# Learning Physical Models that Can Respect Conservation Laws

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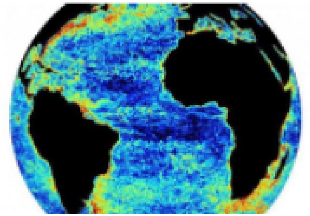
$$\left.\begin{aligned} \mathcal{F}u(t,x) &= 0,\ \ x \in \Omega, \\ u(0,x) &= u_0(x),\ \ x \in \Omega, \\ u(t,x) &= g(t,x),\ \ x \in \partial\Omega, \end{aligned}\right\} , \forall\, t \geq 0,$$

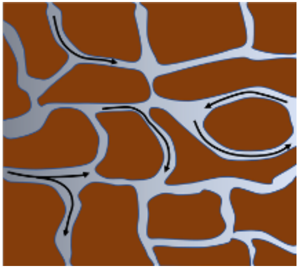
Conservation Law

$$\mathcal{F}u = u_t + \nabla \cdot F(u)$$

Aerodynamics



Ocean & Climate



Reservoir Modeling

# Integral Form of Conservation Laws

$$u_t + \nabla \cdot F(u) = 0$$

$$\int_\Omega u(t,x) d\Omega = \int_\Omega u_0(x) d\Omega - \int_0^t \int_\Gamma F(u) \cdot n d\Gamma dt$$

1D

$$\underbrace{\int_\Omega u(t,x) d\Omega}_{\mathcal{G}u(t,x)} = \underbrace{\int_\Omega u_0(x) d\Omega + \int_0^t (F_{\text{in}} - F_{\text{out}}) dt}_{b(t)}$$

$F_{\text{in}} = F(u, t, x_0)|_{u=g(t,x_0)}$
$F_{\text{out}} = F(u, t, x_N)|_{u=g(t,x_N)}$
$\Omega = [x_0, x_N]$

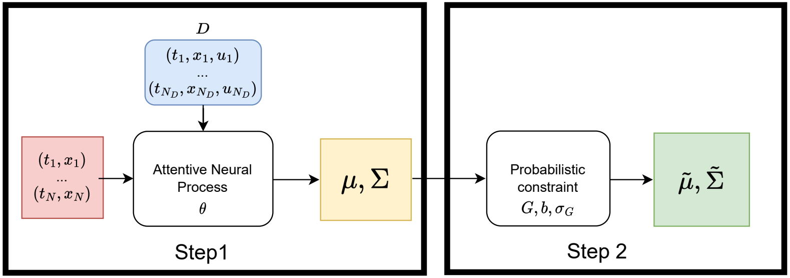
**Algorithm** ProbConserv

1: **Input:** Constraint matrix $G$, constraint value $b$, non-zero noise $\sigma_G$ and input points $(t_1, x_1), \ldots (t_N, x_N)$
2: **Step 1**: Calculate black-box prediction over output grid: $\mu, \Sigma = f_\theta((t_1, x_1), \ldots (t_N, x_N); D)$
3: **Step 2**: Calculate $\tilde{\mu}$ and $\tilde{\Sigma}$ according to Equation 1.
4: **Output:** $\tilde{\mu}, \tilde{\Sigma}$

$$\begin{aligned} \tilde{\mu} &= \mu - \Sigma G^T(\sigma_G^2 I + G\Sigma G^T)^{-1}(G\mu - b) \\ \tilde{\Sigma} &= \Sigma - \Sigma G^T(\sigma_G^2 I + G\Sigma G^T)^{-1} G\Sigma \end{aligned} \quad (1)$$

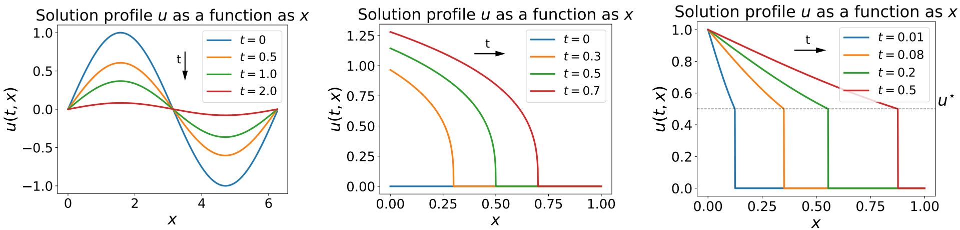
$$b = Gu + \sigma_G \epsilon$$

# Instantiation of Framework ProbConserv-ANP




Schematic for the instantiation of our framework ProbConserv with the ANP (ProbConserv-ANP) as the data-driven black box model in Step 1

