Error estimates for POD Galerkin schemes

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Motivation

- 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 $\delta t^i = 2^{11-i}\,\delta t$, $t_j^i = j\delta t^i$, $1 \le i \le 11$
- Error: $e(n_i) = \delta t^i \sum_{j=1}^{n_i} \int_\Omega \left| y_{FE}(t_j^i, x) - y^\ell(t_j^i, x)\right|^2 \mathrm{d}x$
- Implicit Euler: error $O(\delta t) \Rightarrow e(n_i) \approx O(\delta t_i^2) = O\big(\frac{1}{n_i^2}\big)$
- 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

Outline

- POD method: discrete and continuous version
- Reduced-order modeling for ODE system
- Error analysis
- Numerical examples:
  - laser surface hardening
  - heat equation
  - parameter dependent elliptic PDEs

POD method (discrete version)

- Snapshots: $y_1, \dots, y_n$
- Snapshot ensemble: $\mathcal{V} = \operatorname{span}\{y_1, \dots, y_n\}$, $d = \dim \mathcal{V} \le n$
- Inner product: $\langle \cdot\,, \cdot \rangle$, e.g., $\langle u, v \rangle = u^T v$ for $u, v \in \mathbb{R}^N$
- POD basis of any rank $\ell \in \{1, \dots, d\}$: with weights $\alpha_j \ge 0$

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

- Constrained optimization:

$$\min J(\psi_1, \dots, \psi_\ell) \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

s.t. — subject to

Optimality conditions and computation of POD basis

- EVP for linear and symmetric $\mathcal{R}^n$:

$$\mathcal{R}^n u_i = \sum_{j=1}^{n} \alpha_j \langle u_i, y_j \rangle y_j = \lambda_i u_i$$

and set $\psi_i = u_i$

- EVP for linear, symmetric $n \times n$-matrix $\mathcal{K}^n = ((\langle y_j, y_i \rangle))$:

$$\mathcal{K}^n v_i = \lambda_i v_i$$

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

- Error for the POD basis of rank ℓ:

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

Continuous POD in Hilbert spaces [Henri/Yvon, Kunisch/V., ...]

- Snapshots: $y(\mu)$ for all $\mu \in \mathcal{I}$ ($\mathcal{I} = [0, T]$ or $\mathcal{I} = \mathcal{D}$)
- Snapshot ensemble: $\mathcal{V} = \{y(\mu) \,|\, \mu \in \mathcal{I}\}$, $d = \dim \mathcal{V} \leq \infty$
- POD basis of rank $\ell < d$:

$$\min \int_{\mathcal{I}} \Big\| y(\mu) - \sum_{i=1}^{\ell} \langle y(\mu), \psi_i \rangle \, \psi_i \Big\|^2 \mathrm{d}\mu \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle = \delta_{ij}$$

- Optimality conditions: EVP for linear, symmetric, compact $\mathcal{R}$

$$\mathcal{R}\psi_i^\infty = \int_{\mathcal{I}} \langle \psi_i^\infty, y(\mu) \rangle \, y(\mu) \, \mathrm{d}\mu = \lambda_i^\infty \psi_i^\infty \quad \text{for } i \in \mathbb{N}$$

- Error for the POD basis of rank ℓ:

$$\int_{\mathcal{I}} \Big\| y(\mu) - \sum_{i=1}^{\ell} \langle y(\mu), \psi_i^\infty \rangle \psi_i^\infty \Big\|^2 \mathrm{d}\mu = \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

Relationship between 'discrete' and continuous POD

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

$$\mathcal{R}^n\psi = \sum_{j=1}^{n} \alpha_j \, \langle \psi, y(\mu_j)\rangle y(\mu_j)$$

$$\mathcal{R}\psi = \int_{\mathcal{I}} \langle \psi, y(\mu)\rangle y(\mu)\,\mathrm{d}\mu$$

- Operator convergence of $\mathcal{R}^n - \mathcal{R}$: y smooth and appropriate α_j's
- Perturbation theory [Kato]: $(\lambda_i, \psi_i) \stackrel{n\to\infty}{\longrightarrow} (\lambda_i^\infty, \psi_i^\infty)$ for $1 \le i \le \ell$
- Choice of the weights α_j?: ensure convergence $\mathcal{R}^n \stackrel{n\to\infty}{\longrightarrow} \mathcal{R}$

