Deep adaptive sampling for surrogate modeling

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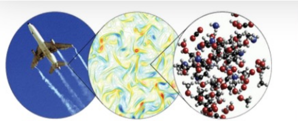
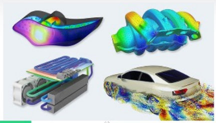
EASIAM

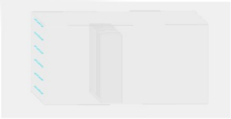
Outline

Background

- Uncertainty quantification
- Inverse design
- Digital twins
- Shape optimization
- Operator learning
- ...







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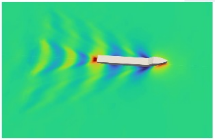
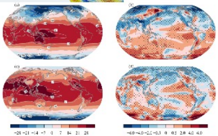
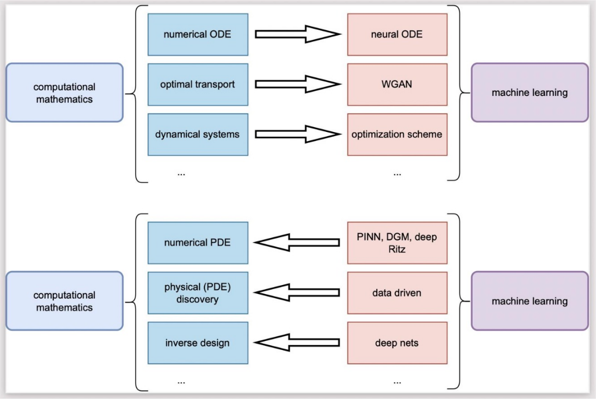
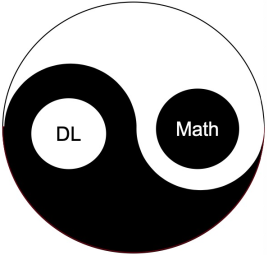




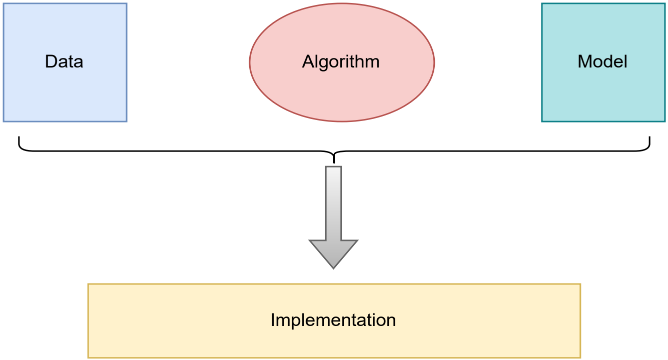
Background





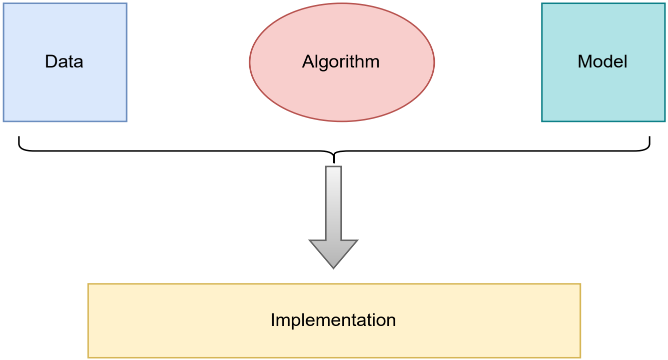
The relationship between math and DL

Big data era: data-driven



- Model: deep neural networks, physical model, or coupling
- Data: labeled, unlabled, random samples ....
- Algorithm: various optimization methods

Big data era: data-driven



data is oil

- model is driven by data
- data has the influence on generalization

Goal

Traditional numerical methods

- high fidelity
- suffers from the curse of dimensionality

Machine (deep) learning approaches

- low fidelity
- weaker dependence on dimensionality

our purpose:
Develop adaptive sampling methods for neural network-based surrogates

Parametric PDEs

Parametric differential equations

$$\mathcal{L}\left(\mathbf{x},\xi;u\left(\mathbf{x},\xi\right)\right)=s(\mathbf{x},\xi)\qquad\forall\left(\mathbf{x},\xi\right)\in\Omega_s\times\Omega_p,$$
$$\mathcal{B}\left(\mathbf{x},\xi;u\left(\mathbf{x},\xi\right)\right)=g(\mathbf{x},\xi)\qquad\forall\left(\mathbf{x},\xi\right)\in\partial\Omega_s\times\Omega_p.$$

For any ξ, compute the solution efficiently without solving the differential equation repeatedly.