$$u_t = \nabla \cdot (k(u) \nabla u)$$



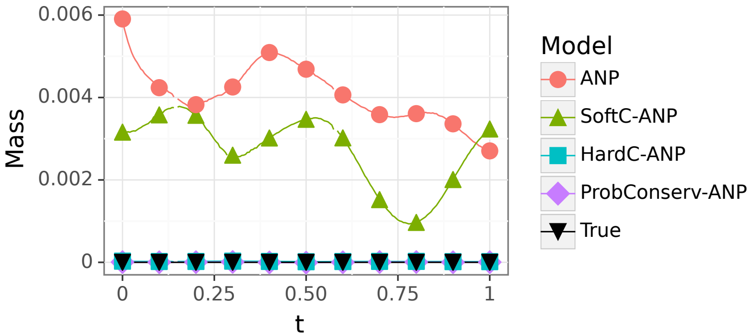

(a) Diffusion equation $k = 1$

(b) PME $k(u) = u^3$

(c) Stefan discont. $k(u)$

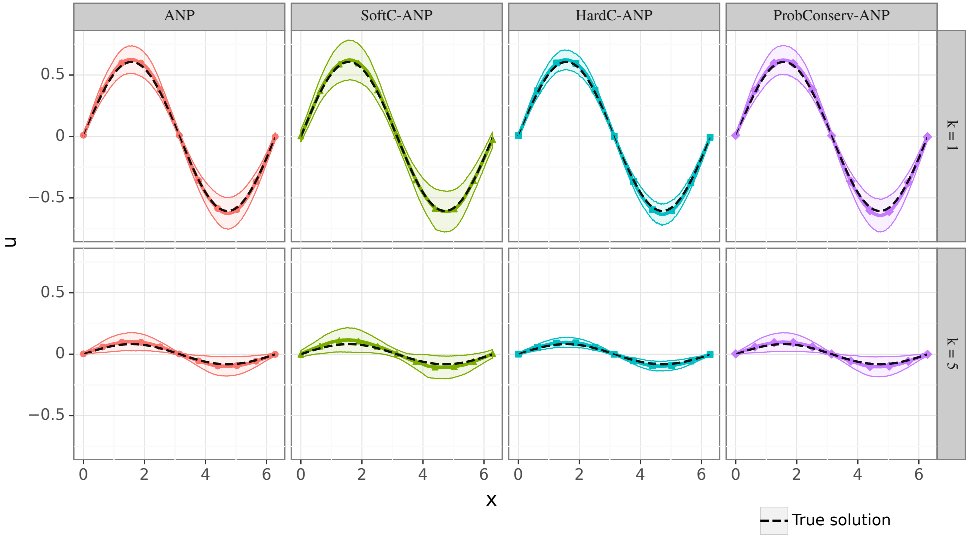
Illustration of the "easy-to-hard" paradigm for the GPME

# Diffusion Equation: Violation of Conservation of Mass




True mass is zero over time: zero net flux from domain boundaries

# Diffusion Equation: Solution Profiles and UQ

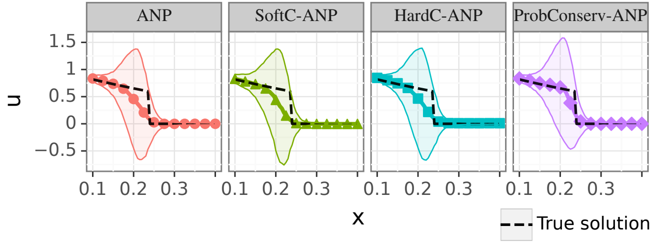



"Easy" problem: uncertainty is relatively homoscedastic

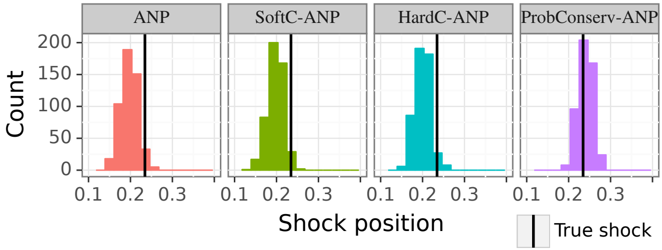
# Diffusion Equation: Error Metrics

| | CE | LL | MSE |
|---|---|---|---|
| ANP | 4.68 (0.10) | 2.72 (0.02) | 1.71 (0.41) |
| SoftC-ANP | 3.47 (0.17) | 2.40 (0.02) | 2.24 (0.78) |
| HardC-ANP | **0** (0.00) | **3.08** (0.04) | **1.37** (0.33) |
| ProbConserv-ANP | **0** (0.00) | 2.74 (0.02) | **1.55** (0.33) |

Mean and standard error for CE $\times 10^{-3}$ (*should be zero*), LL (*higher is better*), MSE $\times 10^{-4}$ (*lower is better*) over $n_{\text{test}} = 50$ runs with variable diffusivity parameter $k \in [1, 5]$ and test-time parameter value $k = 1$




(a) Solution profile




(b) Posterior of the shock position

“Hard” problem: Uncertainty is highly heteroscedastic with largest magnitude near the shock location

# Stefan Equation: Error Metrics

| | CE | LL | MSE |
|---|---|---|---|
| ANP | -1.30 (0.01) | 3.53 (0.00) | 5.38 (0.01) |
| SoftC-ANP | -1.72 (0.04) | **3.57** (0.01) | 6.81 (0.15) |
| HardC-ANP | **0** (0.00) | 2.33 (0.06) | 5.18 (0.02) |
| ProbConserv-ANP | **0** (0.00) | **3.56** (0.00) | **1.89** (0.01) |

Mean and standard error for CE $\times 10^{-2}$ (*should be zero*), LL (*higher is better*), and MSE $\times 10^{-3}$ (*lower is better*) over $n_{\text{test}} = 50$ runs at time $t = 0.05$ with variable parameter $u^\star \in [0.55, 0.7]$ and test-time parameter value $u^\star = 0.6$

**3X decrease in MSE**

# Thank you!

Hansen, D., Maddix, D.C., Alizadeh, S., Gupta, G., Mahoney, M.W., Learning Physical Models that Can Respect Conservation Laws," *Proceedings of the* 40$^{th}$ *International Conference on Machine Learning*, PMLR 202, 2023.

Code: `https://github.com/amazon-science/probconserv`

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