Proper Orthogonal Decomposition (POD) for Nonlinear Systems

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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 or a) in $(*)$ from given (perturbed) measurements u_d for the solution u on (parts of) Γ
- Mathematical formulation: (∞-dim.) optimization problem

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

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:

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

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

- Adjoint system:

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

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

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

- Open-loop control:

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

- 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 POD model reduction

Outline

- Introduction to model reduction
- Balanced truncation method
- Reduced-basis method
- Proper orthogonal decomposition (POD)
    - Burgers equation
    - Navier-Stokes equations
    - energy transport
- Reduced-order modeling (ROM)
    - heat flow
    - λ-ω systems

Introduction

- Linear system (state-space):

$$\dot{x}(t) = Ax(t) + Bu(t), \quad t \geq 0, \quad x(0) = x_\circ$$
$$y(t) = Cx(t) + Du(t)$$

$x(t) \in \mathbb{R}^n$ state, $u(t) \in \mathbb{R}^m$ control, $y(t) \in \mathbb{R}^p$ output/measurement

- Laplace transform: $x \mapsto \int_0^\infty e^{-st} x(t)\, dt$

$$sx(s) - x(0) = Ax(s) + Bu(s)$$
$$y(s) = Cx(s) + Du(s)$$

$\Rightarrow y(s) = \big(C(sI - A)^{-1}B + D\big)u(s) + C(sI - A)^{-1}x_\circ$

- Transfer function for $x_\circ = 0$: $u(s) \mapsto y(s) = G(s)u(s)$ with

$$G(s) = C(sI - A)^{-1}B + D$$

Reduced-order model (ROM)

- Transfer function for $x_\circ = 0$: $u(s) \mapsto y(s) = G(s)u(s)$ with

$$G(s) = C(sI - A)^{-1}B + D$$

- Reduced-order model (ROM) of order $\ell \ll n$:

$$y^\ell(s) = G_\ell(s)u(s) \quad \text{with } G_\ell(s) = C_\ell(sI - A_\ell)^{-1}B_\ell + D$$

- Error bound: $y(s) = G(s)u(s)$ und $y^\ell(s) = G_\ell(s)u(s)$

$$\Rightarrow \qquad \|y - y^\ell\| \le \|G - G_\ell\|\,\|u\|$$

- Goal of model reduction: ROM with $\boxed{\|G - G_\ell\| < \mathrm{tol}}$

Methods

- Linear dynamical systems:
  - balanced truncation
  - moment matching
- Nonlinear dynamical systems:
  - linearize and balanced truncation/moment matching
  - reduced-basis method
  - proper orthogonal decomposition (POD)
- Extension: find $x \in \mathbb{R}^n$ solving

$$F(x; \mu) = 0 \quad \text{in } \mathbb{R}^n$$

or

$$\dot{x}(t) + F(x(t); \mu) = 0 \quad \text{in } \mathbb{R}^n$$

with parameter $\mu \in \mathcal{D} \subset \mathbb{R}^k$

Balanced truncation method

- Linear system:

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t), \quad t \geq 0, \quad x(0) = x_\circ \\ y(t) &= Cx(t) + Du(t) \end{aligned} \qquad (*)$$

$x(t) \in \mathbb{R}^n$ state, $u(t) \in \mathbb{R}^m$ control, $y(t) \in \mathbb{R}^p$ output/measurement

- Transformation of the state space: $x \mapsto \mathrm{x} = \mathcal{T}x$, multiply $(*)$ by $\mathcal{T}$

$$\begin{aligned} \dot{\mathrm{x}}(t) &= \mathcal{T}A\mathcal{T}^{-1}\mathrm{x}(t) + \mathcal{T}Bu(t), \quad t \geq 0, \quad \mathrm{x}(0) = \mathcal{T}x_\circ \\ y(t) &= C\mathcal{T}^{-1}\mathrm{x}(t) + Du(t) \end{aligned}$$

- Transformed matrices:

$$(A, B, C, D) \mapsto (\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}) = (\mathcal{T}A\mathcal{T}^{-1}, \mathcal{T}B, C\mathcal{T}^{-1}, D)$$

- Balanced realization: utilize appropriate $\mathcal{T}$

Balanced realization

- Balanced realization: find appropriate $\mathcal{T}$
- Controllability: (A, B) controllable $\Leftrightarrow$

for any $x_\circ$, x_T there exists $u(t)$ such that $\begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ x(0) = x_\circ \\ x(T) = x_T \end{cases}$