- $\mathcal{L}$: differential operator; $\mathcal{B}$: boundary operator
- $\Omega_s \subset \mathbb{R}^n$: spatial domain with smooth boundary $\partial\Omega_s$
- $\mathbf{x} \in \Omega_s$: spatial variable
- $\Omega_p \subset \mathbb{R}^d$: parametric space
- $\xi \in \Omega_p$: parameters
- we denote $\Omega = \Omega_s \times \Omega_p$ and $\partial\Omega = \partial\Omega_s \times \Omega_p$ for simplicity

Physics-informed surrogate modeling

Why

- fast inference
- tackle high dimensional problems

How: a deep net $u(\mathbf{x}, \xi; \Theta) \to u(\mathbf{x}, \xi)$

$$J(u(\mathbf{x}, \xi; \Theta)) = \| r(\mathbf{x}, \xi; \Theta) \|_{2,\Omega}^2 + \gamma \| b(\mathbf{x}, \xi; \Theta) \|_{2,\partial\Omega}^2 ,$$

$$\| r(\mathbf{x}, \xi; \Theta) \|_{2,\Omega}^2 = \int_{\Omega} r^2(\mathbf{x}, \xi; \Theta) d\mathbf{x} d\xi,$$

$$\| b(\mathbf{x}, \xi; \Theta) \|_{2,\partial\Omega}^2 = \int_{\partial\Omega} b^2(\mathbf{x}, \xi; \Theta) d\mathbf{x} d\xi$$

An optimization problem: $\min_{\Theta} J(u(\mathbf{x}, \xi; \Theta))$

Illustration of the error

Discretization of the loss

$$J_N\left(u(\mathbf{x},\xi;\Theta)\right) = \frac{1}{N_r}\sum_{i=1}^{N_r} r^2(\mathbf{x}_\Omega^{(i)},\xi^{(i)};\Theta) + \gamma\frac{1}{N_b}\sum_{i=1}^{N_b} b^2(\mathbf{x}_{\partial\Omega}^{(i)},\xi^{(i)};\Theta),$$

$\mathbf{x}_\Omega^{(i)}$ drawn from Ω_s, $\mathbf{x}_{\partial\Omega}^{(i)}$ drawn from $\partial\Omega_s$, and $\xi^{(i)}$ drawn from Ω_p.

$$u(\mathbf{x},\xi;\Theta^*) = \arg\min_{\Theta} J(u(\mathbf{x},\xi;\Theta)),$$

$$u(\mathbf{x},\xi;\Theta_N^*) = \arg\min_{\Theta} J_N(u(\mathbf{x},\xi;\Theta)).$$

$$\mathbb{E}\left(\left\|u_{\Theta_N^*} - u\right\|_\Omega\right) \leq \underbrace{\mathbb{E}\left(\left\|u_{\Theta_N^*} - u_{\Theta^*}\right\|_\Omega\right)}_{\text{statistical error}} + \underbrace{\left\|u_{\Theta^*} - u\right\|_\Omega}_{\text{approximation error}}$$

Illustration of the error

Where do the errors come from?

the capability of neural networks $\rightarrow$ approximation error

the strategy of loss discretization $\rightarrow$ statistical error

In this work, we focus on how to reduce the statistical error

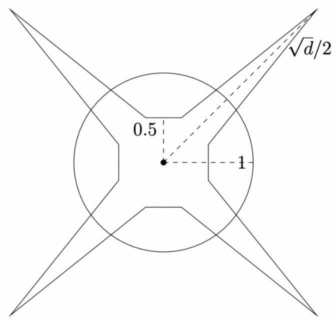
Difficulities

low regularities or high-dimensional

Key point: the strategy to discretize the loss. Uniform random sampling? Quasi-random sampling?

