Proper Orthogonal Decomposition (POD) for Nonlinear Dynamical Systems

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Outline of the talk

- POD and singular value decomposition (SVD)
- Snapshot POD for nonlinear dynamical systems
- Reduced-order modeling (ROM)
- Numerical examples: heat flow, Burgers equation, Navier-Stokes equations
- Continuous POD for nonlinear dynamical systems
- Numerical examples

POD as a minimizing problem

- Given: $y_1, \ldots, y_n \in \mathbb{R}^m$; set $\mathcal{V} = \operatorname{span}\{y_1, \ldots, y_n\} \subset \mathbb{R}^m$
- Goal: Find $\ell \le \dim \mathcal{V}$ orthonormal vectors $\{\psi_i\}_{i=1}^{\ell}$ in $\mathbb{R}^m$ minimizing

$$J(\psi_1, \ldots, \psi_\ell) = \sum_{j=1}^{n} \Big\| y_j - \sum_{i=1}^{\ell} (y_j^T \psi_i) \psi_i \Big\|^2 \longrightarrow \min!$$

with the Euclidean norm $\|y\| = \sqrt{y^T y}$

- Constrained optimization:

$$\min J(\psi_1, \ldots, \psi_\ell) \quad \text{subject to} \quad \psi_i^T \psi_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

Necessary optimality conditions (Part 1)

- Lagrange functional:

$$L(\psi_1, \ldots, \psi_\ell, \lambda_{11}, \ldots, \lambda_{\ell\ell}) = J(\psi_1, \ldots, \psi_\ell) + \sum_{i,j=1}^{\ell} \lambda_{ij}\big(\psi_i^T \psi_j - \delta_{ij}\big)$$

with the Kronecker symbol $\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ otherwise

- Optimality conditions:

$$\begin{aligned} \frac{\partial L}{\partial \psi_i}(\psi_1, \ldots, \psi_\ell, \lambda_{11}, \ldots, \lambda_{\ell\ell}) &= 0 \in \mathbb{R}^m \qquad \text{for } i = 1, \ldots, \ell \\ \frac{\partial L}{\partial \lambda_{ij}}(\psi_1, \ldots, \psi_\ell, \lambda_{11}, \ldots, \lambda_{\ell\ell}) &= 0 \in \mathbb{R} \qquad \text{for } i, j = 1, \ldots, \ell \end{aligned}$$

Necessary optimality conditions (Part 2)

- $L(\psi_1,\ldots,\psi_\ell,\lambda_{11},\ldots,\lambda_{\ell\ell}) = J(\psi_1,\ldots,\psi_\ell) + \sum_{i,j=1}^{\ell} \lambda_{ij}\big(\psi_i^T\psi_j - \delta_{ij}\big)$
- $\dfrac{\partial L}{\partial \psi_i} = 0 \quad \Leftrightarrow \quad \sum_{j=1}^{n} y_j(y_j^T\psi_i) = \lambda_{ii}\psi_i$ and $\lambda_{ij} = 0$ for $i \neq j$
- $\dfrac{\partial L}{\partial \lambda_{ij}} = 0 \quad \Leftrightarrow \quad \psi_i^T\psi_j = \delta_{ij}$
- Setting $\lambda_i = \lambda_{ii}$ and $Y = [y_1,\ldots,y_n] \in \mathbb{R}^{m\times n}$ we have

  $$YY^T\psi_i = \lambda_i\psi_i \quad \text{for } i = 1,\ldots,\ell$$

  i.e., necessary optimality conditions are given by a symmetric $m\times m$ eigenvalue problem
- Here: necessary optimality conditions are already sufficient.