Reduced-order modelling for ODE system

- Initial value problem in $\mathbb{R}^N$:

$$\dot{y}(t) = Ay(t) + f(t, y(t)) \qquad \text{for } t \in (0, T],$$
$$y(0) = y_0$$

  for $y_0 \in \mathbb{R}^N$ and continuous $f : [0, T] \times \mathbb{R}^N \to \mathbb{R}^N$

- Snapshots: $y(t) \in \mathbb{R}^N$ for all $t \in [0, T]$
- Inner product: $\langle u, v \rangle = u^T v$ (Euclidean product)
- POD basis of rank $\ell \leq N$: $\psi_1, \ldots, \psi_\ell \in \mathbb{R}^N$
- Galerkin ansatz: $y^\ell(t) = \sum_{j=1}^{\ell} \big(y^\ell(t)^T \psi_j\big)\psi_j = \sum_{j=1}^{\ell} \mathrm{y}_j^\ell(t)\psi_j$
- Galerkin projection of the ODE:

$$\psi_i^T \dot{y}^\ell(t) = \psi_i^T A y^\ell(t) + \psi_i^T f(t, y^\ell(t)), \quad t \in (0, T], \ i = 1, \ldots, \ell$$
$$\psi_i^T y^\ell(0) = \psi_i^T y_0, \qquad i = 1, \ldots, \ell$$

POD Galerkin projection of the ODE

- Galerkin projection of the ODE: $f \equiv 0$

$$\psi_i^T \dot{y}^\ell(t) = \psi_i^T A y^\ell(t), \qquad t \in (0,T],\ i = 1,\dots,\ell$$
$$\psi_i^T y^\ell(0) = \psi_i^T y_0 \qquad i = 1,\dots,\ell$$

- Inserting Galerkin ansatz:

$$\psi_i^T \dot{y}^\ell(t) = \sum_{j=1}^{\ell} \dot{\mathrm{y}}_j^\ell(t)\psi_i^T\psi_j = \dot{\mathrm{y}}_i^\ell(t)$$

$$\psi_i^T A y^\ell(t) = \psi_i^T \left(\sum_{j=1}^{\ell} \mathrm{y}_j^\ell(t) A\psi_j \right) = \sum_{j=1}^{\ell} \mathrm{y}_j^\ell(t)\psi_i^T A\psi_j$$

- ROM in $\mathbb{R}^\ell$: $\mathrm{y}^\ell = (\mathrm{y}_i^\ell)$, $A^\ell = ((\psi_i^T A\psi_j))$, $y_0^\ell = (\psi_i^T y_0)$

$$\dot{\mathrm{y}}^\ell(t) = A^\ell \mathrm{y}(t) \qquad \text{for } t \in (0,T]$$
$$\mathrm{y}^\ell(0) = y_0^\ell$$

Error analysis — Part 1

- Goal: estimate $\displaystyle\int_0^T \|y(t) - y^\ell(t)\|^2_{\mathbb{R}^N}\,\mathrm{d}t$
- Orthogonal projector onto $V^\ell = \mathrm{span}\,\{\psi_i\}_{i=1}^\ell$:

$$\mathcal{P}^\ell\psi = \sum_{j=1}^{\ell} \left(\psi^T\psi_i\right)\psi_i \quad \text{for } \psi \in \mathbb{R}^N$$

$\Rightarrow y^\ell(0) = \mathcal{P}^\ell y_0 = \mathcal{P}^\ell y(0)$

- POD basis:

$$\int_0^T \left\| y(t) - \sum_{i=1}^{\ell} \left(y(t)^T\psi_i\right)\psi_i \right\|^2 \mathrm{d}t = \int_0^T \left\| y(t) - \mathcal{P}^\ell y(t) \right\|^2 \mathrm{d}t$$

- Decomposition:

$$y(t) - y^\ell(t) = \underbrace{y(t) - \mathcal{P}^\ell y(t)}_{\in (V^\ell)^\perp} + \underbrace{\mathcal{P}^\ell y(t) - y^\ell(t)}_{\in V^\ell} = \varrho^\ell(t) + \vartheta^\ell(t)$$

Error analysis — Part 2

- Decomposition:

$$y(t) - y^\ell(t) = y(t) - \mathcal{P}^\ell y(t) + \mathcal{P}^\ell y(t) - y^\ell(t) = \varrho^\ell(t) + \vartheta^\ell(t)$$

