POD for Nonlinear Systems
Reduced-Order Modeling & Error Estimates

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Model reduction: theory and Applications

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Motivation 1: Parameter identification

- Model equations:

$$
\begin{aligned}
-\mathrm{div}\big(c\nabla u\big) + \beta\cdot\nabla u + au &= f && \text{in } \Omega\subset\mathbb{R}^d \\
c\,\frac{\partial u}{\partial n} + qu &= g_N && \text{on } \Gamma_N\subset\Gamma=\partial\Omega \qquad (*)\\
u &= g_D && \text{on } \Gamma_D=\Gamma\setminus\Gamma_N
\end{aligned}
$$

- Problem: estimate parameters (e.g., c, β, a or q) in $(*)$ from given (perturbed) measurements u_d for the solution u on (parts of) Γ
- Mathematical formulation: (∞-dimensional) optimization problem

$$
\min \int_\Gamma \alpha\,|u-u_d|^2\,\mathrm{d}s + \kappa\,\|p\|^2 \quad \text{s.t.} \quad (p,u) \text{ solves } (*) \text{ and } p\in\mathcal{P}_{\mathrm{ad}}
$$

s.t. — subject to

- Numerical strategy: combine optimization methods with fast (local) rate of convergence and POD model reduction for the PDEs

Motivation 2: Optimal control of time-dependent problems

- Model problem:

$$\min \frac{1}{2}\int_\Omega |y(T)-y_T|^2\,\mathrm{d}x + \frac{\kappa}{2}\int_0^T\int_\Gamma |u|^2\,\mathrm{d}x\mathrm{d}t$$

$$\text{s.t.}\quad \begin{cases} y_t - \Delta y + f(y) & = 0 \quad \text{in } Q=(0,T)\times\Omega \\ y|_\Gamma & = u \quad \text{on } \Sigma=(0,T)\times\Gamma \\ y(0) & = y_\circ \quad \text{on } \Omega\subset\mathbb{R}^d \end{cases}$$

- Adjoint system (for gradient computation):

$$-p_t - \Delta p + f'(y)^* p = 0,\quad p|_\Gamma = 0,\quad p(T) = y_T - y(T)$$

- Optimizer: second-order methods like SQP or (semismooth) Newton
- Challenge: large-scale $\leftrightarrow$ fast/real-time optimizer

Motivation 3: Closed-loop control for time-dependent PDEs

- Open-loop control:

input $u(t) \longrightarrow$
$$\begin{array}{|l|}\hline \dot{x}(t)=f(t,x(t),u(t)) \\ x(0)=x_\circ \in \mathbb{R}^\ell \\ \text{(after spatial discretization)} \\ \hline \end{array}$$
$\longrightarrow$ output $y(t) = Cx(t) + Du(t)$

- Closed-loop control: determine $\mathcal{F}$ with

$$u(t) = \mathcal{F}(t, y(t)) \quad \text{(feedback law)}$$

- Linear case: LQR and LQG design
- Nonlinear case: Hamilton-Jacobi-Bellman equation

$$v_t(t, y_\circ) + H(v_y(t, y_\circ), y_\circ) = 0 \quad \text{in } (0, T) \times \mathbb{R}^\ell$$

- Strategy: ℓ-dim. spatial approximation by, e.g., POD basis

Outline of the first part of the lecture

- Proper orthogonal decomposition (POD)
  - POD and singular value decomposition (SVD)
  - POD method for ordinary differential equations (ODEs)
  - Continuous POD method for ODEs
  - POD method for parabolic partial differential equations (PDEs)
  - POD method for elliptic PDEs
- Reduced-order modeling (ROM)
  - ROM for ODEs and error estimation
  - ROM for λ-ω systems
  - Laser surface hardening
- References

POD method & SVD

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

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

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

- Constrained optimization:

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

- Equivalent problem: Find orthonormal $\psi_1, \ldots, \psi_\ell \in \mathbb{R}^m$ maximizing

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

Necessary optimality conditions (Part 1)

- Lagrange functional:

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

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

- Optimality conditions:

$$\frac{\partial L}{\partial \psi_i}(\psi_1,\dots,\psi_\ell,\lambda_{11},\dots,\lambda_{\ell\ell}) = 0 \in \mathbb{R}^m \qquad \text{for } i = 1,\dots,\ell$$

$$\frac{\partial L}{\partial \lambda_{ij}}(\psi_1,\dots,\psi_\ell,\lambda_{11},\dots,\lambda_{\ell\ell}) = 0 \in \mathbb{R} \qquad \text{for } i,j = 1,\dots,\ell$$

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 $Y \in \mathbb{R}^{m\times n}$: $d = \operatorname{rank} Y$, $\sigma_1 \geq \ldots \geq \sigma_d > 0$, $U = [u_1, \ldots, u_m] \in \mathbb{R}^{m\times m}$ 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 $D = \operatorname{diag}(\sigma_1, \ldots, \sigma_d) \in \mathbb{R}^{d\times d}$. 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: $\mathcal{V} = \text{span}\,\{y_1, \ldots, y_n\} \subset \mathbb{R}^m$ and $d = \dim \mathcal{V}$
  POD basis of rank ℓ: $\psi_i = u_i$ and $\lambda_i = \sigma_i^2 > 0$ for $i = 1, \ldots, \ell \leq d$
- 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:

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

Computation of the POD basis (Part 3)

- Error formula for the POD basis of rank ℓ:

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

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

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

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

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

POD method for ODEs

- Nonlinear dynamical system in $\mathbb{R}^m$:

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

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

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

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

Computation of the POD basis

- EVD for linear and symmetric $\mathcal{R}^n$ in ODE space $\mathbb{R}^m$:

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

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

- EVD for linear and symmetric $\mathcal{K}^n = \big((\alpha_j \, y_j^T y_i)\big)$ 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:

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

Continuous POD method for ODEs [Henri/Yvon, Kunisch/V., ...]

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

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

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

$$\mathcal{R}\psi_i = \int_0^T \big(\psi_i^T y(t)\big)\, y(t)\, \mathrm{d}t = \lambda_i \psi_i \quad \text{for } i \in \mathbb{N}$$

- Error for the POD basis of rank ℓ:

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

Relationship between 'discrete' and continuous POD

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

$$\mathcal{R}^n\psi = \sum_{j=1}^{n} \alpha_j \left(\psi^T y(t_j)\right) y(t_j)$$

$$\mathcal{R}\psi = \int_0^T \left(\psi^T y(t)\right) y(t)\,\mathrm{d}t$$

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

POD method for parabolic PDEs

- Heat equation (for instance):

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

- Variational formulation: for all $\varphi \in H^1(\Omega)$

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

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

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

POD basis computation

- 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: $y_j = y^m(t_j) \in V^m$, $1 \le j \le n$
- Inner product: $\langle u, v\rangle = \int_\Omega uv\,\mathrm{d}x$ or $\langle u, v\rangle = \int_\Omega uv + \nabla u \cdot \nabla v\,\mathrm{d}x$
- Sizes: # FE's $\gg$ # time instances, i.e., $m \gg n$
- Computation of the correlation $\mathcal{K}^n$: $\alpha_j = \frac{1}{n}$

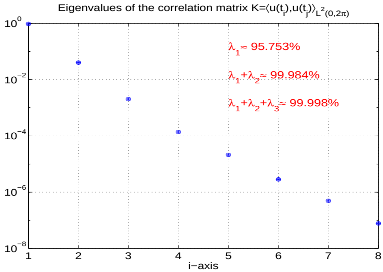
$$\frac{1}{n}\langle y_j^m, y_i^m\rangle = \frac{1}{n}\sum_{k,l=1}^{n} Y_{ik} Y_{jl} \langle \varphi_l, \varphi_k\rangle = \left(\frac{1}{n} Y^T M Y\right)_{ij}$$

