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Model Order Reduction techniques for a parametric nonlinear elliptic problem

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Model Order Reduction and Machine Learning

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Introduction

Parametric PDEs

- Involve *high-dimensional* parameter spaces
- Require *multiple evaluations* for different parameter values
- Significant *computational costs*

Model Order Reduction techniques

- Alleviate the computational burden
- *Reduce* the dimensionality while preserving essential *features*
- Rapid and efficient *approximations* of the solution manifold

Most prominent techniques

- *Proper Orthogonal Decomposition*
- Data-driven methods: *Physics Informed Neural Networks*
- Hybrid approaches: *POD-NN*

Parametric nonlinear elliptic problem

Given

- Two-dimensional spatial domain $\Omega = (0, 1)^2$
- Parameters $\boldsymbol{\mu} = (\mu_0, \mu_1) \in \mathcal{P} = [0.1, 1]^2$
- Homogeneous Dirichlet boundary conditions

$$u(\mathbf{x}, \boldsymbol{\mu}) = 0 \quad \forall\, \mathbf{x} \in \partial\Omega$$

- Source term

$$g(\mathbf{x}; \boldsymbol{\mu}) = 100 \sin(2\pi x_0) \cos(2\pi x_1)$$

Find $u(\boldsymbol{\mu})$ such that

$$\begin{cases} -\Delta u(\boldsymbol{\mu}) + \frac{\mu_0}{\mu_1}\left(e^{\mu_1 u(\boldsymbol{\mu})} - 1\right) = g(\mathbf{x}; \boldsymbol{\mu}) & \text{in } \Omega \\ u(\boldsymbol{\mu}) = 0 & \text{in } \partial\Omega \end{cases}$$

$\forall\, \mathbf{x} = (x_0, x_1) \in \Omega,\ \forall\, \boldsymbol{\mu} \in \mathcal{P}$

Parametric nonlinear elliptic problem

Variational formulation

Find $u(\boldsymbol{\mu}) \in V := H_0^1(\Omega)$ such that

$$\int_\Omega \nabla u(\boldsymbol{\mu}) \cdot \nabla v + \frac{\mu_0}{\mu_1} \int_\Omega \left(e^{\mu_1 u(\boldsymbol{\mu})} - 1\right) v - \int_\Omega g(\mathbf{x}; \boldsymbol{\mu}) v = 0 \quad \forall\, v \in V,\ \forall\, \boldsymbol{\mu} \in \mathcal{P}$$

Introducing

$$f_1(u, v; \boldsymbol{\mu}) = \int_\Omega \nabla u(\boldsymbol{\mu}) \cdot \nabla v$$

$$f_2(u, v; \boldsymbol{\mu}) = \frac{\mu_0}{\mu_1} \int_\Omega \left(e^{\mu_1 u(\boldsymbol{\mu})} - 1\right) v$$

$$f_3(u, v; \boldsymbol{\mu}) = - \int_\Omega g(\mathbf{x}; \boldsymbol{\mu}) v$$

it can be formulated as

$$f(u, v; \boldsymbol{\mu}) := f_1(u, v; \boldsymbol{\mu}) + f_2(u, v; \boldsymbol{\mu}) + f_3(u, v; \boldsymbol{\mu}) = 0$$

Parametric nonlinear elliptic problem

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Find $u(\boldsymbol{\mu}) \in V := H_0^1(\Omega)$ such that

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Introducing

$$f_1(u, v; \boldsymbol{\mu}) = \int_\Omega \nabla u(\boldsymbol{\mu}) \cdot \nabla v$$

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PROBLEM: IS NONLINEAR!

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it can be formulated as

$$f(u, v; \boldsymbol{\mu}) := f_1(u, v; \boldsymbol{\mu}) + f_2(u, v; \boldsymbol{\mu}) + f_3(u, v; \boldsymbol{\mu}) = 0$$

Newton scheme

- Taylor expansion of $f(u, v; \boldsymbol{\mu})$

$$f(u_{n+1}) = f(u_n) + J_f[\delta u]\big|_{u_n}\delta u + O(||\delta u||^2)$$

- $u_{n+1} = u_n + \delta u$ is the estimated solution at the n-th iteration
- The n-th iteration consists in finding δu such that

$$J_f[\delta u]\big|_{u_n}\delta u = -f(u_n, v; \boldsymbol{\mu}) \qquad \forall\, v \in V$$