- Projector onto $V^\ell = \mathrm{span}\,\{\psi_i\}_{i=1}^\ell$: $\mathcal{P}^\ell \psi = \sum_{j=1}^{\ell} \left(\psi^T \psi_i\right) \psi_i$

- Estimate for ϱ^ℓ:

$$\int_0^T \|\varrho^\ell(t)\|^2 \,\mathrm{d}t = \int_0^T \|y(t) - \mathcal{P}^\ell y(t)\|^2 \,\mathrm{d}t = \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

- Differential equation for ϑ^ℓ: for $i \in \{1, \ldots, \ell\}$

$$\begin{aligned}\psi_i^T \dot\vartheta^\ell(t) &= \psi_i^T \left(\mathcal{P}^\ell \dot y(t) - \dot y^\ell(t)\right) = \psi_i^T \left(\dot y(t) - \dot y^\ell(t) + \mathcal{P}^\ell \dot y(t) - \dot y(t)\right)\\ &= \psi_i^T \left(Ay(t) - Ay^\ell(t) + \mathcal{P}^\ell \dot y(t) - \dot y(t)\right)\\ &= \psi_i^T \left(A(\varrho^\ell(t) + \vartheta^\ell(t)) + \mathcal{P}^\ell \dot y(t) - \dot y(t)\right)\end{aligned}$$

Error analysis — Part 3

- Differential equation for ϑ^ℓ: for $i \in \{1, \dots, \ell\}$

$$\psi_i^T \dot{\vartheta}^\ell(t) = \psi_i^T \left(A(\varrho^\ell(t) + \vartheta^\ell(t)) + \mathcal{P}^\ell \dot{y}(t) - \dot{y}(t)\right)$$

- Summation: $\vartheta^\ell(t) = \sum_{i=1}^\ell c_i(t)\psi_i$

$$\vartheta^\ell(t)^T \dot{\vartheta}^\ell(t) = \vartheta^\ell(t)^T \left(A(\varrho^\ell(t) + \vartheta^\ell(t)) + \mathcal{P}^\ell \dot{y}(t) - \dot{y}(t)\right)$$

- Estimation:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\vartheta^\ell(t)\|^2 \le C\left(\|\vartheta^\ell(t)\|^2 + \|\varrho^\ell(t)\|^2 + \|\dot{y}(t) - \mathcal{P}^\ell \dot{y}(t)\|^2\right)$$

- Gronwall lemma: $\vartheta^\ell(0) = \mathcal{P}^\ell y_0 - y^\ell(0) = 0$

$$\|\vartheta^\ell(t)\|^2 \le C\left(\|\varrho^\ell(t)\|^2 + \|\dot{y}(t) - \mathcal{P}^\ell \dot{y}(t)\|^2\right)$$

$$= C\left(\sum_{i=\ell+1}^{\infty} \lambda_i^\infty + \|\dot{y}(t) - \mathcal{P}^\ell \dot{y}(t)\|^2\right)$$

Error estimate for continuous POD

- Error estimate (continuous POD method):

$$\int_0^T \|y(t) - y^\ell(t)\|^2 \,\mathrm{d}t \le 2 \int_0^T \|\varrho^\ell(t)\|^2 + \|\vartheta^\ell(t)\|^2 \,\mathrm{d}t$$

$$\le C\Big(\sum_{i=\ell+1}^{\infty} \lambda_i^\infty + \int_0^T \|\dot y(t) - \mathcal{P}^\ell \dot y(t)\|^2 \,\mathrm{d}t \Big)$$

- Remarks:
  - dependence of the decay of the eigenvalues λ_i
  - dependence on the approximation quality for $\dot y(t)$

- Modified POD method:

$$\min \int_0^T \big\|y(t) - \mathcal{P}^\ell y(t)\big\|^2 + \big\|\dot y(t) - \mathcal{P}^\ell \dot y(t)\big\|^2 \,\mathrm{d}t \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle = \delta_{ij}$$

- Error estimate: $\displaystyle\int_0^T \|y(t) - y^\ell(t)\|^2 \,\mathrm{d}t \le C \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$

