Parameterized Partial Differential Equations and the Proper Orthogonal Decomposition

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Outline

- Parameterized PDEs
- The steady case
- Dimensionality reduction
- Proper orthogonal decomposition
- Projection-based model reduction
- Snapshot selection
- The unsteady case

Parameterized PDE

- Parametrized partial differential equation (PDE)

$$\mathcal{L}(\mathcal{W}, \mathbf{x}, t; \boldsymbol{\mu}) = 0$$

- Associated boundary conditions

$$\mathcal{B}(\mathcal{W}, \mathbf{x}_{\mathsf{BC}}, t; \boldsymbol{\mu}) = 0$$

- Initial condition

$$\mathcal{W}_0(\mathbf{x}) = \mathcal{W}_{\mathsf{IC}}(\mathbf{x}, \boldsymbol{\mu})$$

  - $\mathcal{W} = \mathcal{W}(\mathbf{x}, t) \in \mathbb{R}^q$: state variable
  - $\mathbf{x} \in \Omega \subset \mathbb{R}^d$, $d \leq 3$: space variable
  - $t \geq 0$: time variable
  - $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^p$: parameter vector

Model parameterized PDE

- Advection-diffusion-reaction equation: $\mathcal{W} = \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu})$ solution of

$$\frac{\partial \mathcal{W}}{\partial t} + \mathcal{U} \cdot \nabla \mathcal{W} - \kappa \Delta \mathcal{W} = f_{\mathsf{R}}(\mathcal{W}, t, \boldsymbol{\mu}_{\mathsf{R}}) \text{ for } \mathbf{x} \in \Omega$$

  with appropriate boundary and initial conditions

$$\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) = \mathcal{W}_D(\mathbf{x}, t; \boldsymbol{\mu}_{\mathsf{D}}) \text{ for } \mathbf{x} \in \Gamma_{\mathsf{D}}$$

$$\nabla \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) \cdot \mathbf{n}(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \Gamma_{\mathsf{N}}$$

$$\mathcal{W}(\mathbf{x}, 0; \boldsymbol{\mu}) = \mathcal{W}_0(\mathbf{x}; \boldsymbol{\mu}_{\mathsf{IC}}) \text{ for } \mathbf{x} \in \Omega$$

- Parameters of interest

$$\boldsymbol{\mu} = [\mathcal{U}_1, \cdots, \mathcal{U}_d, \kappa, \boldsymbol{\mu}_{\mathsf{R}}, \boldsymbol{\mu}_{\mathsf{D}}, \boldsymbol{\mu}_{\mathsf{IC}}]$$

Semi-discretized problem

- The PDE is then discretized in space by one of the following methods
  - Finite Differences approximation
  - Finite Element method
  - Finite Volumes method
  - Discontinuous Galerkin method
  - Spectral method....
- This leads to a system of $N_{\mathbf{w}} = q \times N_{\text{space}}$ ordinary differential equations (ODEs)

  $$\boxed{\frac{d\mathbf{w}}{dt} = \mathbf{f}(\mathbf{w}, t; \boldsymbol{\mu})}$$

  in terms of the discretized state variable

  $$\mathbf{w} = \mathbf{w}(t; \boldsymbol{\mu}) \in \mathbb{R}^{N_{\mathbf{w}}}$$

  with initial condition $\mathbf{w}(0; \boldsymbol{\mu}) = \mathbf{w}(\boldsymbol{\mu})$
- This is the high-dimensional model (HDM)

Parameterized solutions

- Example: two dimensional advection-diffusion equation

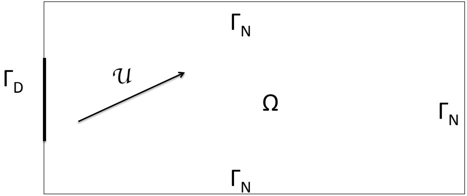
$$\frac{\partial \mathcal{W}}{\partial t} + \mathcal{U} \cdot \nabla \mathcal{W} - \kappa \Delta \mathcal{W} = 0 \text{ for } \mathbf{x} \in \Omega$$

with boundary and initial conditions

$$\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) = \mathcal{W}_D(\mathbf{x}, t; \boldsymbol{\mu}_\mathsf{D}) \text{ for } \mathbf{x} \in \Gamma_\mathsf{D}$$

$$\nabla \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) \cdot \mathbf{n}(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \Gamma_\mathsf{N}$$

$$\mathcal{W}(\mathbf{x}, 0; \boldsymbol{\mu}) = \mathcal{W}_0(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega$$



Parameterized solutions

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with boundary and initial conditions

$$\mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) = \mathcal{W}_D(\mathbf{x}, t; \boldsymbol{\mu}_{\mathsf{D}}) \text{ for } \mathbf{x} \in \Gamma_{\mathsf{D}}$$

$$\nabla \mathcal{W}(\mathbf{x}, t; \boldsymbol{\mu}) \cdot \mathbf{n}(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \Gamma_{\mathsf{N}}$$