Using the properties of the *Gateaux derivative*

$$\int_\Omega \nabla\delta u \cdot \nabla v + \mu_0 \int_\Omega e^{\mu_1 u_n} v = -\int_\Omega \nabla u_n \cdot \nabla v - \frac{\mu_0}{\mu_1}\int_\Omega \left(e^{\mu_1 u_n} - 1\right) v + \int_\Omega g v \quad (1)$$

- Parameters:
  1. Tolerance $= 10^{-5}$
  2. Maximum iterations $= 25$

A priori error estimation

- $u_{ex}(\mathbf{x};\boldsymbol{\mu}) = 16x_0x_1(1-x_0)(1-x_1)$
- $g_{ex}(\mathbf{x};\boldsymbol{\mu}) = 32x_0(1-x_0) + 32x_1(1-x_1) + \frac{\mu_0}{\mu_1}\left(e^{\mu_1 16x_0x_1(1-x_0)(1-x_1)(\mathbf{x};\boldsymbol{\mu})} - 1\right)$

Considering $\mathbb{P}_1$ finite elements and $u \in H^2(\Omega)$

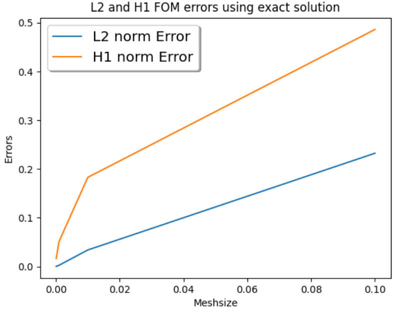
$$\mathcal{E}_{L^2} = ||u - u_h||_{L^2(\Omega)} \sim ch|u|_2$$

$$\mathcal{E}_{H^1_0} = ||u - u_h||_{H^1_0(\Omega)} \sim ch^{\frac{1}{2}}|u|_2$$

If plotted against mesh size h on a *logarithmic* scale, a *linear* decay is expected, with slopes

$$m_{L^2} = 1 \quad m_{H^1} = \frac{1}{2}$$

corresponding to the convergence orders of the errors in the L^2 and H^1 norm, respectively



$$h \in \{0.1, 0.01, 0.001, 0.0001\}$$

$$m_{L^2} = 0.996 \quad m_{H^1} = 0.498$$

Proper Orthogonal Decomposition

Offline phase

- $\mathcal{P}_M = \{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_M\} \subset \mathcal{P}$
- $\{\omega_i = u_\delta(\boldsymbol{\mu}_i)\}_{i=1}^M$ solving (1)
- *Snapshot matrix* $\mathbf{W} = [\omega_1 \,|\, \dots \,|\, \omega_M]$
- *Inner product matrix* $[\mathbb{X}_\delta]_{ij} = (\nabla\phi_i, \nabla\phi_j)_{L^2}$
- *Covariance matrix* $\mathbf{C} = \mathbf{W}^\top \mathbb{X}_\delta \mathbf{W}$
- *Eigenvalues* and *eigenvectors* $\{(\lambda_i, \mathbf{v}_i)\}_{i=1}^M$ of $\mathbf{C}$
- N largest integer s.t. $\frac{\sum_{i=1}^N \lambda_i}{\sum_{j=1}^M \lambda_j} \geq tol$
- *Basis matrix* $\mathbb{B} = [\psi_1 \,|\, \dots \,|\, \psi_N] \quad \psi_i = \frac{\mathbf{W}\mathbf{v}_i}{\|\mathbf{W}\mathbf{v}_i\|_{H_0^1}}$

Online phase

Fixed $\boldsymbol{\mu} \in \mathcal{P}$, during the k-th iteration of the Newton method