Extensions

- Full discrete method: $t_j = j\Delta t$, $Y_j^\ell \approx y(t_j)$

$$\psi_i^T \left(\frac{Y_j^\ell - Y_{j-1}^\ell}{\Delta t} \right) = \psi_i^T A Y_j^\ell + \psi_i^T f(t, Y_j^\ell), \quad j = 1, \dots, m, \; i = 1, \dots, \ell$$
$$\psi_i^T Y_0^\ell = \psi_i^T y_0, \quad i = 1, \dots, \ell$$

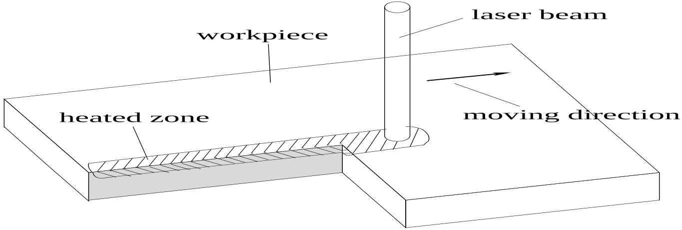
- Discrete POD: $\lambda_i = \lambda_i^n$, $\psi_i = \psi_i^n$
- Error estimate:

$$\sum_{j=1}^n \alpha_j \left\| y(t_j) - Y_j^\ell \right\|_{\mathbb{R}^N}^2 \le C \left((\Delta t)^2 + \sum_{i=\ell+1}^n \lambda_i + \sum_{j=1}^n \alpha_j \left| \psi_i^T \dot{y}(t_j) \right|^2 \right)$$
$$= O\left((\Delta t)^2 + \sum_{i=\ell+1}^\infty \left(\lambda_i^\infty + \int_0^T \left| (\psi_i^\infty)^T \dot{y}(t) \right|^2 \mathrm{d}t \right) \right)$$

- Parameter-dependent elliptic systems

Laser surface hardening [Hömberg/V.]

- Motivation:



- Phase transition of steel:

$$\left.\begin{array}{l}\text{ferrite}\\ \text{pearlite}\\ \text{bainite}\\ \text{martensite}\end{array}\right\} \xrightarrow{\text{heating}} \text{austenite} \xrightarrow{\text{cooling}} \left\{\begin{array}{l}\text{ferrite}\\ \text{pearlite}\\ \text{bainite}\\ \text{martensite}\end{array}\right.$$

Model equations

- Energy balance and Fourier's law:

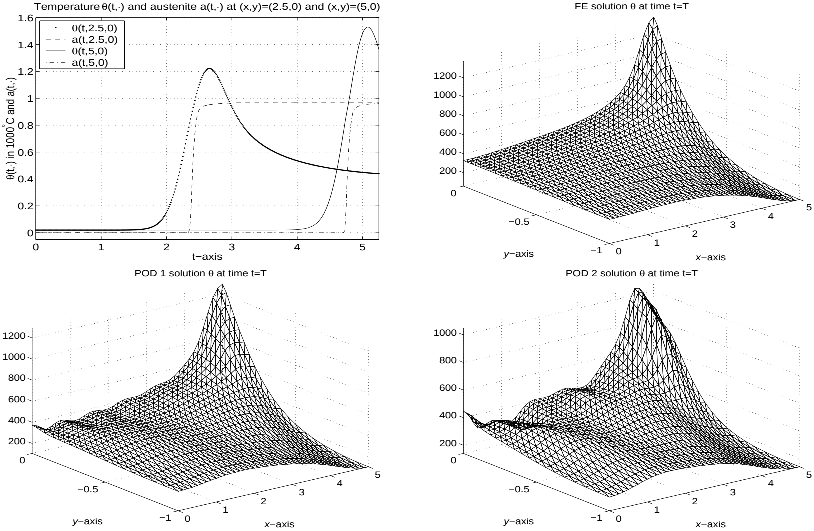
$$\begin{cases} \varrho c_p \theta_t - k\Delta\theta = \alpha u - \varrho L a_t & \text{in } Q = (0,T)\times\Omega \\ \frac{\partial\theta}{\partial n} = 0 & \text{auf } \Sigma = (0,T)\times\partial\Omega \\ \theta(0,\cdot) = \theta_\circ & \text{in } \Omega \subset \mathbb{R}^d \end{cases}$$

- Phase transition of austenite:

$$\begin{cases} a_t = f(\theta, a) & \text{in } Q \\ a(0,\cdot) = 0 & \text{in } \Omega \end{cases}$$