$\Leftrightarrow$ $AW_c + W_cA^T + BB^T = 0$ (Lyapunov eq.), W_c positive definite

- W_c = controllability Gramian
- Observability: (A, C) observable $\Leftrightarrow$

$$u(t),\ y(t) \text{ known} \quad \Rightarrow \quad x(0) = x_\circ \text{ computable}$$

$\Leftrightarrow$ $A^TW_o + W_oA + C^TC = 0$ (Lyapunov eq.), W_o positive definite

- W_o = observability Gramian

Hankel singular values

- Balancing: state space transformation
  $\longrightarrow$ components ordered w.r.t. decay controllability & observability
- Observability Gramian W_o: $A^T W_o + W_o A + C^T C = 0$
- Controllability Gramian W_c: $A W_c + W_c A^T + B B^T = 0$
- Balancing: find $\mathcal{T}$ satisfying

$$\mathcal{W}_c = \mathcal{W}_o = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix}$$

$(\mathcal{A},\mathcal{B},\mathcal{C}) = (\mathcal{T}A\mathcal{T}^{-1}, \mathcal{T}B, C\mathcal{T}^{-1})$
$\mathcal{A}^T\mathcal{W}_o + \mathcal{W}_o\mathcal{A} + \mathcal{C}^T\mathcal{C} = 0$
$\mathcal{A}\mathcal{W}_c + \mathcal{W}_c\mathcal{A}^T + \mathcal{B}\mathcal{B}^T = 0$

- Hankel singular values: $\sigma_1 \geq \ldots \geq \sigma_n \geq 0$
- Balanced Realization: transformation

$$(A, B, C, D) \mapsto (\mathcal{T}A\mathcal{T}^{-1}, \mathcal{T}B, C\mathcal{T}^{-1}, D)$$

Model reduction by balanced truncation

- Hankel singular values:

$$\sigma_i \ll 1 \Rightarrow i\text{-th component of } \mathrm{x}(t) = \mathcal{T}x(t) \text{ small influence}$$

- Truncation: $\mathcal{T}x \approx \mathcal{T}_\ell x^\ell$, $\mathcal{T}_\ell = [\mathcal{T}_{1\ell}, \ldots, \mathcal{T}_{\ell\ell}]$ with $\sigma_{\ell+1} \ll \mathrm{tol}$
- ROM of order $\ell \ll n$: $x^\ell(t) \in \mathbb{R}^\ell$

$$\begin{aligned} \dot{x}^\ell(t) &= A_\ell x(t) + B_\ell u(t), \quad t \geq 0, \quad x^\ell(0) = \mathcal{T}_\ell x_\circ \\ y(t) &= C_\ell x^\ell(t) + Du(t) \end{aligned}$$

with $A_\ell = \mathcal{T}_{1:\ell,1:n} A \mathcal{T}^{-1}_{1:n,1:\ell}$, $B_\ell = \mathcal{T}_{1:\ell,1:n} B$, $C_\ell = C\mathcal{T}^{-1}_{1:n,1:\ell}$

- Error bound:

$$\|G - G_\ell\| \leq 2 \sum_{i=\ell+1}^{n} \sigma_i \quad \text{with} \quad G_\ell = C_\ell \big(sI - A_\ell\big)^{-1} B_\ell + D$$

$$\Rightarrow \|y - y^\ell\| \leq 2\,\|u\| \sum_{i=\ell+1}^{n} \sigma_i$$

Extensions of balanced truncation

- Descriptor systems:

$$E\dot{x}(t) = Ax(t) + Bu(t), \quad t > 0, \quad x(0) = x_\circ$$
$$y(t) = Cx(t) + Du(t)$$

$\longrightarrow$ Multi body systems
$\longrightarrow$ semi-discretized PDEs

- Time-dependent matrices:

$$x_{k+1} = A_k x_k + B_k u_k, \quad k \geq 0, \quad x_0 = x_\circ$$
$$y_k = C_k x_k + D_k u_k$$

- Systems of 2nd order: structure preserving

$$M\ddot{x}(t) + D\dot{x}(t) + Sx(t) = Bu(t), \quad t > 0$$
$$y(t) = Cx(t)$$

MATLAB Control System Toolbox

- Routine `lyap`: solver for Lyapunov equation $A^T X + XA + Q = 0$
- Routine `balreal`: balanced realization
- Routine `minreal`: minimal realization
- Routine `modred`: ROM computation