Computation of the POD basis (Part 1)

- Optimality conditions: $YY^T\psi_i = \lambda_i\psi_i$ for $i = 1, \ldots, \ell$
- Solution by SVD for $Y \in \mathbb{R}^{m\times n}$: $d = \mathrm{rank}\ Y$, $\sigma_1 \geq \ldots \geq \sigma_d > 0$, $U = [u_1, \ldots, u_m] \in \mathbb{R}^{m\times m}$ und $V = [v_1, \ldots, v_n] \in \mathbb{R}^{n\times n}$ orthogonal with

$$U^T YV = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} = \Sigma \in \mathbb{R}^{m\times n}$$

where $D = \mathrm{diag}\,(\sigma_1, \ldots, \sigma_d) \in \mathbb{R}^{d\times d}$. Moreover, for $1 \leq i \leq d$

$$Yv_i = \sigma_i u_i, \;\; Y^T u_i = \sigma_i v_i, \;\; YY^T u_i = \sigma_i^2 u_i, \;\; Y^T Yv_i = \sigma_i^2 v_i$$

- POD basis: $\psi_i = u_i$ and $\lambda_i = \sigma_i^2 > 0$ for $i = 1, \ldots, \ell \leq d = \dim \mathcal{V}$

Computation of the POD basis (Part 2)

- Data ensemble: $\mathcal{V} = \mathrm{span}\,\{y_1, \ldots, y_n\} \subset \mathbb{R}^m$ and $d = \dim \mathcal{V}$
  POD basis of rank ℓ: $\psi_i = u_i$ and $\lambda_i = \sigma_i^2 > 0$ for $i = 1, \ldots, \ell \le d$
- Three choices to compute the ψ_i's
  SVD for $Y \in \mathbb{R}^{m\times n}$: $Yv_i = \sigma_i u_i$
  EVD for $YY^T \in \mathbb{R}^{m\times m}$: $YY^T u_i = \sigma_i^2 u_i$ (if $m \ll n$)
  EVD for $Y^TY \in \mathbb{R}^{n\times n}$: $Y^TYv_i = \sigma_i^2 v_i$ and $u_i = \frac{1}{\sigma_i} Yv_i$ (if $m \gg n$)
- Error formula for the POD basis of rank ℓ:

$$J(\psi_1, \ldots, \psi_\ell) = \sum_{j=1}^{n} \Big\| y_j - \sum_{i=1}^{\ell} \big(y_j^T \psi_i\big)\psi_i \Big\|^2 = \sum_{i=\ell+1}^{d} \lambda_i$$

Computation of the POD basis (Part 3)

- Error formula for the POD basis of rank ℓ:

$$J(\psi_1,\ldots,\psi_\ell)=\sum_{j=1}^{n}\Big\|y_j-\sum_{i=1}^{\ell}\big(y_j^T\psi_i\big)\psi_i\Big\|^2=\sum_{i=\ell+1}^{d}\lambda_i$$

- $YY^T\psi_i=\lambda_i\psi_i$, $1\le i\le\ell$, and $YY^T\psi_i=\sum_{j=1}^{n}\big(y_j^T\psi_i\big)y_j$ give

$$\lambda_i=\lambda_i\psi_i^T\psi_i=\big(YY^T\psi_i\big)^T\psi_i=\Big(\sum_{j=1}^{n}\big(y_j^T\psi_i\big)y_j\Big)^T\psi_i=\sum_{j=1}^{n}\big(y_j^T\psi_i\big)^2$$

- $y_j=\sum_{i=1}^{d}\big(y_j^T\psi_i\big)\psi_i$, $j=1,\ldots,m$, and $\psi_i^T\psi_j=\delta_{ij}$ imply

$$\sum_{j=1}^{n}\Big\|y_j-\sum_{i=1}^{\ell}\big(y_j^T\psi_i\big)\psi_i\Big\|^2=\sum_{j=1}^{n}\sum_{i=\ell+1}^{d}\big|y_j^T\psi_i\big|^2=\sum_{i=\ell+1}^{d}\lambda_i$$