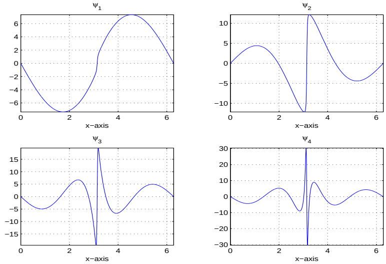
with $M_{ij} = \langle \varphi_j, \varphi_i\rangle$ (mass or stiffness matrix)

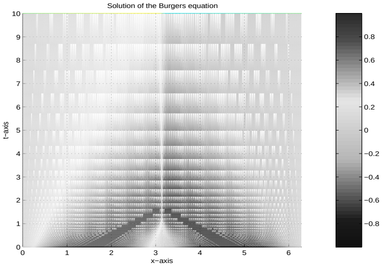
Numerical example: Burgers equation

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

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



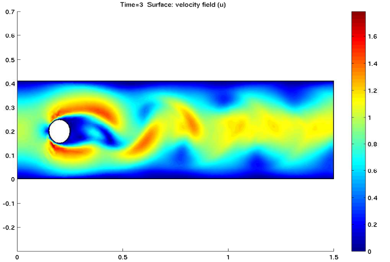


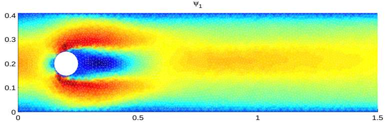


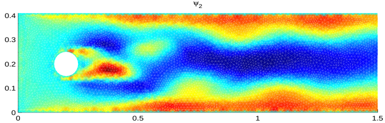
Numerical example: Navier-Stokes equation

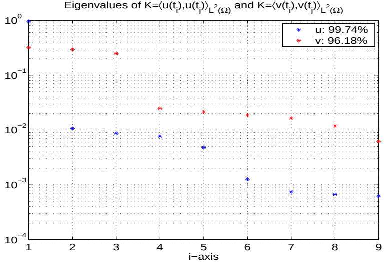
$$\begin{aligned} u_t + uu_x + vu_y + p_x &= \nu\Delta u \quad &&\text{in } Q = (0,T)\times\Omega \\ v_t + uv_x + vv_y + p_y &= \nu\Delta v \quad &&\text{in } Q \\ u_x + v_y &= 0 \quad &&\text{in } Q \end{aligned}$$

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



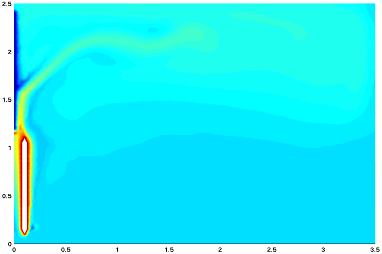




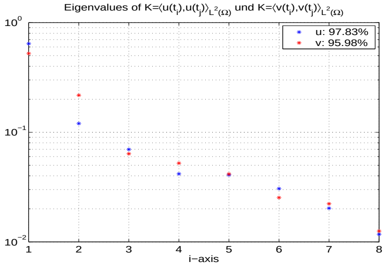


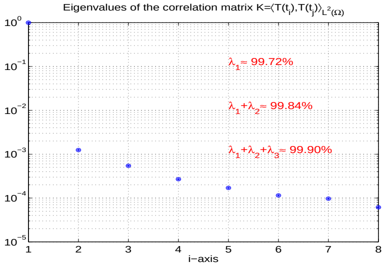
Numerical example: Energy transport (Boussinesq)

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



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





POD for λ-ω systems [Müller/V.]