Advantages/disadvantages of balanced truncation

- Advantages:
  - including system properties
  - explicit error bounds
  - algorithms available
  - applications for sparse matrices
- Disadvantages:
  - only linear systems
  - increasing CPU due to linearization & time-dependent matrices
- Literature:
  - K. Zhou, J.C. Doyle, K. Glover: *Robust and Optimal Control*, Prentice Hall, New Jersey 07458, 1996
  - P. Benner, V. Mehrmann, D.C. Sorensen (eds.): *Dimension Reduction of Large-Scale Systems*, Lecture Notes in Computational Science and Engineering, Vol. 45, Springer-Verlag, 2005

Reduced basis method

- Linear model problem:

$$-\Delta u + \mu u = f \text{ in } \Omega \subset R^3, \quad u = 0 \text{ on } \Gamma, \quad \mathcal{D} = [0, \mu_{\max}]$$

- Discretisation:

$$\big(A + \mu I\big) u^h = F \qquad (*)$$

- Grid in $\mathcal{D}$: $0 = \mu_1 < \mu_2 < \ldots < \mu_\ell = \mu_{\max}$
- Reduced-order space:

$$\mathcal{V}_\ell = \left\{ u^\ell = \sum_{i=1}^{\ell} c_i u^h(\mu_i) \,\middle|\, c_i \in \mathbb{R},\ u^h(\mu_i) \text{ solves } (*) \text{ for } \mu = \mu_i \right\}$$

- ROM of order ℓ: $u^\ell \in \mathcal{V}^\ell$ satisfying

$$\big(V_\ell^T A V_\ell + \mu V_\ell^T V_\ell\big) u^\ell = V_\ell^T F, \quad V_\ell = [u^h(\mu_1), \ldots, u^h(\mu_\ell)]$$

Error bounds and extensions

- Error: ℓ sufficiently large and certain μ_i's

$$\|u^h(\mu) - u^\ell(\mu)\| \leq \sqrt{1 + c_1\mu_{\max}}\,\|u^h(0)\|\,e^{-c_2\ell/2} \quad \text{for all } \mu \in \mathcal{D}$$

- Extensions:
  - $\mathcal{D} \subset \mathbb{R}^k$ with $k > 1$
  - certain nonlinear problems

$$-\Delta u + g(u;\mu) = h(\mu) \quad \text{in } \Omega \subset \mathbb{R}^3$$

  - time-dependent problems

$$u_t - \Delta u + g(u;\mu) = h(\mu) \quad \text{in } (0,T) \times \Omega \subset \mathbb{R}^3$$

$\rightarrow$ interpolation in $\tilde{\mathcal{D}} = \mathcal{D} \times [0,T]$

Advantages/disadvantages of the reduced basis method

- Advantages:
  - reduction based on simulation (data driven)
  - nonlinear problems
  - parameter- and time-dependent problems
  - error bounds for specific interpolation in $\mathcal{D}$
- Disadvantages:
  - not structure preserving
  - no system theoretical results
  - costly interpolation for $k > 1$
- Literature:

  M.A. Grepl, Y. Maday, N.C. Nguyen, A.T. Patera: Efficient reduced-basis treatment of nonaffine and nonlinear partial differential equations, to appear in *Mathematical Modelling and Numerical Analysis* (M^2AN)

Proper orthogonal decomposition

- 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

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

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)

- $L(\psi_1, \ldots, \psi_\ell, \lambda_{11}, \ldots, \lambda_{\ell\ell}) = J(\psi_1, \ldots, \psi_\ell) + \sum_{i,j=1}^{\ell} \lambda_{ij} (\psi_i^T \psi_j - \delta_{ij})$
- $\dfrac{\partial L}{\partial \psi_i} = 0 \quad \Leftrightarrow \quad \sum_{j=1}^{n} y_j (y_j^T \psi_i) = \lambda_{ii} \psi_i$ 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 $i = 1,\dots,\ell$
- Solution by SVD for $Y \in \mathbb{R}^{m\times n}$: $d = \operatorname{rank} Y$, $\sigma_1 \geq \ldots \geq \sigma_d > 0$, $U = [u_1,\dots,u_m] \in \mathbb{R}^{m\times m}$ und $V = [v_1,\dots,v_n] \in \mathbb{R}^{n\times n}$ orthogonal with
$$U^TYV = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} = \Sigma \in \mathbb{R}^{m\times n}$$
where $D = \operatorname{diag}(\sigma_1,\dots,\sigma_d) \in \mathbb{R}^{d\times d}$. Moreover, for $1 \leq i \leq d$
$$Yv_i = \sigma_i u_i,\;\; Y^Tu_i = \sigma_i v_i,\;\; YY^Tu_i = \sigma_i^2 u_i,\;\; Y^TYv_i = \sigma_i^2 v_i$$
- POD basis: $\psi_i = u_i$ and $\lambda_i = \sigma_i^2 > 0$ for $i = 1,\dots,\ell \leq d = \dim\mathcal{V}$