Snapshot POD for dynamical systems

- Nonlinear dynamical system in a Hilbert space X:

$$\dot{y}(t) = f(t, y(t)) \text{ for } t \in (0, T) \quad \text{and} \quad y(0) = y_\circ$$

  with continuous $f : [0, T] \times X \to X$ and given $y_\circ \in X$

- Time grid: $0 \leq t_1 < t_2 < \ldots t_n \leq T$, $\delta t_j = t_j - t_{j-1}$ for $2 \leq j \leq n$
- Available or known snapshots: $y_j = y(t_j) \in X$, $1 \leq j \leq n$
- Snapshot ensemble: $\mathcal{V} = \text{span}\,\{y_1, \ldots, y_n\} \subset X$, $d = \dim \mathcal{V} \leq n$
- POD basis of rank $\ell < d$: with weights $\alpha_j \geq 0$

$$\min \sum_{j=1}^{n} \alpha_j \Big\| y_j - \sum_{i=1}^{\ell} \langle y_j, \psi_i \rangle_X \psi_i \Big\|_X^2 \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle_X = \delta_{ij}$$

- Application: $X = \mathbb{R}^m$ and $\alpha_j = 1$ for $1 \leq j \leq n$

Computation of the POD basis

- EVD for linear and symmetric $\mathcal{R}^n$ in X:

$$\mathcal{R}^n u_i = \sum_{j=1}^{n} \alpha_j \langle u_i, y_j \rangle_X y_j = \sigma_i^2 u_i \qquad (YY^T u_i = \sigma_i^2 u_i)$$

and set $\lambda_i = \sigma_i^2$, $\psi_i = u_i$

- EVD for linear and symmetric $\mathcal{K}^n = \big(\big(\alpha_j \langle y_j, y_i \rangle_X\big)\big)$ in $\mathbb{R}^n$:

$$\mathcal{K}^n v_i = \sigma_i^2 v_i \qquad (Y^T Y v_i = \sigma_i^2 v_i)$$

and set $\lambda_i = \sigma_i^2$, $\psi_i = \frac{1}{\sqrt{\lambda_i}} \sum_{j=1}^{n} \alpha_j (v_i)_j\, y_j$

- Error formula for the POD basis of rank ℓ:

$$\sum_{j=1}^{n} \alpha_j \Big\| y_j - \sum_{i=1}^{\ell} \langle y_j, \psi_i \rangle_X \psi_i \Big\|_X^2 = \sum_{i=\ell+1}^{d} \lambda_i$$

ROM (Part 1)

- Heat equation (for instance):

$$\begin{aligned} y_t - \Delta y &= f && \text{in } Q = (0,T)\times\Omega \\ \frac{\partial y}{\partial n} &= g && \text{on } \Sigma = (0,T)\times\Gamma \\ y(0) &= y_\circ && \text{in } \Omega \end{aligned}$$

- Variational formulation: $V = H^1(\Omega)$, $y(t) \in V$

$$\int_\Omega y_t(t)\varphi + \nabla y(t)\cdot\nabla\varphi \,\mathrm{d}x = \int_\Omega f(t)\varphi\,\mathrm{d}x + \int_\Gamma g(t)\varphi\,\mathrm{d}s \quad \forall\varphi\in V$$

- FE discretization: $y^m(t) \in V^m = \operatorname{span}\{\varphi_1,\ldots,\varphi_m\} \subset V$

$$\int_\Omega y_t^m(t)\varphi + \nabla y^m(t)\cdot\nabla\varphi\,\mathrm{d}x = \int_\Omega f(t)\varphi\,\mathrm{d}x + \int_\Gamma g(t)\varphi\,\mathrm{d}s \;\forall\varphi\in V^m$$

ROM (Part 2)

- Time grid: $0 \le t_1 < t_2 < \ldots t_n \le T$, $\delta t_j = t_j - t_{j-1}$ for $2 \le j \le n$
- FE snapshots: $y_j = y^m(t_j) \in V = H^1(\Omega)$, $1 \le j \le n$
- Topology: $V \subset H = L^2(\Omega)$, $X = H$ or $X = V$
- Sizes: $\#$ FE's $\gg$ $\#$ time instances, i.e., $m \gg n$
- Computation of the correlation $\mathcal{K}^n$: $\alpha_j = \frac{1}{n}$

