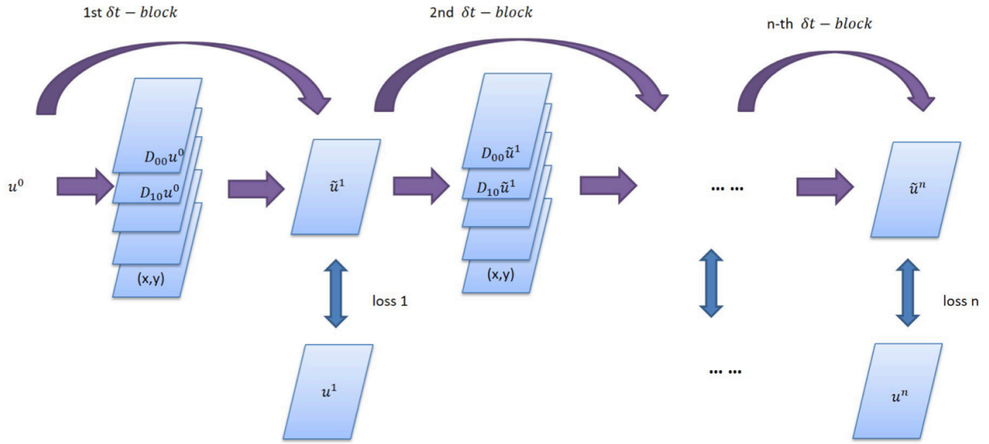
Equation Learning

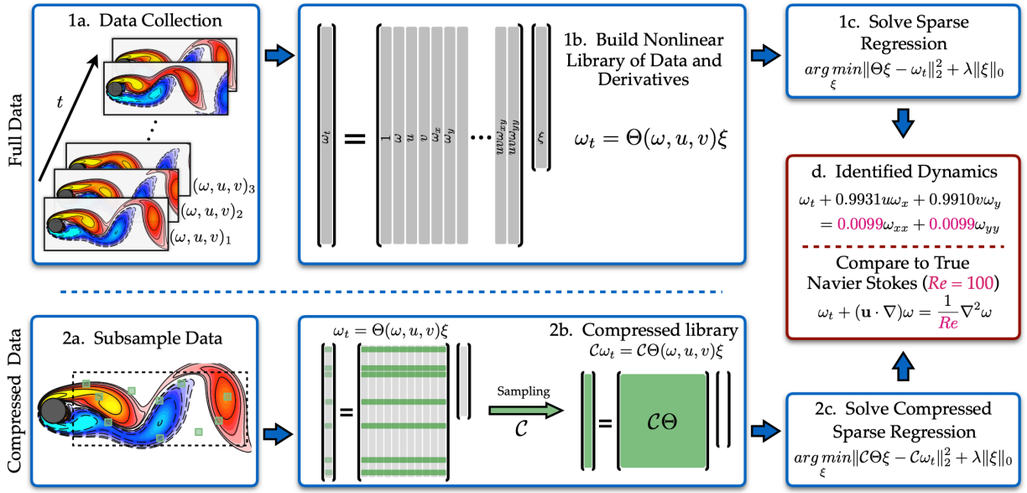


Other Approaches:

- Symbolic Regression (Bongard & Lipson (2007), Schmidt & Lipson (2009))
- SINDy and PDE-Find (Brunton et al. (2016), Rudy et al. (2016))
- PDE-Net (Zichao Long et al. (2018))

Advantages of kernel-based method:

- Handle sparse data (Da Long et al. (2023))
- A priori error estimates (Batlle et al. (2023))



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Kernel Interpolation Problem

Data:

$$\text{inputs } X = (x_1, \ldots, x_n)^\top, \text{ outputs } \; Y = (y_1, \ldots, y_n)^\top$$

Goal:

$$\text{find } f : \mathcal{X} \to \mathbb{R} \text{ such that } f(x_i) = y_i$$

Interpolation Problem:

$$\begin{cases} \underset{f \in \mathcal{H}}{\text{minimize}} & \|f\|_{\mathcal{H}} \\ \text{s.t.} & f(x_i) = y_i \quad \text{for} \quad i = 1, \ldots, n\,. \end{cases}$$

Solution: Using representer theorem, we get a closed form solution

$$f(x) = K(x, X)K(X, X)^{-1}Y,$$

with norm

$$\|f\|_{\mathcal{H}}^2 = Y^\top K(X, X)^{-1}Y\,.$$

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Summary of Methods

Problem:

$$P(x, u^m(x), Du^m(x), D^2u^m(x)) = f^m(x) \qquad \forall x \in \Omega$$

Two Approaches:

- **two-step learning**
  1. approximate the solutions u^m
  2. using the approximant, learn the function P

- **one-step learning**
  4. learn the solution functions u^m and the function P at once