Geometric properties of high-dimensional spaces

uniformly distributed points in high-dimensional spaces



Most of the volume of a high-dimensional cube is located around its corner [Vershynin, High-Dimensional Probability, 2020]. Cube: $[-1, 1]^d$

$$\mathbb{P}(\|\mathbf{x}\|_2^2 \leq 1) \leq \exp(-\frac{d}{10}).$$

Sampling strategy

PDF for sampler

$$p(\mathbf{x},\xi) = p(\mathbf{x}|\xi)p(\xi) \quad \text{or} \quad p(\mathbf{x},\xi) = p(\xi|\mathbf{x})p(\mathbf{x})$$

In practice, the above two PDF models can be further simplified.

- Sample from a joint PDF

$$p(\mathbf{x},\xi) = \hat{r}(\mathbf{x},\xi) \propto r^2(\mathbf{x},\xi;\theta)h(\mathbf{x},\xi),$$

$$p_{\mathbf{x},\xi}(\mathbf{x},\xi;\theta_f) = p_{\mathbf{z}|\xi}(f_{\mathrm{KRnet}}(\mathbf{x},\xi;\theta_f))\left|\det \nabla_{\mathbf{x}} f_{\mathrm{KRnet}}\right|.$$

- Sample from a marginal PDF

$$p(\xi) = \tilde{r}^2(\xi;\theta) = \int_{\Omega_s} r^2(\mathbf{x},\xi;\theta)d\mathbf{x},$$

$$p_\xi(\xi;\theta_f) = p_{\mathbf{z}}(f_{\mathrm{KRnet}}(\xi;\theta_{\mathbf{f}}))\left|\det \nabla_\xi f_{\mathrm{KRnet}}\right|.$$

Deep adaptive sampling for surrogates (DAS^2)

A viewpoint of variance reduction (both $\mathbf{x}$ and ξ)

$$J_r(u(\mathbf{x},\xi;\Theta)) = \int_{\Omega} \frac{r^2(\mathbf{x},\xi;\Theta)}{p(\mathbf{x},\xi)} p(\mathbf{x},\xi) d\mathbf{x} d\xi \approx \frac{1}{N_r} \sum_{i=1}^{N_r} \frac{r^2(\mathbf{x}_\Omega^{(i)},\xi^{(i)};\Theta)}{p(\mathbf{x}_\Omega^{(i)},\xi^{(i)})},$$

where $\{\mathbf{x}_\Omega^{(i)},\xi^{(i)}\}_{i=1}^{N_r}$ from $p(\mathbf{x},\xi)$ instead of a uniform distribution.

A viewpoint of variance reduction (only ξ)

$$J_r(u(\mathbf{x},\xi;\Theta)) = \int_{\Omega_p} \frac{\tilde{r}^2(\xi;\Theta)}{p(\xi)} p(\xi) d\xi \approx \frac{1}{N_{\tilde{r}}} \sum_{i=1}^{N_{\tilde{r}}} \frac{\tilde{r}^2(\xi^{(i)};\Theta)}{p(\xi^{(i)})},$$

where $\tilde{r}^2(\xi;\Theta) \approx \frac{1}{m_\mathbf{x}} \sum_{i=1}^{m_\mathbf{x}} r^2(\mathbf{x}^{(i)},\xi;\Theta)$, $\{\mathbf{x}^{(i)}\}_{i=1}^{m_\mathbf{x}}$ in the spatial domain, $\{\xi^{(i)}\}_{i=1}^{N_{\tilde{r}}}$ from $p(\xi)$.

Deep adaptive sampling for surrogates (DAS^2)

Importance sampling

$$p^* = r^2(\mathbf{x}, \xi; \Theta)/\mu, \ \mu = \int_\Omega r^2(\mathbf{x}, \xi; \Theta) d\mathbf{x} d\xi.$$

Sample from $p(\mathbf{x}, \xi)$ for a fixed Θ: a deep generative model

$$p_{KRnet}(\mathbf{x}, \xi; \Theta_f) \approx \mu^{-1} r^2(\mathbf{x}, \xi; \Theta)$$