Computation of the POD basis (Part 2)

- Data ensemble: $\mathcal{V} = \operatorname{span}\{y_1, \ldots, y_n\} \subset \mathbb{R}^m$ 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 $Y^T Y \in \mathbb{R}^{n \times n}$: $Y^T Y v_i = \sigma_i^2 v_i$ and $u_i = \frac{1}{\sigma_i} Y v_i$ (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:

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

- $YY^T\psi_i = \lambda_i\psi_i$, $1 \le i \le \ell$, 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

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

Properties of the POD basis

- Uncorrelated POD coefficients:

$$\sum_{j=1}^{n} \alpha_j \langle y_j, \psi_i \rangle \, \langle y_j, \psi_k \rangle = \delta_{ik} \lambda_i$$

- Optimality of the POD basis:

$$\sum_{i=1}^{\ell} \sum_{j=1}^{n} \alpha_j \big| \langle y_j, \psi_i \rangle \big|^2 \geq \sum_{i=1}^{\ell} \sum_{j=1}^{n} \alpha_j \big| \langle y_j, \chi_i \rangle \big|^2$$

where $\{\chi_i\}_{i=1}^{\ell}$ orthonormal with respect to $\langle \cdot \, , \cdot \rangle$

Snapshot POD for dynamical systems

- Nonlinear dynamical system:

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

  with continuous f and given $y_\circ$
- 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: $y_j = y(t_j)$, $1 \leq j \leq n$
- Snapshot ensemble: $\mathcal{V} = \mathrm{span}\,\{y_1, \ldots, y_n\}$, $d = \dim \mathcal{V} \leq n$
- POD basis of rank $\ell < d$: with weights $\alpha_j \geq 0$

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

- Inner product: $\langle u, v \rangle = \int_\Omega uv \,\mathrm{d}x$ or $\langle u, v \rangle = \int_\Omega uv + \nabla u \cdot \nabla v \,\mathrm{d}x$

Computation of the POD basis

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

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

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

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

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

POD for λ-ω systems [Müller/V.]

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

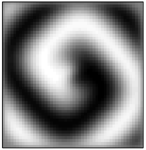
$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} \lambda(s) & -\omega(s) \\ \omega(s) & \lambda(s) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} \sigma\Delta u \\ \sigma\Delta v \end{pmatrix}$$

- Homogeneous boundary conditions:

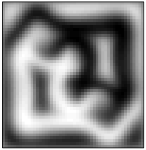
$$u = v = 0 \quad \text{or} \quad \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0$$

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

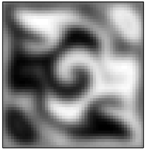
u for β=1 and t=100



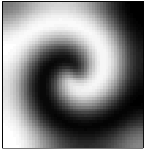
u for β=2 and t=100



u for β=3 and t=100



u for β=1 and t=100

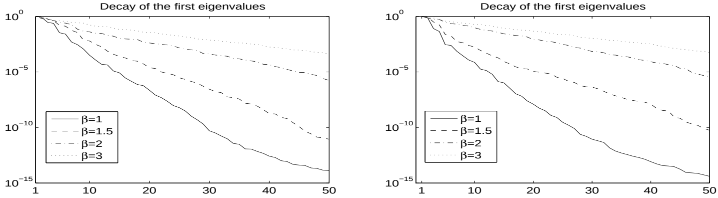


POD basis for λ-ω systems

- 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: $\langle u, v\rangle = \int_\Omega uv\,\mathrm{d}x$

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

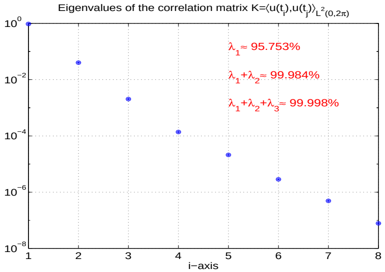
- POD basis computation: $\psi_i = \frac{1}{\sqrt{\lambda_i}}\sum_{j=1}^{n} \alpha_j (v_i)_j \hat{u}_j$