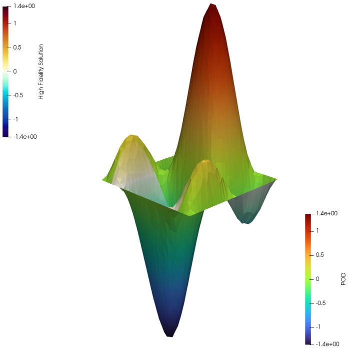
- $\mathbf{A}_\delta(\boldsymbol{\mu})$, $\mathbf{R}_\delta(\boldsymbol{\mu})$, $\mathbf{g}_{i\,\delta}(\boldsymbol{\mu})$
- Reduce the linear system
  $\mathbf{A}_N(\boldsymbol{\mu}) = \mathbb{B}^\top \mathbf{A}_\delta(\boldsymbol{\mu})\mathbb{B}$
  $\mathbf{R}_N(\boldsymbol{\mu}) = \mathbf{B}^\top \mathbb{R}_\delta(\boldsymbol{\mu})\mathbb{B}$
  $\mathbf{g}_{i\,N}(\boldsymbol{\mu}) = \mathbb{B}^\top \mathbf{g}_{i\,\delta}(\boldsymbol{\mu})$
- Find $\delta \mathrm{u}_N^k$
- Update $\mathrm{u}_N^{k+1} = \mathrm{u}_N^k + \delta \mathrm{u}_N^k$
- Project back $\mathrm{u}_{\delta,\,prj}^{k+1} = \mathbb{B}\mathrm{u}_N^{k+1}$

Proper Orthogonal Decomposition

Numerical results

- $h = 0.001$
- $|\mathcal{P}_M| = M = 300$
- $N_{max} = 10$
- $tol = 10^{-7}$
- Fixed $\boldsymbol{\mu} = (0.8, 0.4)$

- $\mathcal{E}^{rel}_{L^2} = \dfrac{||u_\delta(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})||_{L^2(\Omega)}}{||u_\delta(\boldsymbol{\mu})||_{L^2(\Omega)}} = 3.66 \cdot 10^{-4}$
- $\mathcal{E}^{rel}_{H^1_0} = \dfrac{||u_\delta(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})||_{H^1_0(\Omega)}}{||u_\delta(\boldsymbol{\mu})||_{H^1_0(\Omega)}} = 2.22 \cdot 10^{-4}$
- $SpeedUp = \frac{T_{FOM}}{T_{ROM}} = 0.84$



- Satisfactory approximation
- Captures peaks and valleys and preserves global behaviour
- Discrepancies with steep gradients

Physics Informed Neural Networks

- **Inputs:** $\mathbf{x} \in \Omega,\ \boldsymbol{\mu} \in \mathcal{P}$
- **Output:** $u(\mathbf{x}, \boldsymbol{\mu})$

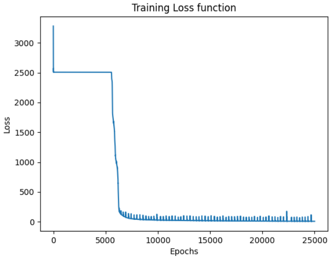
- $MSE \doteq MSE_r(\boldsymbol{\mu}) + \lambda \cdot MSE_b(\boldsymbol{\mu})$
- Residual MSE: for $(\mathbf{x}_i^r, \boldsymbol{\mu}_i^r) \in \Omega \times \mathcal{P}$

$$MSE_r(\boldsymbol{\mu}) \doteq \frac{1}{N_r} \sum_{i=1}^{N_r} |\mathcal{R}(\tilde{\omega}(\mathbf{x}_i^r, \boldsymbol{\mu}_i^r))|^2$$

- Boundary MSE: for $(\mathbf{x}_i^b, \boldsymbol{\mu}_i^b) \in \partial\Omega \times \mathcal{P}$

$$MSE_b(\boldsymbol{\mu}) \doteq \frac{1}{N_b} \sum_{i=1}^{N_b} |\tilde{\omega}(\mathbf{x}_i^b, \boldsymbol{\mu}_i^b) - u(\mathbf{x}_i^b, \boldsymbol{\mu}_i^b)|^2$$

- λ equilibrates the two losses



- $L = 4,\ N_{hl} = n + m + 2 = 7$
- *Sigmoid* activation function
- $trainingSize = 4000$
- $\lambda = 2750$
- $learningRate = 0.01$
- $maxIters = 25000$

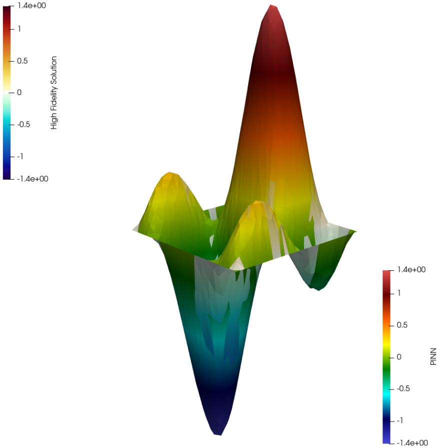
Physics Informed Neural Networks

Numerical results

- $h = 0.001$
- Fixed $\boldsymbol{\mu} = (0.8, 0.4)$
- $|\mathcal{P}_{test}| = 100$