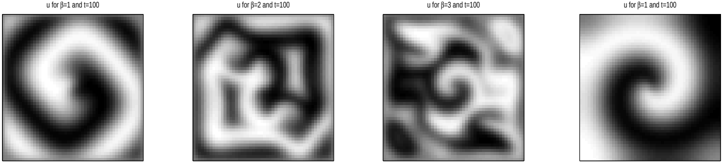
- PDEs: $s = u^2 + v^2$, $\lambda(s) = 1 - s$, $\omega(s) = -\beta s$

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} \lambda(s) & -\omega(s) \\ \omega(s) & \lambda(s) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} \sigma \Delta u \\ \sigma \Delta v \end{pmatrix}$$

- Homogeneous boundary conditions:

$$u = v = 0 \quad \text{or} \quad \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0$$

- Initial conditions: $u_\circ(x_1, x_2) = x_2 - 0.5$, $v_\circ(x_1, x_2) = (x_1 - 0.5)/2$

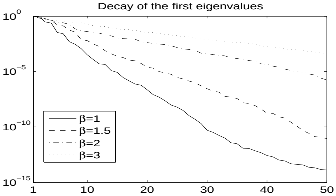


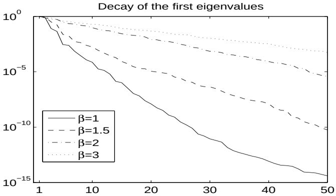
POD basis for λ-ω systems

- Offsets: $\bar{u}(x) = \frac{1}{n}\sum_{j=1}^{n} u(t_j, x)$ or $\bar{u} \equiv 0$
- Snapshots: $\hat{u}_j(x) = u(t_j, x) - \bar{u}(x)$ for $1 \le j \le n$
- POD eigenvalue problem: $\langle u, v\rangle = \int_\Omega uv\,\mathrm{d}x$

$$\mathcal{K}v_i = \lambda v_i, \; 1 \le i \le \ell, \quad \text{with } \mathcal{K}_{ij} = \int_\Omega \hat{u}_j(x)\hat{u}_i(x)\,\mathrm{d}x$$

- POD basis computation: $\psi_i = \frac{1}{\sqrt{\lambda_i}}\sum_{j=1}^{n} \alpha_j (v_i)_j \hat{u}_j$





POD method for elliptic PDEs

- Helmholtz equation (for instance): $f \in [f_{\min}, f_{\max}]$

$$
\begin{aligned}
-\Delta p(f) - k^2 p(f) &= q(f) && \text{in } \Omega \\
\frac{\jmath}{\varrho_\circ \omega} \frac{\partial p(f)}{\partial n} &= 0 && \text{on } \Gamma_{\mathrm{N}} \\
\frac{\jmath}{\varrho_\circ \omega} \frac{\partial p(f)}{\partial n} &= \frac{p(f)}{Z(f)} && \text{on } \Gamma_{\mathrm{R}}
\end{aligned}
$$

with $p : \Omega \to \mathbb{C}$, $c = 343,8 \left[\frac{\mathrm{m}}{\mathrm{s}}\right]$, $\omega = 2\pi f$, $k = \frac{\omega}{c}$, $\varrho_\circ = 1,2 \left[\frac{\mathrm{kg}}{\mathrm{m}^3}\right]$

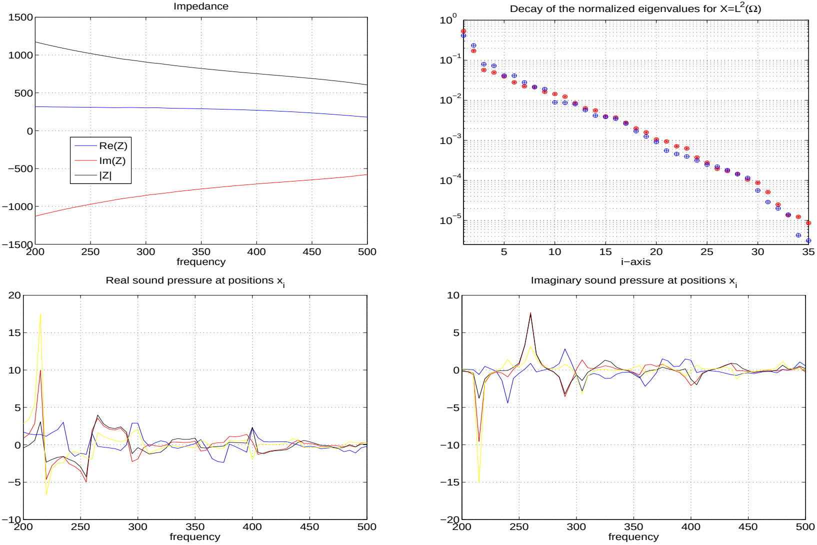
- Variational formulation: for all $\varphi \in H^1(\Omega; \mathbb{C})$