- Intensity of the laser: $u = u(t) \in L^2(0,T)$
- Nonlinearity: $f_+(\theta,a) = \max\{a_{eq}(\theta) - a, 0\}/\tau(\theta)$, $\tau(\theta) > 0$

FE and POD temperatures at $t = T$



POD error

- Measures for the error:

$$\Psi^i = \frac{\max_{0\le j\le N} \|\theta^j_\ell - \theta^j_{FE}\|_{L^\infty(\Omega)}}{\max_{0\le j\le N} \|\theta^j_{FE}\|_{L^\infty(\Omega)}} \quad \text{with} \quad \begin{cases} i=1 & \text{POD with DQ} \\ i=2 & \text{POD without DQ} \end{cases}$$

	$X = L^2(\Omega)$		$X = H^1(\Omega)$	
ℓ	Ψ^1	Ψ^2	Ψ^1	Ψ^2
10	24.1%	40.6%	21.0%	40.1%
25	1.6%	26.9%	4.0%	24.6%

- Heuristic: $\mathcal{E}(\ell) = \sum_{i=1}^{\ell} \lambda_i \Big/ \sum_{i=1}^{d} \lambda_i \cdot 100\% \;\ge 94\%$

	$\ell = 10$	$\ell = 15$	$\ell = 20$	$\ell = 25$
$\mathcal{E}(\ell)$, $X = L^2(\Omega)$	94.3	98.4	99.5	99.8
$\mathcal{E}(\ell)$, $X = H^1(\Omega)$	77.7	87.4	92.5	95.7

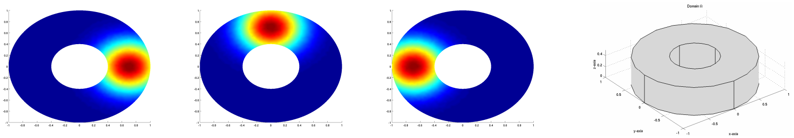
Heat equation

- Model equations:

$$
\begin{aligned}
y_t(t,\mathrm{x}) - \Delta y(t,\mathrm{x}) &= 0 && \text{for all } (t,\mathrm{x}) \in Q = (0,T)\times\Omega \\
\frac{\partial y}{\partial n}(t,\mathrm{x}) &= 0 && \text{for all } (t,\mathrm{x}) \in \Sigma_1 = (0,T)\times\Gamma_1 \\
\frac{\partial y}{\partial n}(t,\mathrm{x}) &= 100 g(t,x) && \text{for all } (t,\mathrm{x}) \in \Sigma_2 = (0,T)\times\Gamma_2 \\
y(0,\mathrm{x}) &= 0 && \text{for all } \mathrm{x} = (x,y,z) \in \Omega \subset \mathbb{R}^3
\end{aligned}
$$

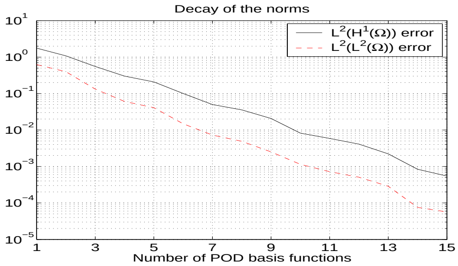
- Boundary condition:

$$\exp\Big(-\big[(x-0.7\cos(2\pi t))^2 + (y-0.7\sin(2\pi t))^2\big]\Big)$$



FE and POD results

Computing the FE mesh and matrices	50.0 seconds
FE solve	49.9 seconds
Computing 15 POD basis functions	87.1 seconds
Computing the reduced-order model, $\ell = 15$	$<$ 2.0 seconds
POD solve, $\ell = 15$	$<$ 0.1 seconds



Estimate the decay of the eigenvalues

- Error estimate: $\|y^\ell - y\|^2 \sim \sum_{i=\ell+1}^{\infty} \lambda_i$
- Ansatz: $\lambda_i = \lambda_1 e^{-\alpha(i-1)}$ for $i \geq 1$
- Error quotient:

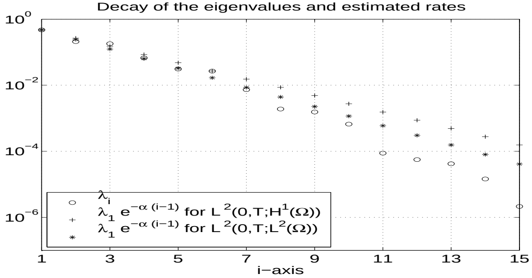
$$\frac{\|y^\ell - y\|^2}{\|y^{\ell+1} - y\|^2} \sim \frac{\sum_{i=\ell+1}^{\infty} \lambda_i}{\sum_{i=\ell+2}^{\infty} \lambda_i} = \frac{\sum_{i=\ell+1}^{\infty} e^{-\alpha(i-1)}}{\sum_{i=\ell+2}^{\infty} e^{-\alpha(i-1)}} = \frac{\sum_{i=0}^{\infty} \left(e^{-\alpha}\right)^i}{\sum_{i=0}^{\infty} \left(e^{-\alpha}\right)^i - 1} = e^{\alpha}$$

- Experimental order of decay:

$$EOD := \frac{1}{\ell_{\max}} \sum_{\ell=1}^{\ell_{\max}} Q(\ell)$$

with $Q(\ell) = \ln \frac{\|y^\ell - y\|^2}{\|y^{\ell+1} - y\|^2} \sim \alpha$

Experimental order of decay



- ○ decay of the eigenvalues
- $+$ estimated decay with error norm

$$\|u\| = \left(\int_0^T \int_\Omega |u(t,x)|^2 + |\nabla u(t,x)|^2 \,\mathrm{d}x\mathrm{d}t\right)^{1/2}$$

- $*$ estimated decay with error norm $\|u\| = \left(\int_0^T \int_\Omega \left|u(t,x)\right|^2 \mathrm{d}x\mathrm{d}t\right)^{1/2}$

Parameter-dependent systems

- Model equations: $\beta(x) = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

$$\begin{aligned} -2\Delta u + \beta \cdot \nabla u + a u &= 1 && \text{in } \Omega = (0,1)\times(0,1) \\ 2\,\frac{\partial u}{\partial n} + \frac{3}{2}\,u &= -1 && \text{on } \Gamma \end{aligned}$$

- Snapshots: (FE) solutions $\{u_j\}_{j=1}^{102}$ for $a_j = -51.5 + j$
- POD basis of rank ℓ:

$$\min \sum_{j=1}^{102} \Big\| u_j - \sum_{i=1}^{\ell} \langle u_j, \psi_i \rangle\, \psi_i \Big\| \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle = \delta_{ij} \qquad (\mathbf{P}^\ell)$$

with $\langle \varphi, \phi \rangle = \int_\Omega \varphi\phi \,\mathrm{d}x$ and $\|\varphi\| = \sqrt{\langle \varphi, \varphi \rangle}$

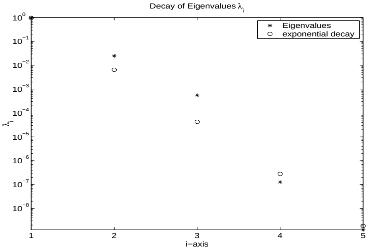
- Solution to $(\mathbf{P}^\ell)$: correlation matrix $K_{ij} = \langle u_i, u_j \rangle$

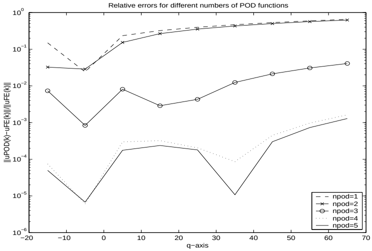
$$K v_i = \lambda_i v_i, \quad \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_\ell, \quad \psi_i = \frac{1}{\sqrt{\lambda_i}} \sum_{j=1}^{102} (v_i)_j u_j$$

Reduced-order modeling (ROM)

- Ansatz: $u^\ell = \sum_{i \le \ell} u_i^\ell \psi_i$ and Galerkin projection
- Error estimate: $\int \|u^\ell(a) - u(a)\|^2 \,\mathrm{d}a \sim \sum_{i>\ell} \lambda_i$
- Exponential decay of the eigenvalues: $\lambda_i = \lambda_1 e^{-\eta(i-1)}$
- Experimental order of decay (EOD):

$$EOD := \frac{1}{\ell_{\max}} \sum_{\ell=1}^{\ell_{\max}} Q(\ell) \quad \text{with} \quad Q(\ell) = \ln \frac{\int \|u^\ell(a) - u(a)\|^2 \,\mathrm{d}a}{\int \|u^{\ell+1}(a) - u(a)\|^2 \,\mathrm{d}a} \sim \eta$$





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