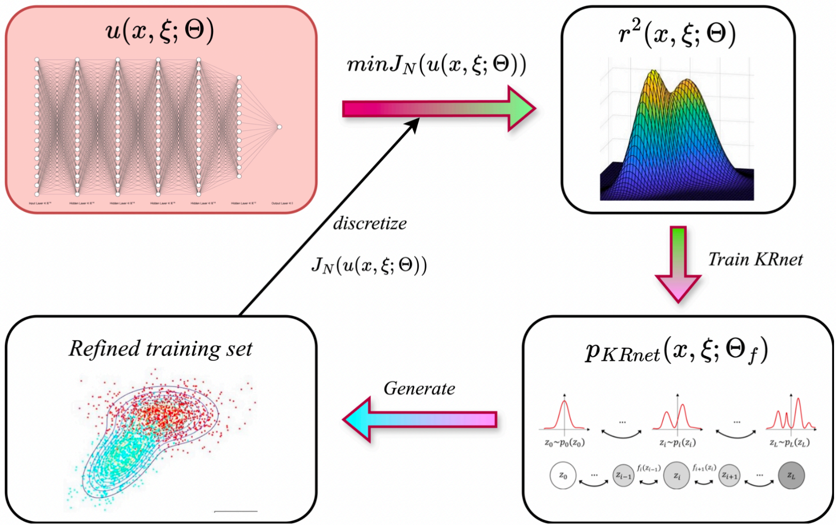
where $p_{KRnet}(\mathbf{x}, \xi; \Theta_f)$ is a PDF induced by KRnet [Tang, Wan and Liao, 2020]; [Tang, Wan and Liao, 2021]

"Error estimator": $\hat{r}(\mathbf{x}, \xi) \propto r^2(\mathbf{x}, \xi; \Theta)$

$$D_{KL}(\hat{r}(\mathbf{x}, \xi) \| p_{KRnet}(\mathbf{x}, \xi; \Theta_f)) = \int_B \hat{r} \log \hat{r} d\mathbf{x} d\xi - \int_B \hat{r} \log p_{KRnet} d\mathbf{x} d\xi.$$

$$\min_{\Theta_f} H(\hat{r}, p_{KRnet}) = -\int_B \hat{r} \log p_{KRnet} d\mathbf{x} d\xi.$$

Algorithm of DAS^2



Analysis

Assumptions [T. De Ryck and S. Mishra, 2022]

- $\theta \in \Theta = [-a, a]^D$: trainable parameters of u_θ where $a > 0$ is a constant.
- $\mathscr{M}_1 : \theta \mapsto J_{r,N}$ and $\mathscr{M}_2 : \theta \mapsto J_r$: Lipschitz continuous in the ℓ_∞ sense with Lipschitz constant $\mathfrak{L}$ for $\theta \in \Theta$.
- Let $c > 0$ be a constant that is independent of Θ. Assume that $J_{r,N} \in [0, c]$ for all $\theta \in \Theta$.

Theorem (Wang, Tang, Zhai, Wan, and Yang, 2024)

Let θ_N^* be a minimizer of $J_{r,N}$ where the collocation points are independently drawn from a given probability distribution. Given $\varepsilon \in (0, 1)$, the following inequality holds under the above assumptions

$$J_r(u_{\theta_N^*}) \leq \varepsilon^2 + J_{r,N}(u_{\theta_N^*})$$

with probability at least $1 - (4a\mathfrak{L}/\varepsilon^2)^D \exp(-N_r\varepsilon^4/2c^2)$.

Numerical results: physics-informed operator learning

The following dynamical system

$$\begin{cases} \dfrac{\mathrm{d}u(x,\xi)}{\mathrm{d}x} = e^{-D\|\boldsymbol{\xi}-\mathbf{0.5}\|^2} f(x,\xi), \quad x \in [0,1], \\ u(0,\xi) = 0, \end{cases}$$

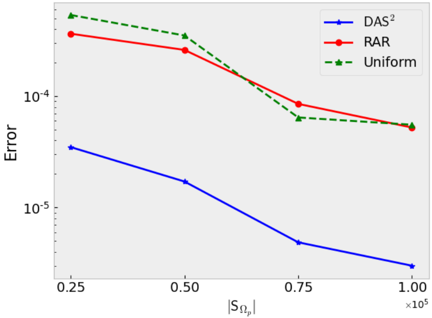
- $D = 6$: a fixed parameter
- $\xi \in \Omega_p = [-1,1]^8$