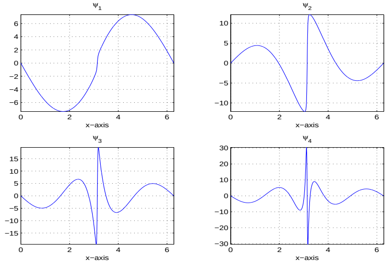


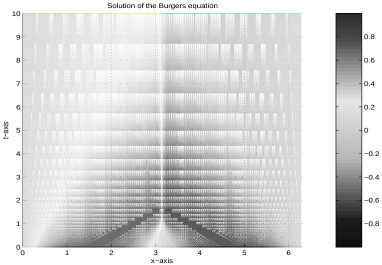
Numerical example: Burgers equation

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

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

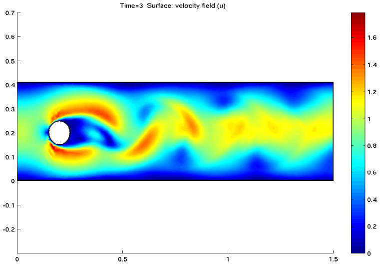






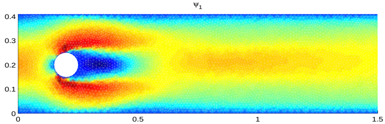
Numerical example: Navier-Stokes equation

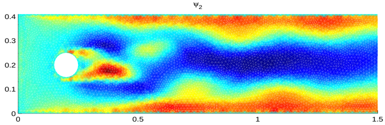
$$
\begin{aligned}
u_t + uu_x + vu_y + p_x &= \nu\Delta u && \text{in } Q = (0,T)\times\Omega \\
v_t + uv_x + vv_y + p_y &= \nu\Delta v && \text{in } Q \\
u_x + v_y &= 0 && \text{in } Q
\end{aligned}
$$

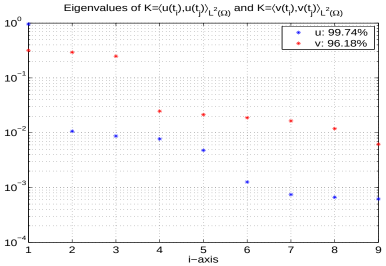


- $\nu = 5\cdot 10^{-3}$
- 3×4804 finite elements (Femlab)
- Time integration with Matlab's ode15s
- Snapshots $\mathcal{V}(u) = \mathrm{span}\,\{u(t_1),\dots,u(t_{21})\}$

  and $\mathcal{V}(v) = \mathrm{span}\,\{v(t_1),\dots,v(t_{21})\}$



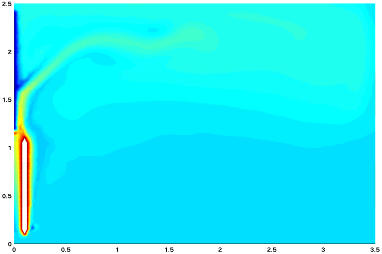


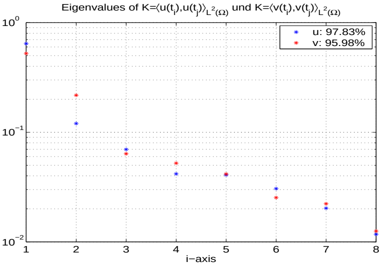


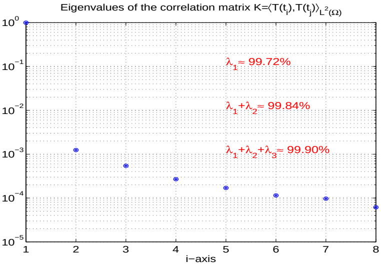
Numerical example: Energy transport (Boussinesq)

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

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







Reduced-order modeling (ROM)

- 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:

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

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

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

ROM for heat equation

- 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 $\mathcal{K}^n$: $\alpha_j = \frac{1}{n}$

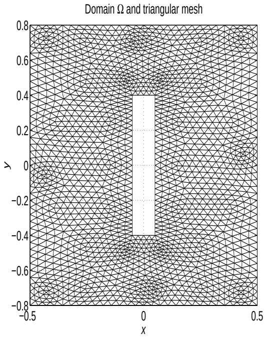
$$\frac{1}{n}\langle y_j^m, y_i^m\rangle = \frac{1}{n}\sum_{k,l=1}^{n} Y_{ik}Y_{jl}\langle \varphi_l, \varphi_k\rangle = \left(\tfrac{1}{n}Y^T MY\right)_{ij}$$