$$
\int_\Omega \nabla p(f) \cdot \overline{\nabla \varphi} - k^2 p(f) \overline{\varphi} \, \mathrm{d}x + \frac{\jmath \varrho_\circ \omega}{Z(f)} \int_{\Gamma_R} p(f) \overline{\varphi} \, \mathrm{d}s = \int_\Omega q(f) \overline{\varphi} \, \mathrm{d}x
$$

- FE discretization: $p^m(f) \in V^m = \mathrm{span}\,\{\varphi_1, \ldots, \varphi_m\}$

$$
\int_\Omega \nabla p^m(f) \cdot \overline{\nabla \varphi_i} - k^2 p^m(f) \overline{\varphi}_i \, \mathrm{d}x + \frac{\jmath \varrho_\circ \omega}{Z(f)} \int_{\Gamma_R} p^m(f) \overline{\varphi}_i \, \mathrm{d}s = \int_\Omega q(f) \overline{\varphi}_i \, \mathrm{d}x
$$

Impedance identification [Hepberger/Acoustic Competence Center/V.]



ROM for ODE system & error estimation

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

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

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

- Snapshots: $y(t) \in \mathbb{R}^m$ for all $t \in [0, T]$
- POD basis of rank $\ell \leq m$: $\psi_1, \ldots, \psi_\ell \in \mathbb{R}^m$
- Galerkin ansatz: $y^\ell(t) = \sum_{j=1}^{\ell} \left(\psi_j^T y^\ell(t)\right) \psi_j = \sum_{j=1}^{\ell} \mathrm{y}_j^\ell(t)\psi_j$
- Galerkin projection of the ODE:

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

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:

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

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

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

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

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

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

- Estimate for ϱ^ℓ:

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

- 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 $i \in \{1, \ldots, \ell\}$

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

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

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

- Estimation:

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

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

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

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

Error estimate for continuous POD

- Error estimate (continuous POD method):

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

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

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

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

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

Extensions

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

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

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

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

- nonlinear parabolic PDEs and parameter-dependent elliptic systems

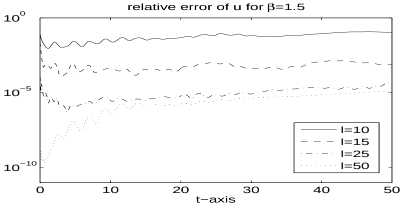
ROM for λ-ω systems [Müller/V.]

- Inner product: $\langle u, v \rangle = \int_\Omega uv \,\mathrm{d}x$
- POD Galerkin ansatz:

$$u_\ell(t,x) = \bar{u}(x) + \sum_{j=1}^{\ell} u_\ell^j(t)\psi_j(x), \quad v_\ell(t,x) = \bar{v}(x) + \sum_{j=1}^{\ell} v_\ell^j(t)\phi_j(x)$$

- Reduced-order model (ROM):
  - insert ansatz into PDEs
  - multiply by POD basis functions ψ_i respectively ϕ_i
  - integrate over Ω
- Numerical results:

$$t \mapsto \frac{\|u_\ell(t)-u(t)\|^2}{\|u(t)\|^2}$$



Relative POD errors for λ-ω systems

- Offsets: $u_{\mathrm{m}}(x) = \frac{1}{n}\sum_{j=1}^{n} u(t_j, x)$
- Relative POD errors:

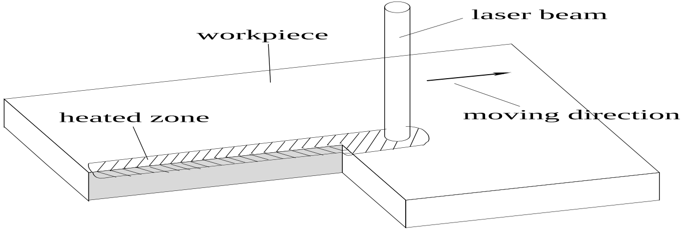
	$\bar{u} = 0$	$\bar{u} = u_{\mathrm{m}}$
$\ell = 10$	0.005890	0.005945
$\ell = 15$	0.000350	0.000335
$\ell = 50$	0.000009	0.000009

	$\bar{u} = 0$	$\bar{u} = u_{\mathrm{m}}$
$\ell = 40$	0.577442	0.460188
$\ell = 45$	0.898613	0.297619
$\ell = 50$	0.071035	0.001774

$$E_{\mathrm{rel}}(u) = \frac{\sum_{j=1}^{n} \alpha_j \, \|u_\ell(t_j) - u_h(t_j)\|^2}{\sum_{j=1}^{n} \alpha_j \, \|u_h(t_j)\|^2} \quad \text{for } \beta = 1.5 \text{ (left) and } \beta = 2 \text{ (right)}$$

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:

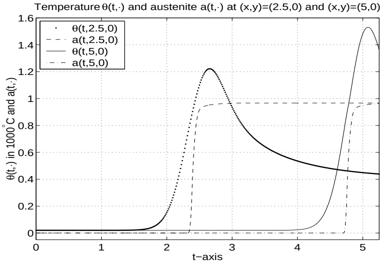
$$\begin{cases} \varrho c_p \theta_t - k\Delta\theta = \alpha u - \varrho L a_t & \text{in } Q = (0,T)\times\Omega \\ \frac{\partial\theta}{\partial n} = 0 & \text{auf } \Sigma = (0,T)\times\partial\Omega \\ \theta(0,\cdot) = \theta_\circ & \text{in } \Omega\subset\mathbb{R}^d \end{cases}$$

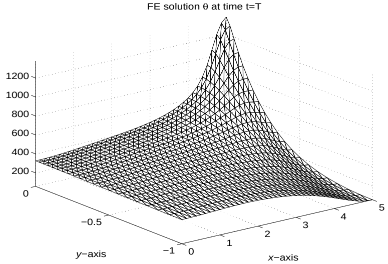
- Phase transition of austenite:

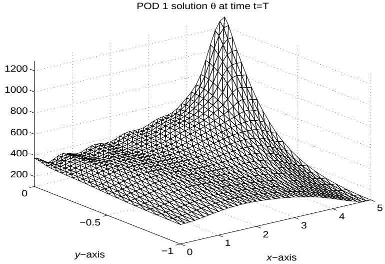
$$\begin{cases} a_t = f(\theta,a) & \text{in } Q \\ a(0,\cdot) = 0 & \text{in } \Omega \end{cases}$$

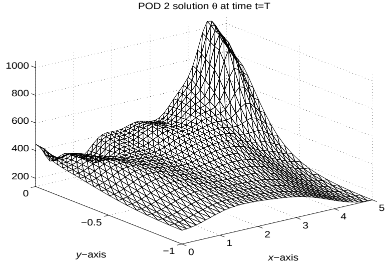
- Intensity of the laser: $u = u(t) \in L^2(0,T)$
- Nonlinearity: $f_+(\theta,a) = \max\left\{a_{eq}(\theta) - a, 0\right\}/\tau(\theta),\ \tau(\theta) > 0$

FE and POD temperatures at $t = T$









POD error

- Measures for the error:

$$\Psi^i = \frac{\max\limits_{0\le j\le N}\Big(\sup\limits_{x\in\Omega}|\theta_\ell^j(x)-\theta_{FE}^j(x)|\Big)}{\max\limits_{0\le j\le N}\Big(\sup\limits_{x\in\Omega}|\theta_{FE}^j(x)|\Big)} \quad \text{with} \quad \begin{cases} i=1 & \text{POD with derivatives} \\ i=2 & \text{POD without derivatives} \end{cases}$$

	$X = L^2(\Omega)$		$X = H^1(\Omega)$	
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

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