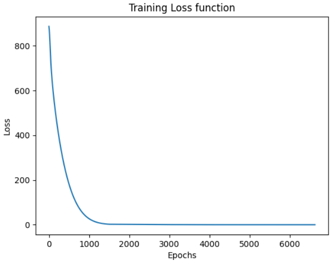
- $\mathcal{E}_{L^2}^{rel} = 1.44 \cdot 10^{-2}$
- $\mathcal{E}_{H_0^1}^{rel} = 5.05 \cdot 10^{-2}$
- $SpeedUp = 158$

- Captures overall structure and main features
- Discrepancies with steep gradients or rapid variations
- Less accurate than POD



POD-NN

- POD generates reduced space V_N
- FFNN $\Pi^{NN}(\boldsymbol{\mu}) : \mathcal{P} \to V_N$
- $u_\delta(\boldsymbol{\mu})$ reconstructed
- $\mathcal{L} = \sum_{\boldsymbol{\mu} \in \mathcal{P}_{train}} ||\Pi^{NN}(\boldsymbol{\mu}) - \mathbb{P}_g u_\delta(\boldsymbol{\mu})||^2$
- Optimal projection $\mathbb{P}_g u_\delta(\boldsymbol{\mu}) = \mathbb{B}(\mathbb{B}^\top \mathbb{X}_\delta \mathbb{B})^{-1} \mathbb{B}^\top \mathbb{X}_\delta u_\delta(\boldsymbol{\mu})$



- *Offline* phase
  - Build $\mathbb{B}_N$ via POD's *offline phase*
  - Solve $\mathbb{X}_N u_{N_i} = \mathbb{B}^\top \mathbb{X}_\delta u_\delta(\boldsymbol{\mu})$
  - Train the FFNN $\Pi^{NN}(\boldsymbol{\mu})$
- *Online* phase
  - $\boldsymbol{\mu}^* \mapsto \Pi^{NN}(\boldsymbol{\mu}^*)$
  - $u_\delta^{prj} = \mathbb{B}\Pi^{NN}(\boldsymbol{\mu}^*)$

- $L = 4,\ N_1 = 2,\ N_{hl} = 30,\ N_L = |V_N|$
- *Tanh* activation function
- $trainingSize = 300$
- $tol = 10^{-6}$
- $learningRate = 0.001$

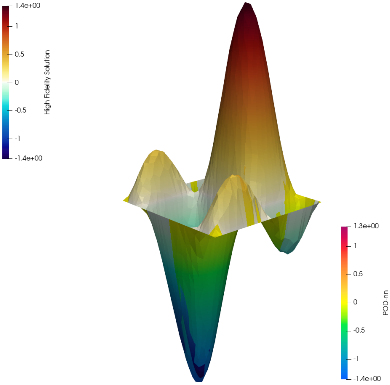
POD-NN

Numerical results

- $h = 0.001$
- Fixed $\boldsymbol{\mu} = (0.8, 0.4)$
- $|\mathcal{P}_{test}| = 100$

- $\mathcal{E}^{rel}_{L^2} = 7.88 \cdot 10^{-3}$
- $\mathcal{E}^{rel}_{H^1} = 5.31 \cdot 10^{-3}$
- $SpeedUp = 1235$

- Captures global structure and main features
- Discrepancies on extreme values and rapid variations



Conclusions

	L^2 norm Error	H^1 norm Error	SpeedUp
POD	$3.66 \cdot 10^{-4}$	$2.22 \cdot 10^{-4}$	0.84
PINN	$1.44 \cdot 10^{-2}$	$5.05 \cdot 10^{-2}$	158
POD-NN	$7.88 \cdot 10^{-3}$	$5.31 \cdot 10^{-3}$	1235

- POD offers the highest accuracy
- Nonlinearity issue $\rightarrow$ No significant reduction in computational time
- PINN has the worst relative errors
- POD-NN strikes the best balance
  - Almost as accurate as the POD
  - Highest SeepUp