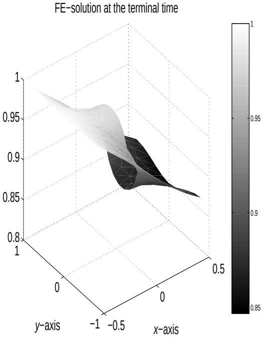
  with $M_{ij} = \langle \varphi_j, \varphi_i\rangle$ (mass or stiffness matrix)
- ROM for heat equation: $y^\ell(t) \in V^\ell = \mathrm{span}\,\{\psi_1, \ldots, \psi_\ell\} \subset V^m$

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

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 $0 = t_1 < \ldots < t_n = 5$

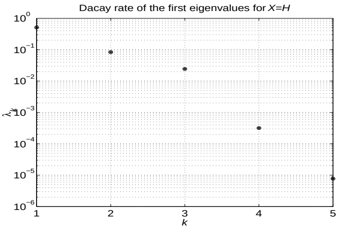
Heat flow in a block (Part 2)

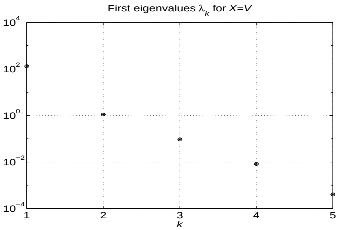
- FE space $V^m = \mathrm{span}\,\{\varphi_1, \ldots, \varphi_m\}$, $m = 1844$
- Time grid: $T = 5$, $n = 126$, $\delta t = \frac{T}{n-1}$, $t_j = (j-1)\delta t$, $1 \le j \le n$
- Snapshots: $y_j^m = \sum_{i=1}^{m} Y_{ij}\varphi_i$, $1 \le j \le n$
- Inner product: $\langle u, v\rangle = \int_\Omega uv\,\mathrm{d}x$ or $\langle u, v\rangle = \int_\Omega uv + \nabla u \cdot \nabla v\,\mathrm{d}x$
- Computation of the correlation matrix $(m \gg n)$: $\mathcal{K}^n = \frac{1}{n} Y^T M Y$ with $M = ((\langle \varphi_j, \varphi_i\rangle))$
- EVD for $\mathcal{K}^n$: $\left(\frac{1}{n} Y^T M Y\right) v_i = \lambda_i v_i$ 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:

$$\langle u, v\rangle = \begin{cases} \int_\Omega uv\,\mathrm{d}x & \text{left plot} \\ \int_\Omega uv + \nabla u \cdot \nabla v\,\mathrm{d}x & \text{right plot} \end{cases}$$



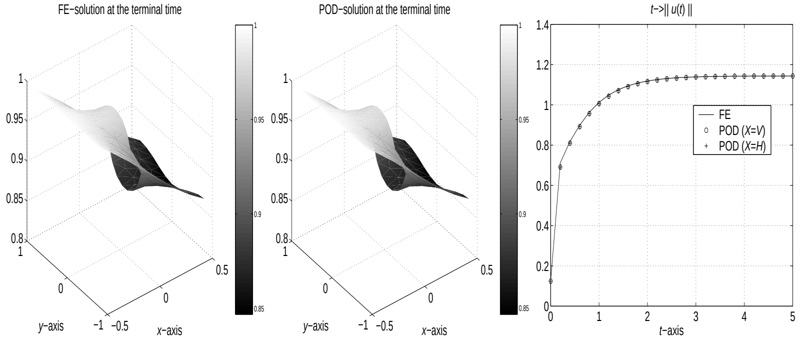


- Approximation property, e.g., for $\ell = 5$

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

Heat flow in a block (Part 4)

- ROM: $\ell = 5$ POD basis functions
- FE-/POD-solution and error:



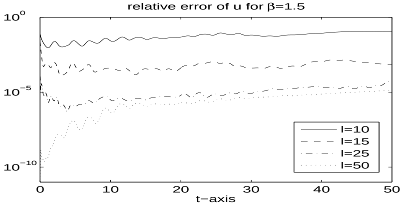
ROM for λ-ω systems

- 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

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

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- Kunisch & V.: Control of Burgers' equation by a reduced order approach using proper orthogonal decomposition, JOTA, 102:345-371, 1999
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