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Two-step learning

Problem:

$$P(x, u^m(x), Du^m(x), D^2u^m(x)) = f^m(x) \qquad \forall x \in \Omega$$

Kernel Interpolation Problem:

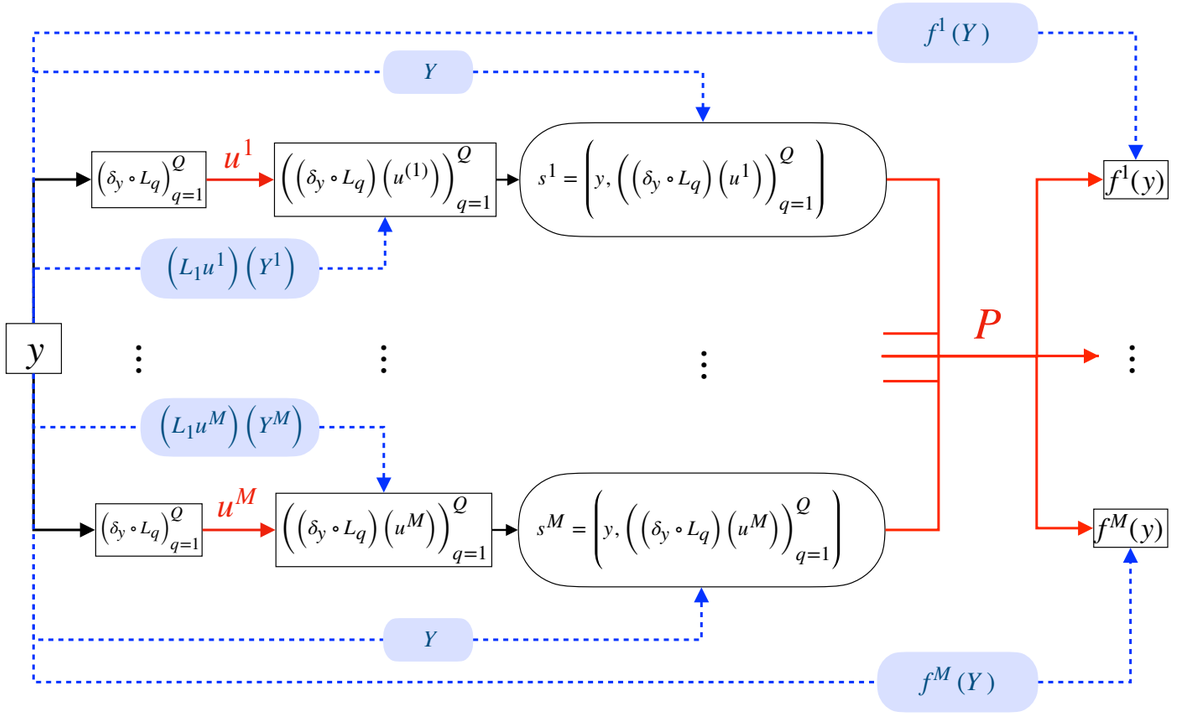
1. Learn u^m's:

$$\begin{cases} \underset{v^m \in \mathcal{H}_K}{\text{minimize}} & \|v^m\|_{\mathcal{H}_K} \\ \text{s.t.} & v^m(X_N) = u^m(X_N) \end{cases}$$

2. Learn P: for minimizer v_N^m,

- compute Dv_N^m and $D^2v_N^m$,
- define $\phi_N^m := (v_N^m(X_N), Dv_N^m(X_N), D^2v_N^m(X_N))$,
- solve

$$\underset{Q \in \mathcal{H}_\Gamma}{\text{minimize}} \quad \|Q\|_{\mathcal{H}_\Gamma}^2 + \lambda \sum_{m=1}^{M} \|Q\left(X_N, \phi_N^m\right) - f^m(X_N)\|_2^2$$



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One-step learning

Problem:

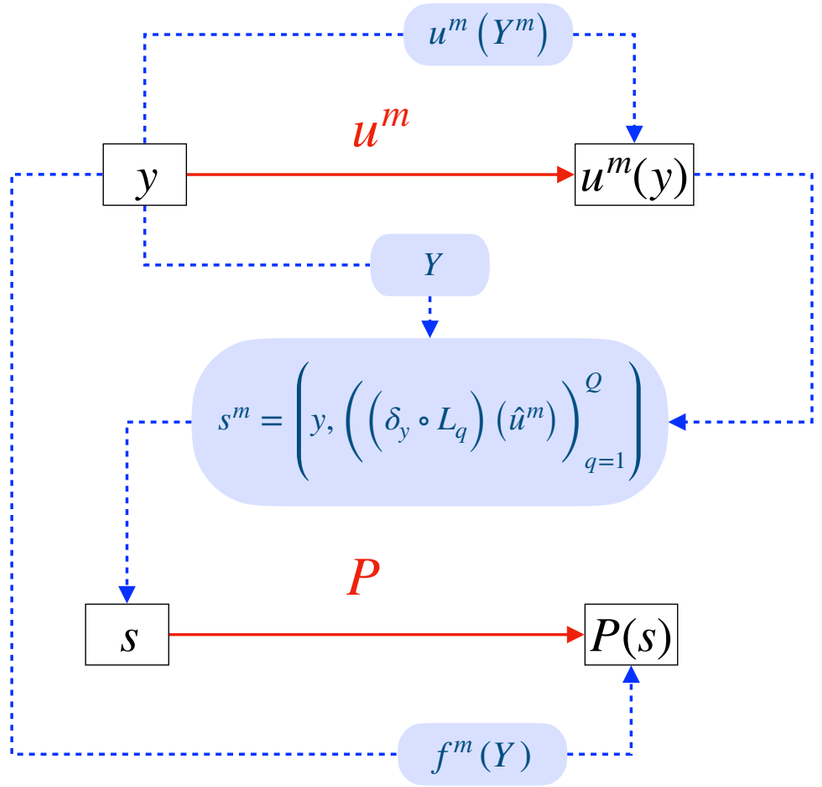
$$P(x, u^m(x), Du^m(x), D^2u^m(x)) = f^m(x) \qquad \forall x \in \Omega$$

Kernel Interpolation Problem:

- solve

$$\begin{cases} \underset{Q \in \mathcal{H}_\Gamma, v^m \in \mathcal{H}_K}{\text{minimize}} \ \|Q\|_\Gamma^2 + \lambda \sum_{m=1}^{M} \|v^m\|_K^2 \\ \text{s.t.} \qquad v^m(X_N) = u^m(X_N), \qquad \text{for} \quad m = 1, \ldots, M, \\ \qquad\quad Q\left(X_N, \phi_N^m\right) = f^m(X_N), \qquad \text{for} \quad m = 1, \ldots, M, \end{cases}$$

where $\phi_N^m := (v^m(X_N), Dv^m(X_N), D^2v^m(X_N))$.



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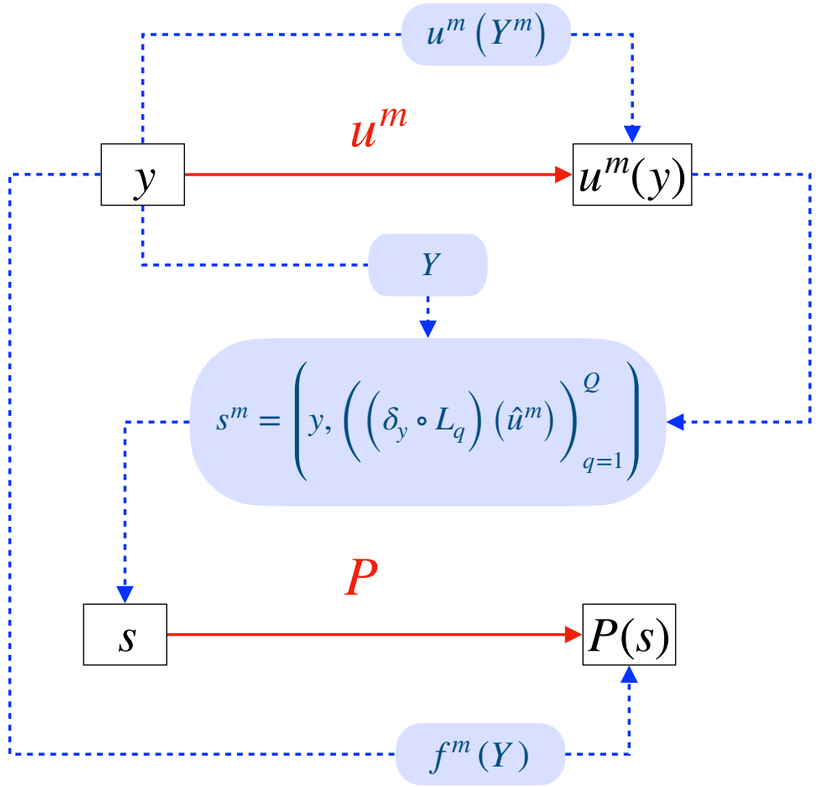
One-step learning

- introduce latent variables Z_N^m such that $Z_N^m = \phi_N^m$,
- rewrite the problem as

$$
\begin{cases}
\underset{Q \in \mathcal{H}_\Gamma, v^m \in \mathcal{H}_K, Z_N^m}{\text{minimize}} \; \|Q\|_\Gamma^2 + \lambda \sum_{m=1}^{M} \|v^m\|_K^2 \\
\text{s.t.} \quad v^m(X_N) = u^m(X_N), \quad \text{for} \quad m = 1, \ldots, M, \\
\qquad\quad Q\left(X_N, Z_N^m\right) = f^m(X_N), \quad \text{for} \quad m = 1, \ldots, M, \\
\qquad\quad Z_N^m = \phi_N^m, \quad \text{for} \quad m = 1, \ldots, M\,.
\end{cases}
$$