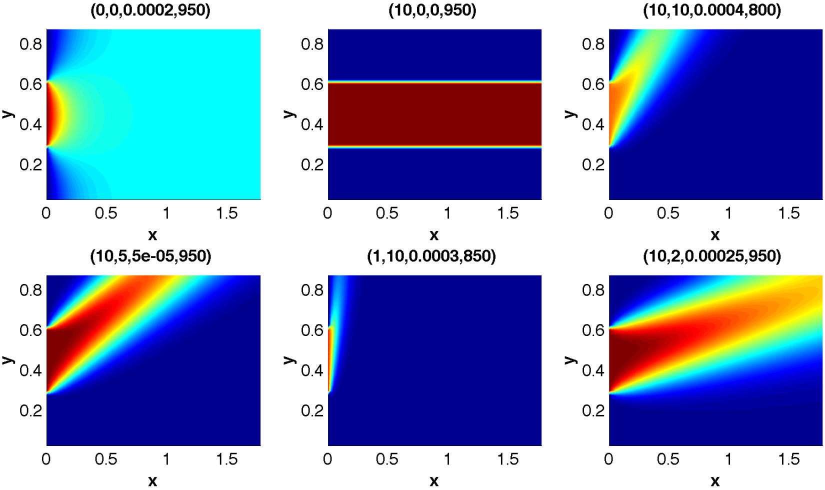
$$\mathcal{W}(\mathbf{x}, 0; \boldsymbol{\mu}) = \mathcal{W}_0(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega$$

- 4 parameters of interest

$$\boldsymbol{\mu} = [\mathcal{U}_1, \mathcal{U}_2, \kappa, \boldsymbol{\mu}_{\mathsf{D}}] \in \mathbb{R}^4$$

- $\mathbf{w} \in \mathbb{R}^{N_{\mathbf{w}}}$ with $N_{\mathbf{w}} = 2,701$

Parameterized solutions



Steady parameterized PDE

- Steady parameterized HDM

$$\mathbf{f}(\mathbf{w};\boldsymbol{\mu}) = \mathbf{0}$$

- Linear case

$$\mathbf{A}(\boldsymbol{\mu})\mathbf{w} = \mathbf{b}(\boldsymbol{\mu})$$

- Example: steady advection-diffusion equation

Dimensionality reduction

- Consider the manifold of solutions

$$\mathcal{M} = \{\mathbf{w}(\boldsymbol{\mu}) \text{ s.t. } \boldsymbol{\mu} \in \mathcal{D}\} \subset \mathbb{R}^{N_{\mathbf{w}}}$$

- Often $\dim(\mathcal{M}) \ll N_{\mathbf{w}}$
- Therefore, $\mathcal{M}$ could be described in terms of a much smaller set of variables, rather than $\{\mathbf{e}_1, \cdots, \mathbf{e}_{N_{\mathbf{w}}}\}$
- Hence dimensionality reduction

Dimensionality reduction

- First idea: use solutions of the equation to describe $\mathcal{M}$
- Consider pre-computed solution $\{\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)\}$ where $\{\boldsymbol{\mu}_1, \cdots, \boldsymbol{\mu}_m\} \subset \mathcal{D}$
- Let $\boldsymbol{\mu} \in \mathcal{D}$. Then approximate $\mathbf{w}(\boldsymbol{\mu})$ as

$$\mathbf{w}(\boldsymbol{\mu}) \approx \alpha_1(\boldsymbol{\mu})\mathbf{w}(\boldsymbol{\mu}_1) + \cdots + \alpha_m(\boldsymbol{\mu})\mathbf{w}(\boldsymbol{\mu}_m)$$

where $\{\alpha_1(\boldsymbol{\mu}), \cdots, \alpha_m(\boldsymbol{\mu})\}$ are coefficients to be determined

Reduced-order basis

- There may be redundancies in the solutions $\{\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)\}$.
- Better approach: remove the redundancies by considering an equivalent independent set $\{\mathbf{v}_1, \cdots, \mathbf{v}_k\}$ with $k \leq m$ such that

$$\text{span}\,\{\mathbf{v}_1, \cdots, \mathbf{v}_k\} = \text{span}\,\{\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)\}$$

- $\mathbf{V} = [\mathbf{v}_1, \cdots, \mathbf{v}_k] \in \mathbb{R}^{N_{\mathbf{w}} \times k}$ is a reduced-order basis with $k \ll N_{\mathbf{w}}$

Basis construction

- Lagrange basis

$$\text{span}\left\{\mathbf{v}_1, \cdots, \mathbf{v}_k\right\} = \text{span}\left\{\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)\right\}$$

- Hermite basis

$$\text{span}\left(\mathbf{v}_1, \cdots, \mathbf{v}_k)\right\} = \text{span}\left\{\mathbf{w}(\boldsymbol{\mu}_1), \frac{\partial \mathbf{w}}{\partial \mu_1}(\boldsymbol{\mu}_1), \cdots, \frac{\partial \mathbf{w}}{\partial \mu_p}(\boldsymbol{\mu}_1), \mathbf{w}(\boldsymbol{\mu}_2), \cdots\right\}$$

Data compression

- It is possible to remove more information from the snapshots $\{\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)\}$
- Consider the snapshot matrix $\mathbf{W} = [\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)]$
- Can we quantify the main information contained in $\mathbf{W}$ and discard the rest (noise)?
- This amount to data compression
- Here orthogonal projection will be used to compress the data