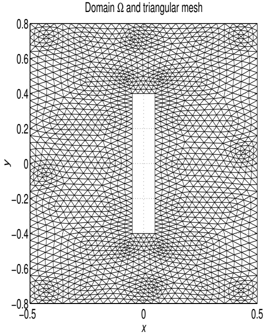
$$\tfrac{1}{n}\,\langle y_j^m, y_i^m\rangle_X = \frac{1}{n}\sum_{k,l=1} Y_{ik} Y_{jl}\langle \varphi_l, \varphi_k\rangle_X = \Big(\tfrac{1}{n} Y^T M Y\Big)_{ij}$$

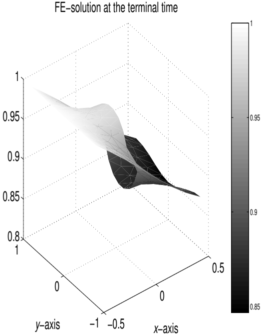
with $M_{ij} = \langle \varphi_j, \varphi_i\rangle_X$ (mass $[X = H]$ or stiffness matrix $[X = V]$)
- ROM for heat equation: $y^\ell(t) \in V^\ell = \mathrm{span}\,\{\psi_1, \ldots, \psi_\ell\} \subset V^m$

$$\int_\Omega y_t^\ell(t)\psi + \nabla y^\ell(t)\cdot\nabla\psi\,\mathrm{d}x = \int_\Omega f(t)\psi\,\mathrm{d}x + \int_\Gamma g(t)\psi\,\mathrm{d}s \;\; \forall \psi \in V^\ell$$

Heat flow in a block (Part 1)

$$
\begin{aligned}
y_t - \Delta y &= 0 && \text{in } Q = (0,5) \times \Omega \\
y &= 1 && \text{on } \Gamma_1 = \{(-0.5, y) : -0.8 \le y \le 0.8\} \\
\frac{\partial y}{\partial n} &= -0.1 && \text{on } \Gamma_2 = \{(0.5, y) : -0.8 \le y \le 0.8\} \\
\frac{\partial y}{\partial n} &= 0 && \text{on } \partial\Omega \setminus (\Gamma_1 \cup \Gamma_2) \\
y(0,\cdot) &= 0 && \text{in } \Omega \subset \mathbb{R}^2
\end{aligned}
$$





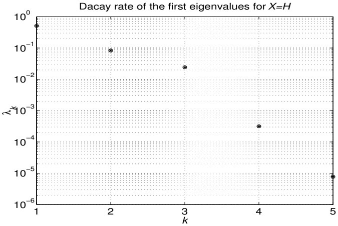
Triangulation of Ω and FE solution at $T = 5$ computed with 1844 degrees of freedom, backward Euler and $n = 126$ equidistant time instances $0 = t_1 < \ldots < t_n = 5$

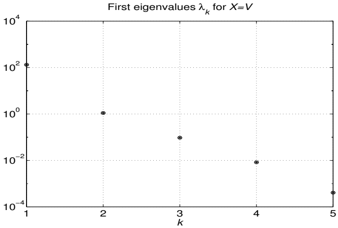
Heat flow in a block (Part 2)

- FE space $V^m = \mathrm{span}\,\{\varphi_1, \ldots, \varphi_m\} \subset H^1(\Omega) \subset L^2(\Omega)$, $m = 1844$
- Time grid: $T = 5$, $n = 126$, $\delta t = \frac{T}{n-1}$, $t_j = (j-1)\delta t$, $1 \le j \le n$
- Snapshots: $y_j^m = \sum_{i=1}^{m} Y_{ij}\varphi_i$, $1 \le j \le n$
- Topology for POD: $X = L^2(\Omega)$ or $X = H^1(\Omega)$
- Computation of the correlation matrix $(m \gg n)$: $\mathcal{K}^n = \frac{1}{n} Y^T M Y$ with $M = ((\langle \varphi_j, \varphi_i \rangle_X))$
- EVD for $\mathcal{K}^n$: $\big(\frac{1}{n} Y^T M Y\big) v_i = \lambda_i v_i$ and $\psi_i = \frac{1}{n\sqrt{\lambda_i}} \sum_{j=1}^{n} (v_i)_j\, y_j^m \in V^m$

Heat flow in a block (Part 3)