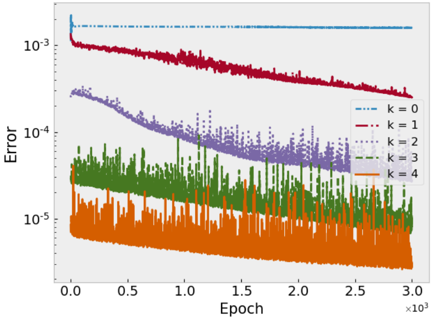
Goal: learn the sulution operator from f to the solution u without any paired input-output data

f is drawn from V_{poly} where

$$V_{\text{poly}} = \left\{ \sum_{i=0}^{d-1} \xi_i T_i(x) : |\xi_i| \leq M \right\}.$$

Numerical results: physics-informed operator learning





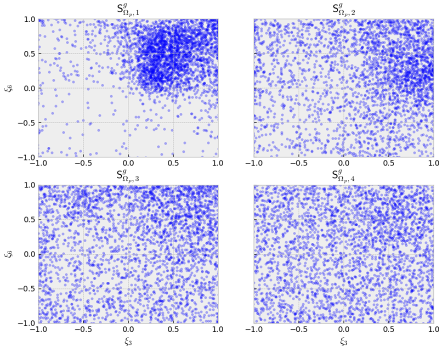
$$u_\theta(x, \xi) \approx \sum_{i=1}^{l} q_{\theta_1}^{(i)}(x) t_{\theta_2}^{(i)}(\xi) + b_0,$$

marginal PDF for sampling

Numerical results: physics-informed operator learning

The results and evolution of samples

sampling strategy \ $\lvert S_{\Omega_p} \rvert$	2.5×10^4	5×10^4	7.5×10^4	1×10^5
Uniform (0.006s)	5.4×10^{-4}	3.5×10^{-4}	6.4×10^{-5}	5.5×10^{-5}
RAR (0.006s)	3.6×10^{-4}	2.6×10^{-4}	8.5×10^{-5}	5.2×10^{-5}
DAS^2 (0.03s)	3.5×10^{-5}	1.7×10^{-5}	4.9×10^{-6}	3.0×10^{-6}



Numerical results: parametric optimal control problems

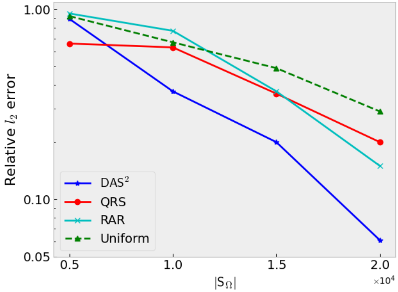
$$
\begin{cases}
\min\limits_{y(\mathbf{x},\xi),u(\mathbf{x},\xi)} J\left(y\left(\mathbf{x},\xi\right),u\left(\mathbf{x},\xi\right)\right) = \frac{1}{2}\left\|y(\mathbf{x},\xi)-y_d(\mathbf{x},\xi)\right\|_{2,\Omega}^2 + \frac{\alpha}{2}\left\|u(\mathbf{x},\xi)\right\|_{2,\Omega}^2, \\
\text{subject to} \begin{cases} -\Delta y(\mathbf{x},\xi) = u(\mathbf{x},\xi) & \text{in } \Omega, \\ y(\mathbf{x},\xi) = 1 & \text{on } \partial\Omega, \end{cases} \\
\text{and} \quad u_a \le u(\mathbf{x},\xi) \le u_b \quad \text{a.e. in } \Omega,
\end{cases}
$$

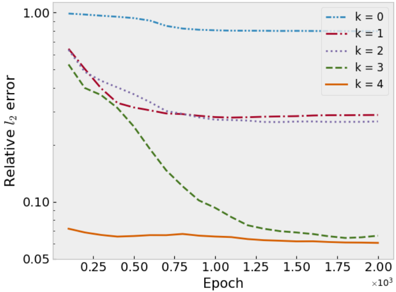
where $\Omega_p = (\xi_1, \xi_2)$ is the paramter.
$\Omega(\boldsymbol{\xi}) = ([0,2]\times[0,1])\backslash B((1.5,0.5),\xi_1)$ and the desired state is given by

$$
y_d(\boldsymbol{\xi}) = \begin{cases} 1 & \text{in } \Omega_1 = [0,1]\times[0,1], \\ \xi_2 & \text{in } \Omega_2(\boldsymbol{\xi}) = ([1,2]\times[0,1])\backslash B((1.5,0.5),\xi_1), \end{cases}
$$

where $B((1.5,0.5),\xi_1)$ is a ball of radius ξ_1 with center $(1.5,0.5)$, $\alpha = 0.001$ and $\boldsymbol{\xi} \in \Omega_p = [0.05,0.45]\times[0.5,2.5]$.