Orthogonal projection

- Let $\mathbf{V} \in \mathbb{R}^{N_{\mathbf{w}} \times k}$ be an orthogonal matrix ($\mathbf{V}^T\mathbf{V} = \mathbf{I}_k$) which columns span $\mathcal{S}$, a subspace of dimension k
- Let $\mathbf{x} \in \mathbb{R}^{N_{\mathbf{w}}}$. The orthogonal projection of $\mathbf{x}$ onto the subspace $\mathcal{S}$ is

$$\mathbf{V}\mathbf{V}^T\mathbf{x}$$

  - Projection matrix

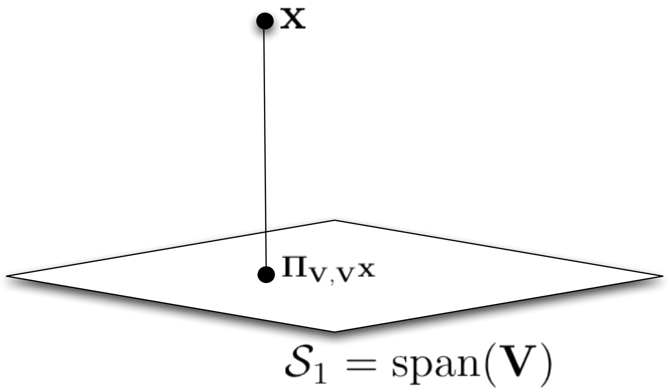
$$\mathbf{\Pi}_{\mathbf{V},\mathbf{V}} = \mathbf{V}(\mathbf{V}^T\mathbf{V})^{-1}\mathbf{V}^T = \mathbf{V}\mathbf{V}^T$$

  - special case 1: if $\mathbf{x}$ belongs to $\mathcal{S}$

$$\mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\mathbf{x} = \mathbf{V}\mathbf{V}^T\mathbf{x} = \mathbf{x}$$

  - special case 2: if $\mathbf{x}$ is orthogonal to $\mathcal{S}$

$$\mathbf{\Pi}_{\mathbf{V},\mathbf{V}}\mathbf{x} = \mathbf{V}\mathbf{V}^T\mathbf{x} = \mathbf{0}$$


$\mathbf{x}$
$\Pi_{\mathbf{V},\mathbf{V}}\mathbf{x}$
$\mathcal{S}_1 = \mathrm{span}(\mathbf{V})$

Proper Orthogonal Decomposition

- POD seeks the subspace $\mathcal{S}$ of a given dimension k minimizing the projection error of the snapshots $\{\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)\}$
- Mathematical formulation $\mathcal{S} = \text{range}(\mathbf{V})$ where

$$\mathbf{V} = \underset{\mathbf{Y}}{\text{argmin}} \sum_{i=1}^{m} \|\mathbf{w}(\boldsymbol{\mu}_i) - \mathbf{\Pi}_{\mathbf{Y},\mathbf{Y}}\mathbf{w}(\boldsymbol{\mu}_i)\|_2^2$$

$$\text{s.t. } \mathbf{Y}^T\mathbf{Y} = \mathbf{I}_k$$

POD by eigenvalue decomposition

- Minimization problem

$$\mathbf{V} = \underset{\mathbf{Y}^T\mathbf{Y}=\mathbf{I}_k}{\operatorname{argmin}} \sum_{i=1}^{m} \|\mathbf{w}(\boldsymbol{\mu}_i) - \boldsymbol{\Pi}_{\mathbf{Y},\mathbf{Y}}\mathbf{w}(\boldsymbol{\mu}_i)\|_2^2$$

- Equivalent maximization problem

$$\begin{aligned}
\mathbf{V} &= \underset{\mathbf{Y}^T\mathbf{Y}=\mathbf{I}_k}{\operatorname{argmax}} \sum_{i=1}^{m} \left\|\mathbf{Y}\mathbf{Y}^T\mathbf{w}(\boldsymbol{\mu}_i)\right\|_2^2 \\
&= \underset{\mathbf{Y}^T\mathbf{Y}=\mathbf{I}_k}{\operatorname{argmax}} \left\|\mathbf{Y}^T\mathbf{W}\right\|_F^2 \\
&= \underset{\mathbf{Y}^T\mathbf{Y}=\mathbf{I}_k}{\operatorname{argmax}} \text{trace}\left(\mathbf{Y}^T\mathbf{W}\mathbf{W}^T\mathbf{Y}\right)
\end{aligned}$$

- Solution: $\mathbf{V}$ is the matrix of eigenvectors $\{\phi_1, \cdots, \phi_k\}$ associated with the k largest eigenvalues of $\mathbf{K} = \mathbf{W}\mathbf{W}^T$