- Decay of the first eigenvalues for $X = L^2(\Omega)$ and $X = H^1(\Omega)$



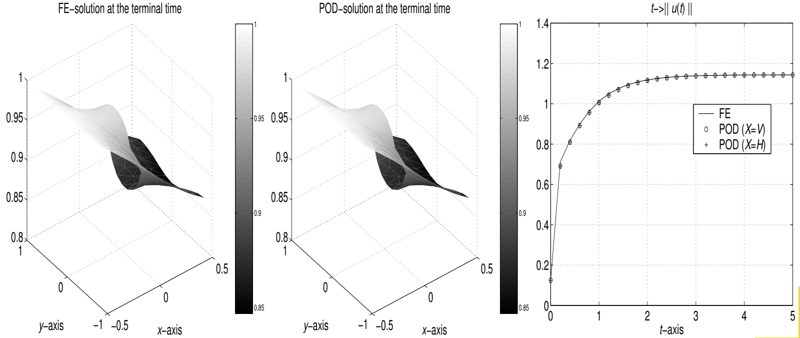


- Rapid decay of the eigenvalues, e.g., for $\ell = 5$

$$\frac{1}{n} \sum_{j=1}^{n} \Big\| y_j^m - \sum_{i=1}^{5} \langle y_j^m, \psi_i \rangle_X \psi_i \Big\|_X^2 = \sum_{i=6}^{126} \lambda_i < 2 \cdot 10^{-6}$$

Heat flow in a block (Part 4)

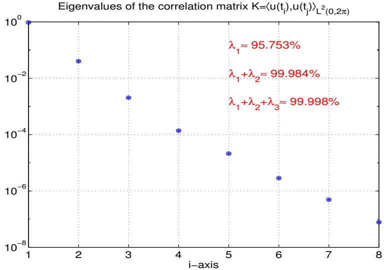
- ROM: $\ell = 5$ POD basis functions, $X = L^2(\Omega)$ and $X = H^1(\Omega)$
- FE-/POD-solution and error:

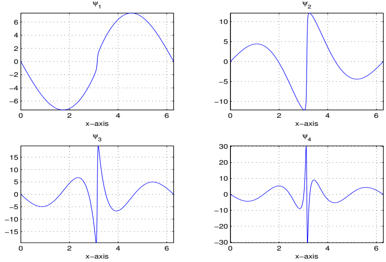


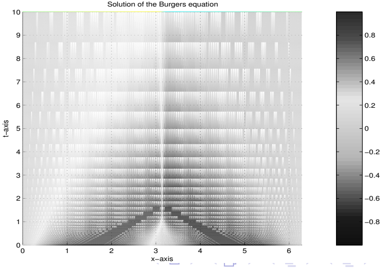
Burgers equation

$$
\begin{aligned}
y_t - \nu y_{xx} + y y_x &= f && \text{in } Q = (0,T) \times \Omega \\
y(\cdot, 0 = y(\cdot, 1) &= 0 && \text{on } (0,T) \\
y(0, \cdot) &= y_\circ && \text{in } \Omega = (0, 2\pi) \subset \mathbb{R}
\end{aligned}
$$

- $y_\circ(x) = \sin(x)$ and $\nu = 0.01$
- 1258 finite elements
- Time integration with Matlab's ode15s
- Snapshots $\mathcal{V} = \mathrm{span}\,\{y(t_1), \ldots, y(t_{100})\}$