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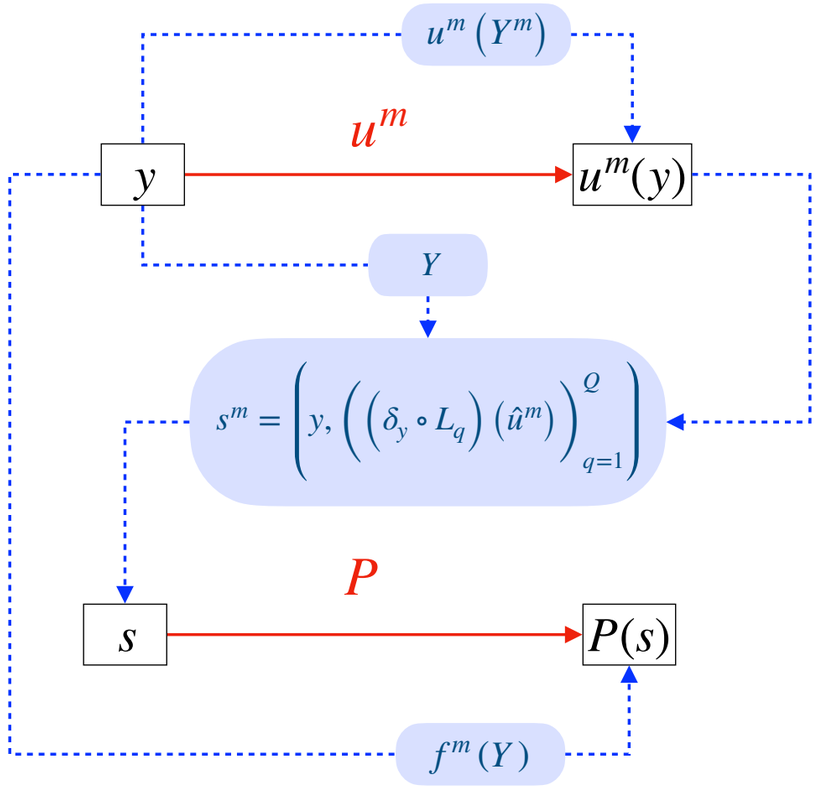
One-step learning

- define $S_N^m := (X_N, Z_N^m)$,
- using representer theorem, reduce the problem to

$$\begin{cases} \underset{Z_N^m}{\text{minimize}} & f(X_N)^\top \Gamma(S_N, S_N)^{-1} f(X_N) + \lambda \sum_{m=1}^{M} \left(Z_N^m\right)^\top K(\phi_N^m, \phi_N^m)^{-1} Z_N^m \\ \text{s.t.} & Z_{N,0}^m = u^m(X_N), \qquad \text{for} \quad m = 1, \ldots, M\,. \end{cases}$$

- solve numerically using a Levenberg–Marquardt-type algorithm



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Convergence Guarantees

Theorem (convergence guarantee)

Assumptions:

- the kernel $K : \Omega \times \Omega \to \mathbb{R}$ is such that $\mathscr{H}_K \subset H^s(\Omega)$ for some $s > d/2 + \text{order}_P$
- the kernel $\Gamma : \mathbb{R}^{d+q} \times \mathbb{R}^{d+q} \to \mathbb{R}$ be such that $\mathscr{H}_\Gamma \subset H^{s'}(\mathbb{R}^{d+q})$ for some $s' > \frac{q}{2}$
- the fill distance between $x_j \in \Omega$ goes to zero as $N \to \infty$
- the fill distance $h_{S_N,\mathbb{R}^{d+q}} \to 0$ as $M \to \infty$

Let $v_N^m, Q_{M,N}$ be the minimizers of the kernel interpolation problem.

$$\lim_{N\to\infty} v_N^m = u^m, \qquad \text{pointwise and in} \quad H^t(t < s) \quad \text{in} \quad \Omega$$

$$\lim_{M\to\infty} \lim_{N\to\infty} Q_{M,N} = P, \qquad \text{pointwise and in} \quad H^{t'}(t' < s') \quad \text{in} \quad \mathbb{R}^{d+q}$$

+ A priori Error Estimates for u^m and P

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Example: Darcy Flow

Problem:

$$P(x, u(x), Du(x), D^2u(x)) = \nabla \cdot \big(a(x)\nabla u(x)\big) = f(x), \quad \forall x \in (0,1)^2$$