The method of snapshots

- POD: $\mathbf{V}$ is the matrix of eigenvectors $\{\boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_k\}$ associated with the k largest eigenvalues of $\mathbf{K} = \mathbf{W}\mathbf{W}^T$
- $\mathbf{K} \in \mathbb{R}^{N_{\mathbf{w}} \times N_{\mathbf{w}}}$ is a large, dense matrix
- Its rank is at most $m \ll N_{\mathbf{w}}$
- In 1987, Sirovich developed the method of snapshots by noticing that $\mathbf{R} = \mathbf{W}^T\mathbf{W} \in \mathbb{R}^{m \times m}$ has the same non-zero eigenvalues $\{\lambda_i\}_{i=1}^r$ as $\mathbf{K}$
- $r = \text{rank}(\mathbf{R}) \leq m \leq N_{\mathbf{w}}$ and

$$\mathbf{R}\boldsymbol{\psi}_i = \lambda\boldsymbol{\psi}_i, \;\; i = 1, \cdots, r$$

- Exercise: relationship between $\{\boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_r\}$ and $\{\boldsymbol{\psi}_1, \cdots, \boldsymbol{\psi}_r\}$?

The method of snapshots

- Step 1: compute the eigenpairs $\{\lambda_i, \boldsymbol{\psi}_i\}_{i=1}^r$ associated with $\mathbf{R}$

$$\mathbf{R}\boldsymbol{\psi}_i = \lambda\boldsymbol{\psi}_i, \;\; i = 1, \cdots, r$$

- Step 2: compute $\boldsymbol{\phi}_i = \frac{1}{\sqrt{\lambda_i}}\mathbf{W}\boldsymbol{\psi}_i, \; i = 1, \cdots, r$
- In matrix form $\boldsymbol{\Phi} = \mathbf{W}\boldsymbol{\Psi}\boldsymbol{\Lambda}^{-\frac{1}{2}}$
- POD reduced basis of dimension $k \leq r$:

$$\mathbf{V} = [\boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_k]$$

POD by singular value decomposition

- The POD basis $\mathbf{V}$ can also be computed by singular value decomposition (SVD)
- SVD of $\mathbf{W}$:

$$\mathbf{W} = \mathbf{U}_r \boldsymbol{\Sigma}_r \mathbf{Z}_r^T$$

  - $\mathbf{U}_r = [\mathbf{u}_1, \cdots, \mathbf{u}_r] \in \mathbb{R}^{N_{\mathbf{w}} \times r}$: left singular vectors ($\mathbf{U}_r^T \mathbf{U}_r = \mathbf{I}_r$)
  - $\boldsymbol{\Sigma}_r = \text{diag}(\sigma_1, \cdots, \sigma_r) \in \mathbb{R}^{r \times r}$: singular values
  - $\mathbf{Z}_r = [\mathbf{z}_1, \cdots, \mathbf{z}_r] \in \mathbb{R}^{m \times r}$: right singular vectors ($\mathbf{Z}_r^T \mathbf{Z}_r = \mathbf{I}_r$)
- POD reduced basis of dimension $k \leq r$

$$\mathbf{V} = [\mathbf{u}_1, \cdots, \mathbf{u}_k]$$

POD basis size selection

- The POD basis $\mathbf{V}$ can also be computed by singular value decomposition (SVD)
- SVD of $\mathbf{W}$:

$$\mathbf{W} = \mathbf{U}_r \mathbf{\Sigma}_r \mathbf{Z}_r^T$$

- POD reduced basis of dimension $k \leq r$

$$\mathbf{V}_k = [\mathbf{u}_1, \cdots, \mathbf{u}_k]$$

- Relative projection error

$$e(k) = \frac{\|\mathbf{W} - \mathbf{V}_k \mathbf{V}_k^T \mathbf{W}\|_F}{\|\mathbf{W}\|_F} = \sqrt{\frac{\sum_{i=k+1}^r \sigma_i^2}{\sum_{i=1}^r \sigma_i^2}}$$

- Typically k is chosen so that $e(k) < 0.1$

Projection-based model reduction

- High-dimensional model (HDM)

$$\mathbf{A}(\boldsymbol{\mu})\mathbf{w} = \mathbf{b}(\boldsymbol{\mu})$$

- Reduced-order modeling assumption using a reduced basis $\mathbf{V}$

$$\mathbf{w}(\boldsymbol{\mu}) \approx \mathbf{V}\mathbf{q}(\boldsymbol{\mu})$$

  - $\mathbf{q}(\boldsymbol{\mu})$: reduced (generalized) coordinates
- Inserting in the HDM equation

$$\mathbf{A}\mathbf{V}\mathbf{q} \approx \mathbf{b}$$

- $N_{\mathbf{w}}$ equations in terms of k unknowns $\mathbf{q}$
- Associated residual

$$\mathbf{r}(\mathbf{q}) = \mathbf{A}(\boldsymbol{\mu})\mathbf{V}\mathbf{q} - \mathbf{b}(\boldsymbol{\mu})$$

Galerkin projection

- Residual equation

$$\mathbf{r}(\mathbf{q}) = \mathbf{A}(\boldsymbol{\mu})\mathbf{V}\mathbf{q} - \mathbf{b}(\boldsymbol{\mu})$$

- $N_{\mathbf{w}}$ equations with k unknowns
- Galerkin projection enforces the orthogonality of $\mathbf{r}(\mathbf{q})$ to range$(\mathbf{V})$:

$$\mathbf{V}^T\mathbf{r}(\mathbf{q}) = \mathbf{0}$$

- Reduced equations:

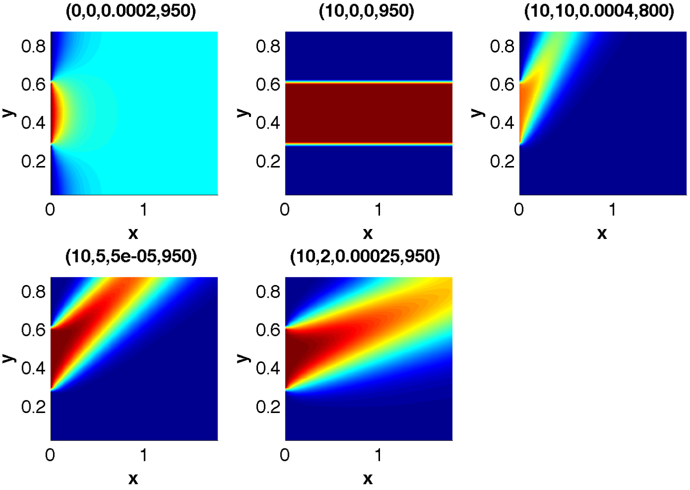
$$\mathbf{V}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{V}\mathbf{q} = \mathbf{V}^T\mathbf{b}(\boldsymbol{\mu})$$

- k equations in terms of k unknowns

$$\mathbf{A}_k(\boldsymbol{\mu})\mathbf{q} = \mathbf{b}_k(\boldsymbol{\mu})$$

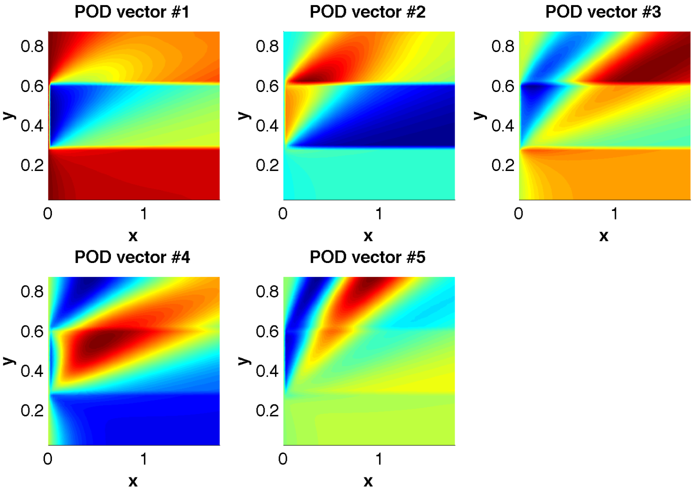
Application to the steady advection diffusion equation

- $m = 5$ snapshots $\{\boldsymbol{\mu}_i\}_{i=1}^{5}$



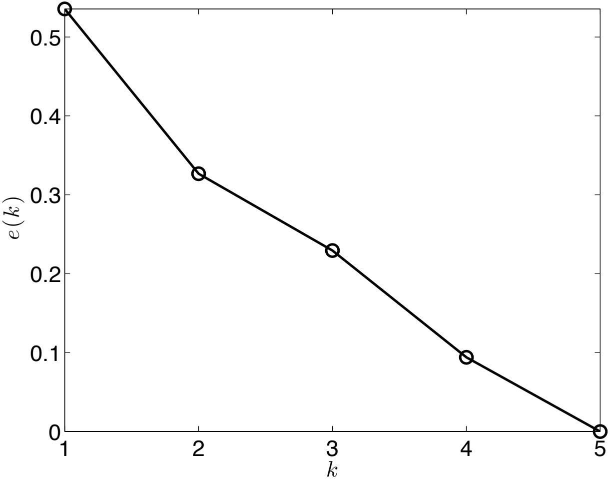
Application to the steady advection diffusion equation

- $m = 5$ snapshots $\{\boldsymbol{\mu}_i\}_{i=1}^5 \Rightarrow$ POD basis of dimension $k = 5$



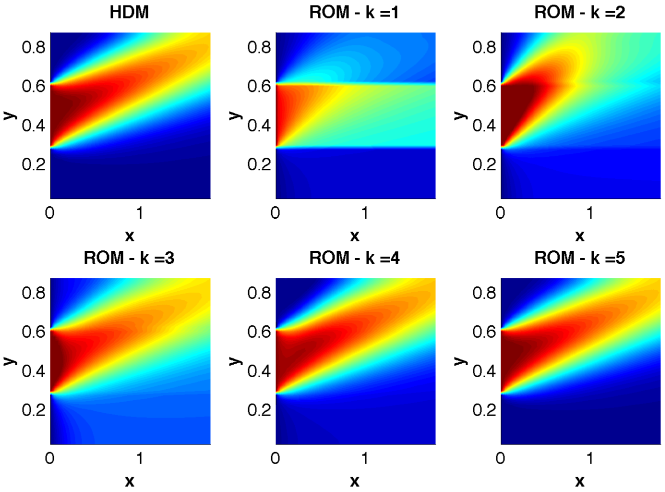
Application to the steady advection diffusion equation