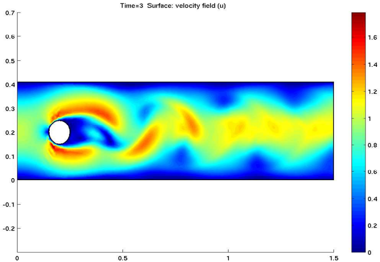




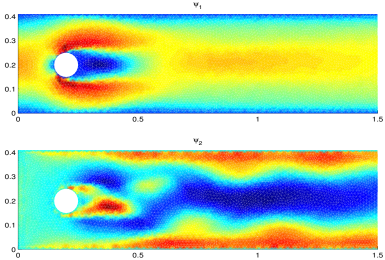


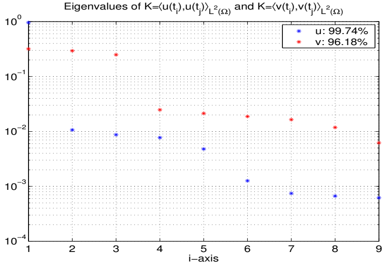
Navier-Stokes equation

$$\begin{aligned} u_t + uu_x + vu_y + p_x &= \nu\Delta u && \text{in } Q = (0,T)\times\Omega \\ v_t + uv_x + vv_y + p_y &= \nu\Delta v && \text{in } Q \\ u_x + v_y &= 0 && \text{in } Q \end{aligned}$$



- $\nu = 5 \cdot 10^{-3}$
- 3×4804 finite elements (Femlab)
- Time integration with Matlab's ode15s
- Snapshots $\mathcal{V}(u) = \text{span}\,\{u(t_1),\dots,u(t_{21})\}$ and $\mathcal{V}(v) = \text{span}\,\{v(t_1),\dots,v(t_{21})\}$

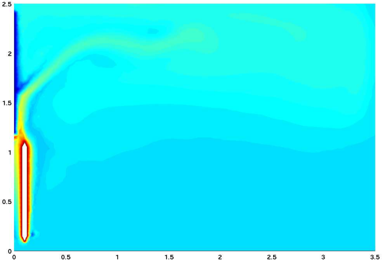


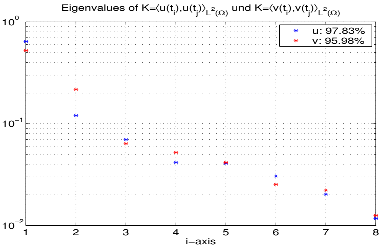


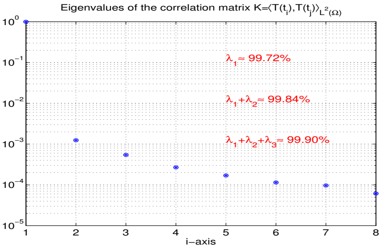
Energy transport (Boussinesq)

$$
\begin{aligned}
u_t + uu_x + vu_y + p_x &= \nu\Delta u && \text{in } Q\\
v_t + uv_x + vv_y + p_y &= \nu\Delta v + \beta\theta && \text{in } Q\\
u_x + v_y &= 0 && \text{in } Q\\
\theta_t + u\theta_x + v\theta_y &= \alpha\Delta\theta && \text{in } Q
\end{aligned}
$$

- $\alpha = 10^{-5}$, $\beta = 10^{-2}$, $\nu = 10^{-4}$
- 4×3512 finite elements (Femlab)
- Time integration with Matlab's ode15s
- Snapshots at $t_1, \ldots, t_{21}$ for u, v and θ







Discussions

- Problems:

  Choice of the grid $0 \le t_1 < \ldots < t_n \le T$, i.e., of the snapshots
  Dependence of $\{(\lambda_i, \psi_i)\}_{i=1}^{\ell}$ on the time grid $\{t_j\}_{j=1}^{n}$
  Choice for the weights α_j

- Procedere: continuous version of POD

Continuous POD for dynamical system

- Nonlinear dynamical system in a Hilbert space X:

$$\dot{y}(t) = f(t, y(t)) \text{ for } t \in (0, T) \quad \text{and} \quad y(0) = y_\circ$$

with continuous $f : [0, T] \times X \to X$ and given $y_\circ \in X$

- Available or known snapshots: $y(t) \in X$ for all $t \in [0, T]$
- Snapshot ensemble: $\mathcal{V} = \{y(t) \,|\, t \in [0, T]\} \subset X$, $d = \dim \mathcal{V} \leq \infty$
- POD basis of rank $\ell < d$:

$$\min \int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i \rangle_X \psi_i \Big\|_X^2 \,\mathrm{d}t \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle_X = \delta_{ij}$$