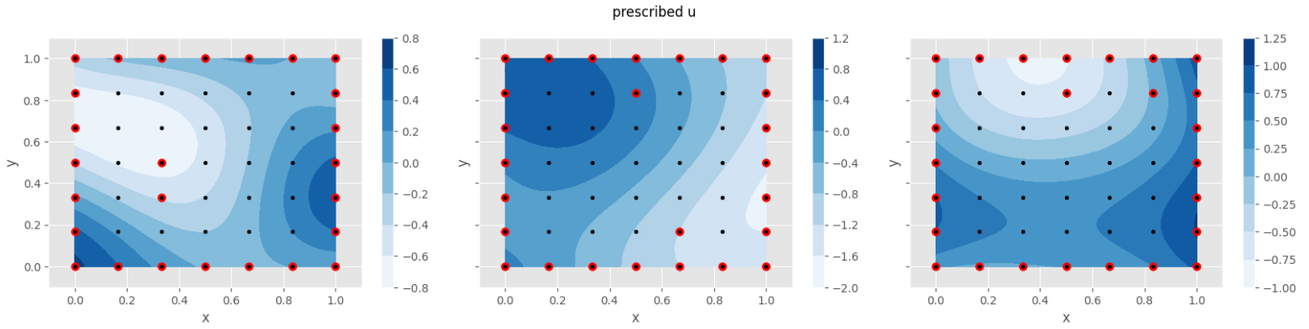
Data:

- $M = 3$ pairs of (u^m, f^m), for $m \in \{1,2,3\}$ prescribe functions $u^m \sim GP(0,K)$
- 7×7 data points X, $N = 26$ observation points X_N^m

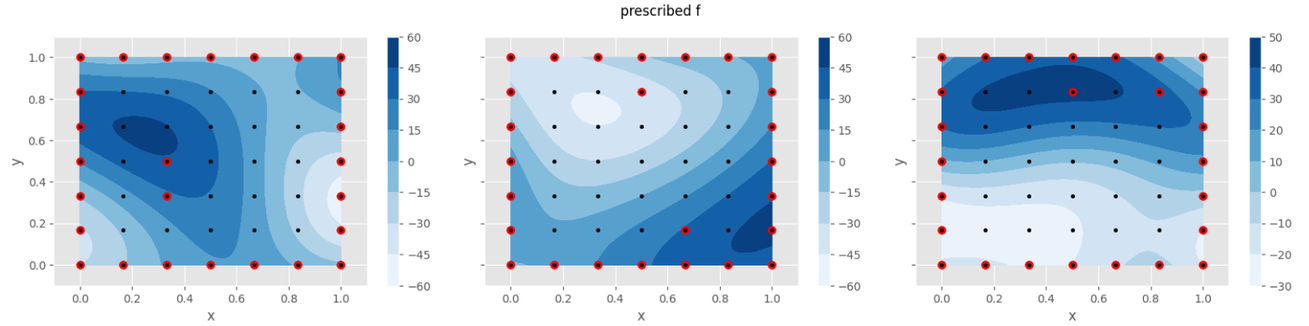
Objective:

learn P and u^m's

$u^m(X), u^m(X_N^m)$



$f^m(X), f^m(X_N^m)$



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Example: Darcy Flow

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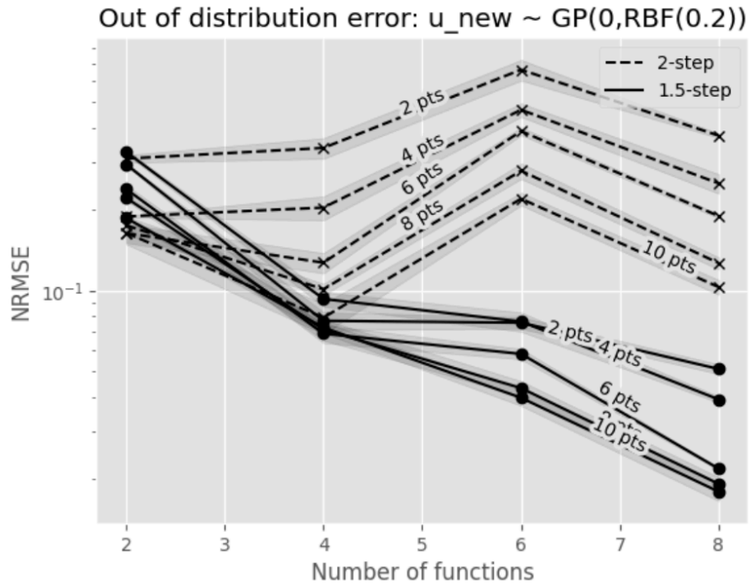

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Example: Burgers' Equation

Problem:

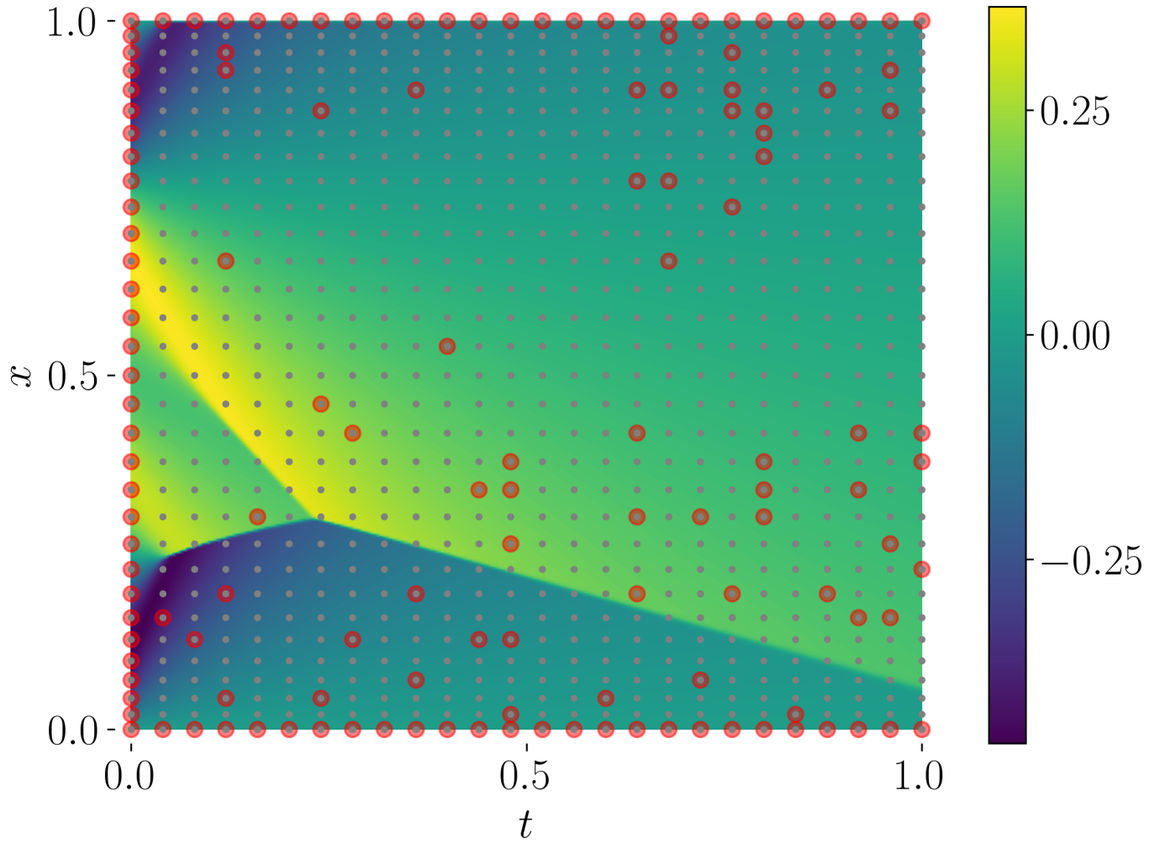
$$P(u)(y) = \partial_t u - 5u\partial_x u - 0.001\partial_{xx} u, \quad \forall y = (t, x) \in [0,1] \times (0,1)$$

Data:

- $M = 1$ pairs of (u^1, f^1)
- 806 data points Y, $N = 60$ observation points Y_N^1

Objective:

learn P and u^1



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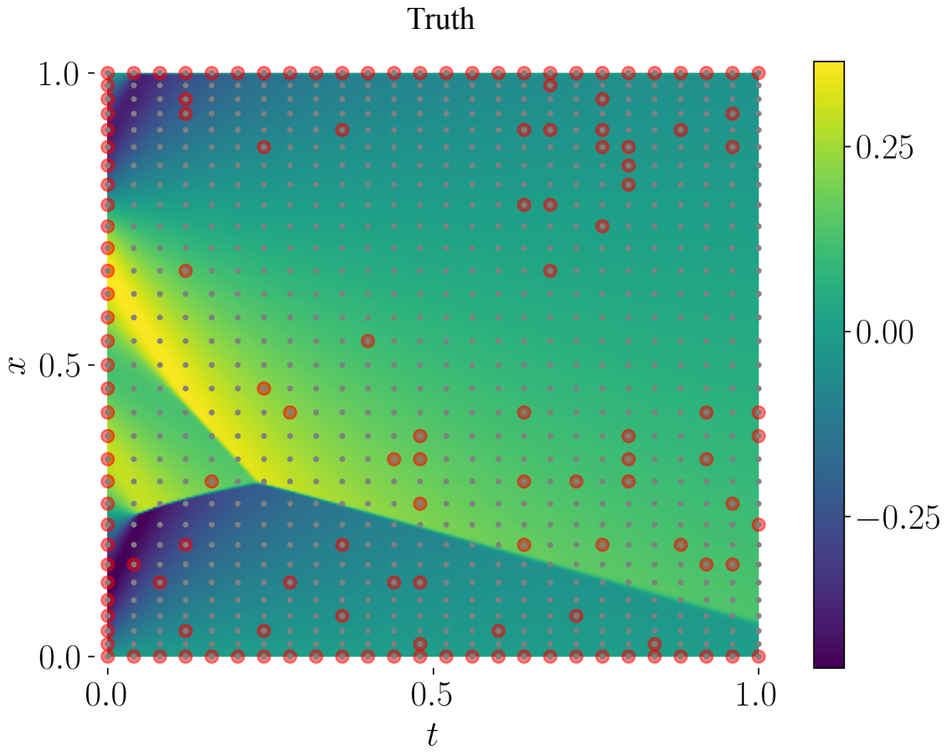