- Projection error



Application to the steady advection diffusion equation

- $\boldsymbol{\mu}_5 = (\mathcal{U}_1, \mathcal{U}_2, \kappa, \boldsymbol{\mu}_{\mathsf{D}}) = (1, 10, 3 \times 10^{-4}, 850)$



Exercise: Petrov-Galerkin projection

- Other approach to get a unique solution to

$$\mathbf{A}(\boldsymbol{\mu})\mathbf{V}\mathbf{q} \approx \mathbf{b}(\boldsymbol{\mu})$$

- Least-squares approach

$$\mathbf{q} = \underset{\mathbf{y}}{\operatorname{argmin}} \|\mathbf{A}(\boldsymbol{\mu})\mathbf{V}\mathbf{y} - \mathbf{b}(\boldsymbol{\mu})\|_2$$

- Exercise: give the equivalent set of equations satisfied by $\mathbf{y}$
- Solution:

$$\mathbf{V}^T\mathbf{A}(\boldsymbol{\mu})^T\mathbf{A}(\boldsymbol{\mu})\mathbf{V}\mathbf{q} = \mathbf{V}^T\mathbf{A}(\boldsymbol{\mu})^T\mathbf{b}(\boldsymbol{\mu})$$

Offline/online decomposition for parametric systems

- Offline phase: computation of $\mathbf{V}$ from snapshots $\{\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)\}$
- Online phase: construction and solution of $\mathbf{V}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{V}\mathbf{q} = \mathbf{V}^T\mathbf{b}(\boldsymbol{\mu})$
- Issue: constructing $\mathbf{A}_k(\boldsymbol{\mu}) = \mathbf{V}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{V}$ and $\mathbf{b}_k(\boldsymbol{\mu}) = \mathbf{V}^T\mathbf{b}(\boldsymbol{\mu})$ is expensive
- Exception in the case of affine parameter dependence: $q_A \ll N_{\mathbf{w}}$ and $q_b \ll N_{\mathbf{w}}$

$$\mathbf{A}(\boldsymbol{\mu}) = \sum_{i=1}^{q_A} f_A^{(i)}(\boldsymbol{\mu})\mathbf{A}^{(i)}, \quad \mathbf{b}(\boldsymbol{\mu}) = \sum_{i=1}^{q_b} f_b^{(i)}(\boldsymbol{\mu})\mathbf{b}^{(i)}$$

- Then

$$\mathbf{A}_k(\boldsymbol{\mu}) = \sum_{i=1}^{q_A} f_A^{(i)}(\boldsymbol{\mu})\mathbf{V}^T\mathbf{A}^{(i)}\mathbf{V}, \quad \mathbf{b}(\boldsymbol{\mu}) = \sum_{i=1}^{q_b} f_b^{(i)}(\boldsymbol{\mu})\mathbf{V}^T\mathbf{b}^{(i)}$$

- The following small dimensional matrices can be computed offline

$$\mathbf{A}_k^{(i)} = \mathbf{V}^T\mathbf{A}^{(i)}\mathbf{V} \in \mathbb{R}^{k\times k}, \; i = 1, \cdots, q_A$$

$$\mathbf{b}_k^{(i)} = \mathbf{V}^T\mathbf{b}^{(i)} \in \mathbb{R}^{k}, \; i = 1, \cdots, q_b$$

Snapshot selection

- For a given number of snapshots m, what are the best snapshot parameter locations
$$\boldsymbol{\mu}_1, \cdots, \boldsymbol{\mu}_m \in \mathcal{D}?$$
- The snapshots $\{\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_m)\}$ should be optimally placed so that they capture the physics over the parameter space $\mathcal{D}$
- Difficult problem $\Rightarrow$ use a heuristic approach (Greedy algorithm)

Greedy approach

- Start by randomly selecting a parameter value $\boldsymbol{\mu}_1$ and compute $\mathbf{w}(\boldsymbol{\mu}_1)$
- For $i = 1, \cdots m$, find the parameter $\boldsymbol{\mu}_i$ which presents the highest error between the ROM solution $\mathbf{Vq}(\boldsymbol{\mu})$ and the HDM solution $\mathbf{w}(\boldsymbol{\mu})$
- This however requires knowing the HDM solution (unknown)
- Instead, for $i = 1, \cdots m$, find the parameter $\boldsymbol{\mu}_i$ for which the residual $\mathbf{r}(\mathbf{q}(\boldsymbol{\mu})) = \mathbf{AVq}(\boldsymbol{\mu}) - \mathbf{b}(\boldsymbol{\mu})$ is the highest