Computation of the POD basis

- EVD for linear and symmetric $\mathcal{R}$ in X:

$$\mathcal{R}u_i = \int_0^T \langle u_i, y(t)\rangle_X y(t)\,\mathrm{d}t = \sigma_i^2 u_i \qquad (YY^T u_i = \sigma_i^2 u_i)$$

and set $\lambda_i^\infty = \sigma_i^2$, $\psi_i^\infty = u_i$

- EVD for linear and symmetric $\mathcal{K}$ in $L^2(0,T)$:

$$(\mathcal{K}v_i)(t) = \int_0^T \langle y(s), y(t)\rangle_X v_i(s)\,\mathrm{d}t = \sigma_i^2 v_i(t) \quad (Y^T Y v_i = \sigma_i^2 v_i)$$

and set $\lambda_i^\infty = \sigma_i^2$, $\psi_i^\infty = \frac{1}{\sqrt{\lambda_i^\infty}} \sum_{j=1}^n \alpha_j (v_i)_j y_j$

- Error formula for the POD basis of rank ℓ:

$$\int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i^\infty\rangle_X \psi_i^\infty \Big\|_X^2 \mathrm{d}t = \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

Relation to Snapshot POD

- Operators $\mathcal{R}^n$ and $\mathcal{R}$:

$$\mathcal{R}^n\psi = \sum_{j=1}^{n} \alpha_j \langle \psi, y_j \rangle_X y_j \qquad \text{for } \psi \in X$$

$$\mathcal{R}\psi = \int_0^T \langle \psi, y(t) \rangle_X y(t)\,\mathrm{d}t \qquad \text{for } \psi \in X$$

- Convergence of $\|\mathcal{R} - \mathcal{R}^n\|$: $y_j = y(t_j)$ and appropriate α_j's
- Perturbation theory [Kato]:

$$\lambda_i \stackrel{n\to\infty}{\longrightarrow} \lambda_i^\infty \qquad \text{for } 1 \le i \le \ell$$

$$\psi_i \stackrel{n\to\infty}{\longrightarrow} \psi_i^\infty \qquad \text{for } 1 \le i \le \ell$$

$$\sum_{i=1}^{d(n)} \lambda_i \stackrel{n\to\infty}{\longrightarrow} \sum_{i=1}^{\infty} \lambda_i^\infty$$

Relation to Snapshot POD

- Choice of times: capture the dynamics $y([0,T])$ as good as possible
- Choice of weights: ensure operator convergence $\mathcal{R}^n \to \mathcal{R}$

- Burgers equation:

$$
\begin{aligned}
y_t - \nu y_{xx} + y y_x &= f && \text{in } Q = (0,T)\times\Omega\\
y(\cdot,0 = y(\cdot,1) &= 0 && \text{on } (0,T)\\
y(0,\cdot) &= 0 && \text{in } \Omega = (0,1) \subset \mathbb{R}
\end{aligned}
$$

- exact solution $y(t,x) = (x^2 - x)\sin(2\pi t)$ and $f = y_t - \nu y_{xx} + y y_x$
- FE with error $< 10^{-10}$ and fine time grid with $n = 5\cdot 2^{11}$, $\delta t = \frac{T}{n}$
- Snapshots at $t_1^i, \ldots, t_{n_i}^i$ with $\delta t^i = 2^{11-i}\,\delta t$, $t_j^i = j\delta t^i$, $0 \le i \le 11$
- Error: $e(n_i) = \delta t^i \sum_{j=1}^{n_i} \|y_{FE}(t_j^i) - y_{POD}(t_j^i)\|^2_{L^2(\Omega)}$
- Implicit Euler: error $O(\delta t) \Rightarrow e(n_i) \approx O(\delta t_i^2) = O\left(\frac{1}{n_i^2}\right)$
- Quotient: $n_i^2 = 4n_{i-1}^2 \Rightarrow \frac{e(n_{i-1})}{e(n_i)} \approx 4$

i	1	2	3	4	5	6	7	8	9	10	11
$\frac{e(n_{i-1})}{e(n_i)}$	3.11	3.55	3.77	3.88	3.94	3.96	3.97	3.98	3.98	3.96	3.92

References

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