Numerical results: parametric optimal control problems





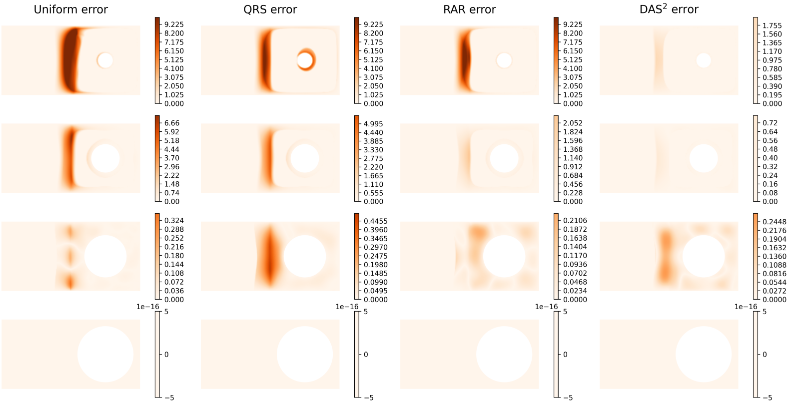
$$l(\mathbf{x}, \xi) = x_1(2 - x_1)x_2(1 - x_2)(\xi_1^2 - (x_1 - 1.5)^2 - (x_2 - 0.5)^2).$$

$$u(\mathbf{x}, \xi) \approx u_{\theta_u}(\mathbf{x}, \xi),\ y(\mathbf{x}, \xi) \approx l(\mathbf{x}, \xi) y_{\theta_y}(\mathbf{x}, \xi) + 1,\ p(\mathbf{x}, \xi) \approx l(\mathbf{x}, \xi) p_{\theta_p}(\mathbf{x}, \xi)$$

$$\Omega := \{(\mathbf{x}, \xi) | 0 \leq x_1 \leq 2, 0 \leq x_2 \leq 1, 0.05 \leq \xi_1 \leq 0.45, 0.5 \leq \xi_2 \leq 2.5,$$
$$(x_1 - 1.5)^2 + (x_2 - 0.5)^2 \geq \xi_1^2\}.$$

joint PDF model for sampling

Numerical results: parametric optimal control problems



top to bottom: $\xi = (0.10, 2.5)$ $\xi = (0.20, 2.0)$ $\xi = (0.30, 1.5)$ $\xi = (0.40, 0.5)$.

Numerical results: parametric optimal control problems

sampling strategy \ $\lvert S_\Omega \rvert$	0.5×10^4	1×10^4	1.5×10^4	2×10^4
Uniform (0.1s)	0.92	0.67	0.49	0.29
QRS (0.1s)	0.66	0.63	0.36	0.20
RAR (0.1s)	0.95	0.77	0.37	0.15
DAS^2 (0.1s)	0.89	0.37	0.20	0.06

- 11×11 grid in the parametric space
- dolfin-adjoint solver for a fixed parameter
- dolfin-adjoint solver : 18804 seconds

Parametric lid-driven cavity flow problems

$$\begin{cases} \mathbf{u}(\mathbf{x},\xi)\cdot\nabla\mathbf{u}(\mathbf{x},\xi)+\nabla p(\mathbf{x},\xi)=\dfrac{1}{Re(\xi)}\Delta\mathbf{u}(\mathbf{x},\xi) & \text{in } \Omega, \\ \nabla\cdot\mathbf{u}(\mathbf{x},\xi)=0 & \text{in } \Omega, \\ \mathbf{u}(\mathbf{x},\xi)=\mathbf{g}(\mathbf{x},\xi) & \text{on } \partial\Omega, \end{cases}$$