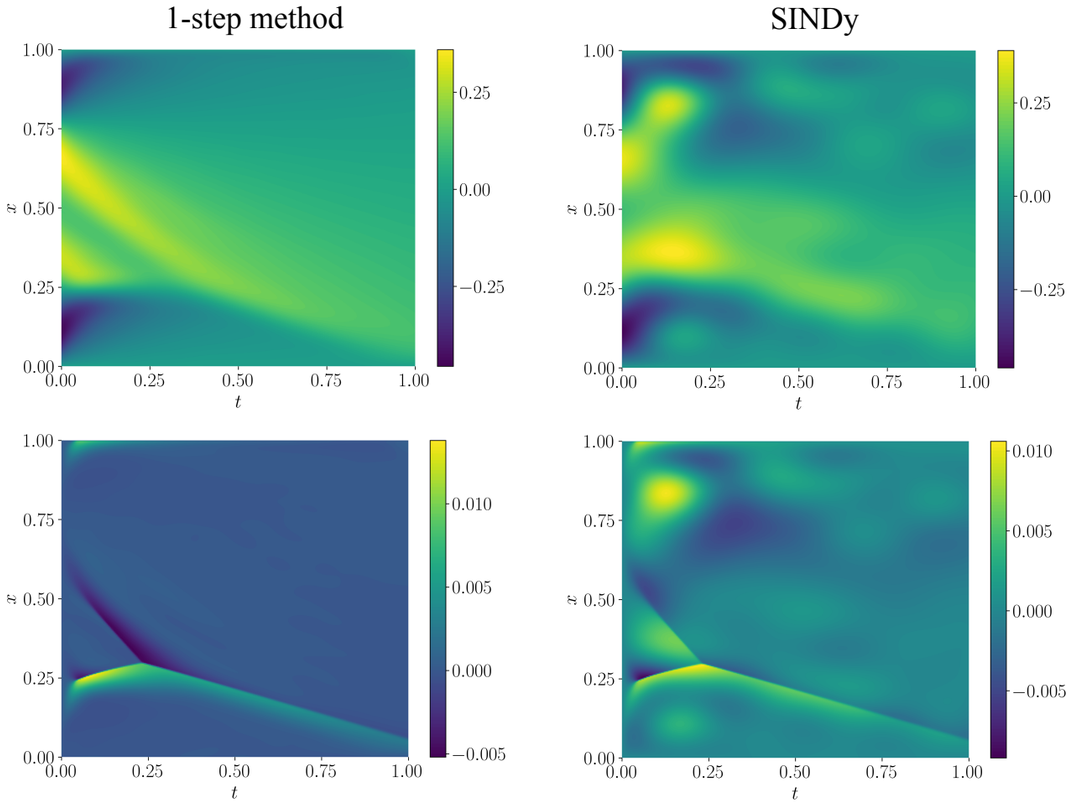

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Application: Jupiter's radiation environment

Collaboration with JPL Natural Space Environments Group

Problem:

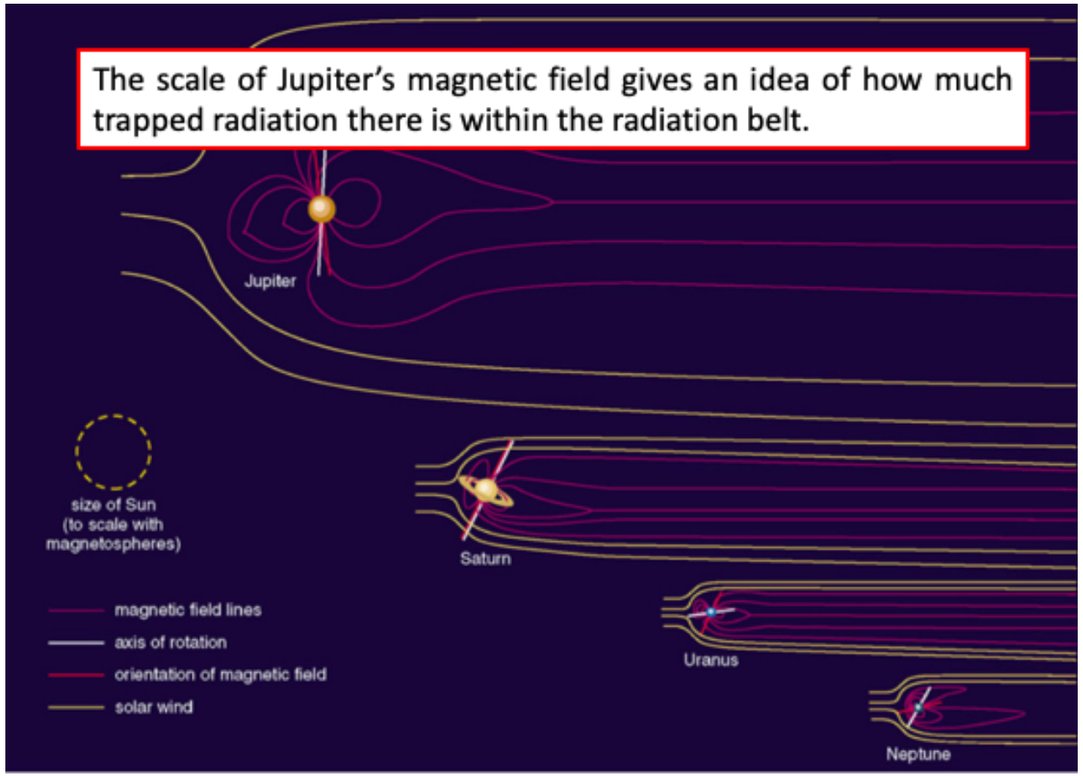
$$\partial_t f = \nabla \cdot (D \nabla f) + \nabla \cdot (cf)$$

Data:

Values of f at 6000 points in the domain

Objective:

learn f in the entire domain and learn the unknown coefficients c and D



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Application: Stress Transfer & Earthquake Dynamics

Collaboration with USC Department of Chemical Engineering and Materials Science

Problem:

$$\nabla \cdot \left(G \nabla u_x\right) + \frac{G}{1-2\nu}\frac{\partial \varepsilon_v}{\partial x} - \alpha \frac{\partial p}{\partial x} = 0$$

$$\nabla \cdot \left(G \nabla u_y\right) + \frac{G}{1-2\nu}\frac{\partial \varepsilon_v}{\partial y} - \alpha \frac{\partial p}{\partial y} = 0$$

$$\nabla \cdot \left(G \nabla u_z\right) + \frac{G}{1-2\nu}\frac{\partial \varepsilon_v}{\partial z} - \alpha \frac{\partial p}{\partial z} = \rho_b g$$

$$\frac{1}{M}\frac{\partial p}{\partial t} + \alpha \frac{\partial \varepsilon_v}{\partial t} - \nabla \cdot \left(\frac{k}{\mu}\nabla p - \rho_f g\right) = 0$$

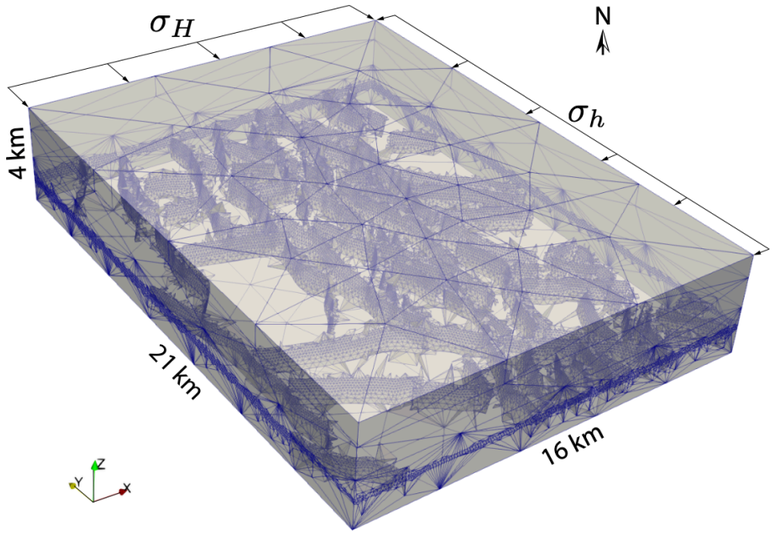
Data:

Values of u and p, each on 5 million points in the domain

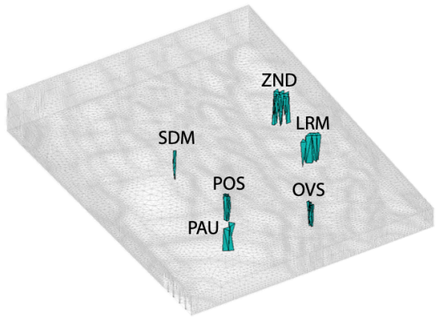
Objective:

learn u and p in the entire domain and learn all the unknown coefficients

a. Mesh showing 115 faults



b. Reservoir domain and well locations



c. Faults color-coded by dip angles