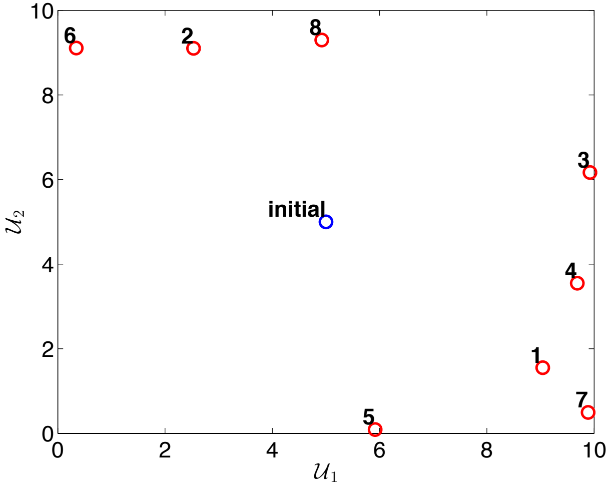
$$\boldsymbol{\mu}_i = \underset{\boldsymbol{\mu} \in \mathcal{D}}{\operatorname{argmin}} \|\mathbf{A}(\boldsymbol{\mu})\mathbf{Vq}(\boldsymbol{\mu}) - \mathbf{b}(\boldsymbol{\mu})\|_2$$

  where $\mathbf{V}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{Vq}(\boldsymbol{\mu}) = \mathbf{V}^T\mathbf{b}(\boldsymbol{\mu})$
- The parameter domain $\boldsymbol{\mu} \in \mathcal{D}$ can be in practice replaced by a search over a finite set

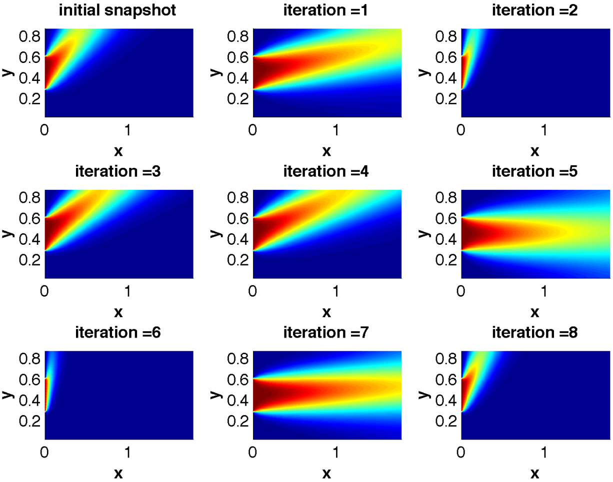
$$\boldsymbol{\mu} \in \{\boldsymbol{\mu}^{(1)}, \cdots, \boldsymbol{\mu}^{(N)}\} \subset \mathcal{D}$$

Application to the steady advection diffusion equation

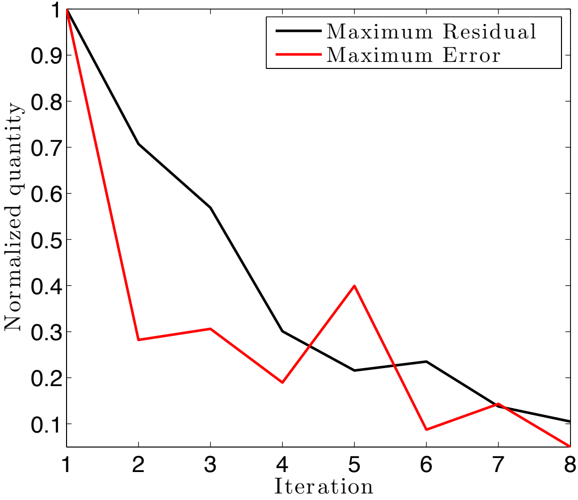
- Parameter domain $(\mathcal{U}_1, \mathcal{U}_2) \in [0, 10] \times [0, 10]$



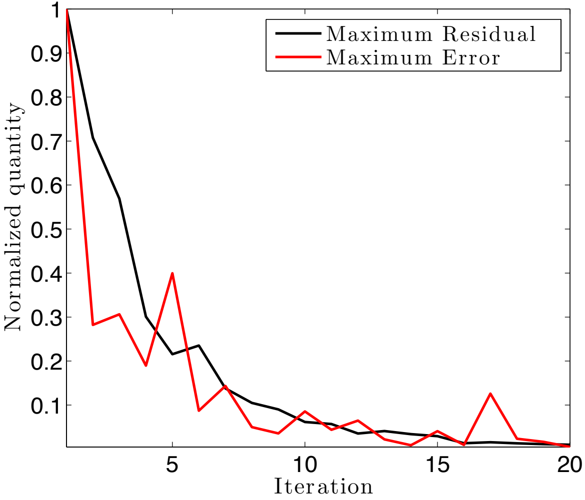
Application to the steady advection diffusion equation



Application to the steady advection diffusion equation



Application to the steady advection diffusion equation



POD in time

- Consider an unsteady linear parametric problem

$$\frac{d\mathbf{w}}{dt}(t) = \mathbf{A}(\boldsymbol{\mu})\mathbf{w}(t) - \mathbf{b}(\boldsymbol{\mu})\mathbf{u}(t)$$

  where $u(t)$ is given for a time interval $t \in [t_0,\ t_{N_t}]$
- For a given parameter $\boldsymbol{\mu}$, POD can also provide an optimal reduced basis associated with the minimization problem

$$\min_{\mathbf{V}^T\mathbf{V}=\mathbf{I}_k} \int_{t_0}^{t_{N_t}} \left\|\mathbf{w}(t,\boldsymbol{\mu}) - \mathbf{V}\mathbf{V}^T\mathbf{w}(t,\boldsymbol{\mu})\right\|_2^2 dt$$