- $\mathbf{u}(\mathbf{x},\xi)=[u(\mathbf{x},\xi),v(\mathbf{x},\xi)]^{\mathsf{T}},\mathbf{x}=[x,y]^{\mathsf{T}}$
- $Re(\xi)=\xi\in\Omega_p=[100,1000]$
- The physical domain is $\Omega_s=[0,1]\times[0,1]$
- Boundary conditions

$$\mathbf{g}(\mathbf{x},\xi)=\begin{cases}[1,0]^{\mathsf{T}}, y=1; \\ [0,0]^{\mathsf{T}}, \text{ otherwise.}\end{cases}$$

Goal: obtaining all-at-once solutions for $Re\in[100,1000]$

Parametric lid-driven cavity flow problems

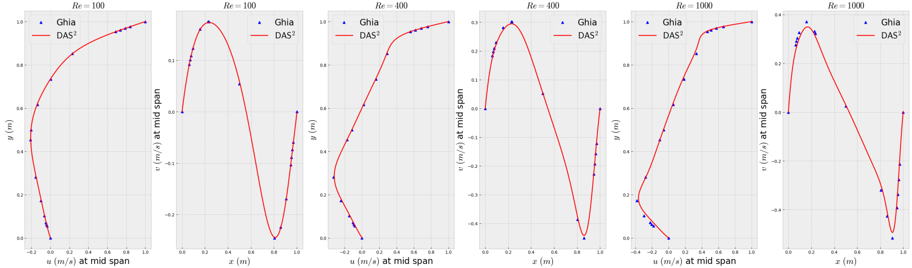
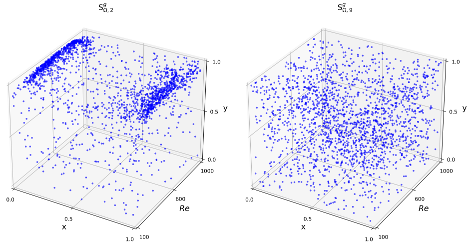
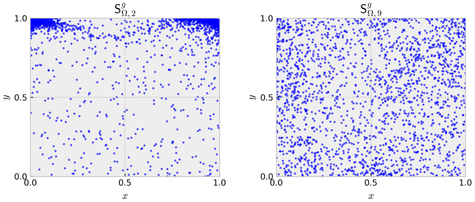


Figure: The velocity components at the location of mid-span lines for surrogate modeling of parametric lid-driven cavity flow problems ($Re \in [100, 1000]$). The results for $Re = 100, 400, 1000$ are chosen for visualization.

Parametric lid-driven cavity flow problems



(a) 3d points



(b) 2d projection onto *xy*-plane

Parametric lid-driven cavity flow problems

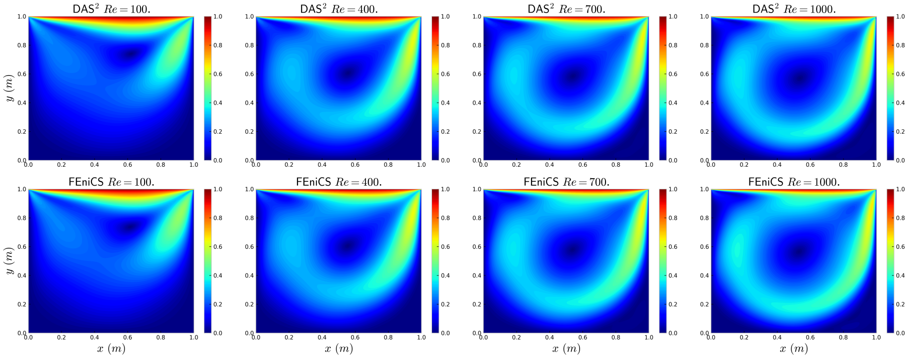


Figure: The visualization of $|\mathbf{u}| = \sqrt{u^2 + v^2}$ for surrogate modeling of parametric lid-driven cavity flow problems, $Re \in [100, 1000]$. The l_2 relative errors are $1.5\%, 1.1\%, 3.1\%, 4.8\%$ for $Re = 100, 400, 700, 1000$ respectively.

- Inference time of DAS^2: 0.02 seconds,
- The computation time of FEniCS: 309.94 seconds

Summary and outlook

summary

- illustrate that DAS^2 is necessary for parametric PDEs
- significantly improve the accuracy for low-regularity problems especially for high-dimensional or parametric problems

outlook

- incoporate tensor networks into deep adaptive sampling
- large scale problems
- more applications

Thank you for your attention
Q & A