- Solution by the method of snapshots: consider the solutions in time $\mathbf{w}(t_0,\boldsymbol{\mu}), \cdots, \mathbf{w}(t_{N_t},\boldsymbol{\mu})$. An approximation of the minimization problem is

$$\min_{\mathbf{V}^T\mathbf{V}=\mathbf{I}_k} \sum_{i=0}^{N_t} \delta_i \left\|\mathbf{w}(t_i,\boldsymbol{\mu}) - \mathbf{V}\mathbf{V}^T\mathbf{w}(t_i,\boldsymbol{\mu})\right\|_2^2$$

  where $\delta_0, \cdots, \delta_{N_t}$ are appropriate quadrature weights

POD in time (continued)

- Equivalent maximization problem

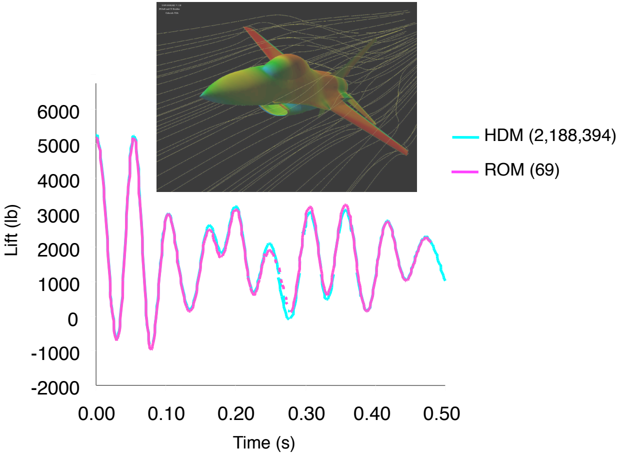
$$\max_{\mathbf{V}^T\mathbf{V}=\mathbf{I}_k} \sum_{i=0}^{N_t} \delta_i \left\|\mathbf{V}^T\mathbf{w}(t_i,\boldsymbol{\mu})\right\|_2^2$$

- Solution by POD by the method of snapshots with the associated snapshot matrix

$$\mathbf{W} = [\sqrt{\delta_0}\mathbf{w}(t_0,\boldsymbol{\mu}),\cdots,\sqrt{\delta_{N_t}}\mathbf{w}(t_{N_t},\boldsymbol{\mu})]$$

POD: Application to linearized aeroelasticity

- $M_\infty = 0.99$
- $N_{\mathbf{w}} = 2,188,394$, $m = 99$ snapshots, $k = 60$ retained POD vectors



Global vs. local strategies

- Global strategy
  - build a ROB $\mathbf{V}$ that captures the behavior of unsteady systems for all $\boldsymbol{\mu} \in \mathcal{D}$
  - POD based on snapshots

$$\{\mathbf{w}(t_0, \boldsymbol{\mu}_1), \cdots, \mathbf{w}(t_{N_t}, \boldsymbol{\mu}_1), \mathbf{w}(t_0, \boldsymbol{\mu}_2), \cdots, \mathbf{w}(t_{N_t}, \boldsymbol{\mu}_m)\}$$

  - not optimal for a given $\boldsymbol{\mu}_i$
- Local strategy
  - build a separate ROB $\mathbf{V}(\boldsymbol{\mu})$ for every value of $\boldsymbol{\mu} \in \mathcal{D}$
  - database approach: build offline a set of ROBs $\{\mathbf{V}(\boldsymbol{\mu}_i)\}_{i=1}^{m}$ and use them online to build $\mathbf{V}(\boldsymbol{\mu})$ for $\boldsymbol{\mu} \in \mathcal{D}$
  - each ROB $\mathbf{V}(\boldsymbol{\mu}_i)$ is optimal at $\boldsymbol{\mu} = \boldsymbol{\mu}_i$
  - requires an adaptation approach online (see Lecture 3)

References

- Lecture notes on projection-based model reduction: http://www.stanford.edu/∼amsallem/CA-CME345-Ch3.pdf
- Lecture notes on POD: http://www.stanford.edu/∼amsallem/CA-CME345-Ch4.pdf
- Holmes, P., Lumley, J., and Berkooz, G., Turbulence, Coherent Structures, Dynamical Systems and Symmetry, Cambridge Univ. Press, Cambridge, England, U.K., 1996.
- Sirovich, L.: Turbulence and the dynamics of coherent structures. Part I: coherent structures. Quarterly of applied mathematics 45(3), 561-571 (1987).
- Patera A. and Rozza G., Reduced Basis Approximation and a Posteriori Error Estimation for Parametrized Partial Differential Equations, Version 1.0, Copyright MIT 2006, to appear in (tentative rubric) MIT Pappalardo Graduate Monographs in Mechanical Engineering.
- Haasdonk, B., Ohlberger, M.: Efficient reduced models and a-posteriori error estimation for parametrized dynamical systems by offline/online decomposition. Stuttgart Research Centre for Simulation Technology (SRC SimTech) Preprint Series 23 (2009)