

# Model Reduction using Proper Orthogonal Decomposition and Applications in Optimization

Workshop on RB and POD Model-Order Reduction, Konstanz

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# POD-Galerkin ansatz

## MOTIVATION:

Find finite elements  $\{u_1, \dots, u_l\}$  which reflect the dynamics of the evolution equation

$$\begin{cases} \dot{y}(t) - Ay(t) &= f(t) \\ y(0) &= y_0 \end{cases},$$

i.e.  $y^l(t) := \sum_{i=1}^l y_i(t)u_i$  determined by solving the reduced Galerkin system

$$\begin{cases} \mathbf{M}(u)\dot{y}(t) - \mathbf{A}(u)y(t) &= \mathbf{F}(u)(t) \\ \mathbf{M}(u)y(0) &= y_0(u) \end{cases},$$

is a good approximation for  $y$  where  $l$  is quite small.



# Singular value decomposition

Let  $y_1, \dots, y_n \in \mathbb{R}^m$  the columns of a matrix  $Y \in \mathbb{R}^{m \times n}$  of rank  $d$ .

Then there are  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_d > 0$  and orthogonal matrices  $U \in \mathbb{R}^{m \times m}$  and  $V \in \mathbb{R}^{n \times n}$  such that

$$U^t Y V = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} =: \Sigma \in \mathbb{R}^{m \times n}, \quad D = \text{diag}(\sigma) \in \mathbb{R}^{d \times d}.$$



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- The columns  $u_1, \dots, u_m$  of  $U$  are the eigenvectors of  $Y Y^t$  corresponding to the eigenvalues  $\sigma_1^2, \dots, \sigma_d^2, 0, \dots, 0$ .
- Analogously, the columns  $v_1, \dots, v_n$  of  $V$  are the eigenvectors of  $Y^t Y$  corresponding to the eigenvalues  $\sigma_1^2, \dots, \sigma_d^2, 0, \dots, 0$ .
- The columns of  $Y$  can be represented by

$$y_j = \sum_{i=1}^d \langle y_j, u_i \rangle u_i.$$



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- The representation

$$Y = U \Sigma V^t$$

is called the **Proper Orthogonal Decomposition (POD)** of  $Y$ .

- The orthogonal subbasis  $U^l := \{u_1, \dots, u_l\}$  of the image  $\text{Im}(Y)$  is called the **POD-basis of rank  $l$**  ( $l \leq d$ ).
- The optimal representation of  $y$  as a linear combination with  $l$  vectors is

$$y \approx \sum_{i=1}^l \langle y, u_i \rangle u_i :$$



# POD as best-approximation

**THEOREM.** The minimization problem

$$\left\{ \begin{array}{l} \min_{(\tilde{u}_1, \dots, \tilde{u}_l)} \sum_{j=1}^n \left\| y_j - \sum_{i=1}^l \langle y_j, \tilde{u}_i \rangle \tilde{u}_i \right\|^2 \\ \text{subject to } \langle \tilde{u}_i, \tilde{u}_j \rangle = \delta_{ij} \end{array} \right.$$

is solved by the POD-basis  $(u_1, \dots, u_l)$ .



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is solved by the POD-basis  $(u_1, \dots, u_l)$ .

The [Pythagoras theorem](#) states that this optimization problem is equivalent to

$$\left\{ \begin{array}{l} \max_{(\tilde{u}_1, \dots, \tilde{u}_l)} \sum_{j=1}^n \sum_{i=1}^l |\langle y_j, \tilde{u}_i \rangle|^2 \\ \text{subject to } \langle \tilde{u}_i, \tilde{u}_j \rangle = \delta_{ij} \end{array} \right.$$



# POD as best-approximation

To solve the constraint maximization problem, we introduce the **Lagrange function**

$$\mathcal{L} : \mathbb{R}^{m \times l} \times \mathbb{R}^{l \times l}$$

by

$$\mathcal{L}(\tilde{U}, \Lambda) := \sum_{j=1}^n \sum_{i=1}^l |\langle y_j, \tilde{u}_i \rangle|^2 + \sum_{j=1}^l \sum_{i=1}^l \lambda_{ij} (\delta_{ij} - \langle \tilde{u}_i, \tilde{u}_j \rangle).$$



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The first-order optimality conditions

$$\frac{\partial}{\partial \tilde{u}_i} \mathcal{L}(\tilde{U}, \Lambda) = 0$$

can be transformed into

$$\underbrace{\sum_{j=1}^n \langle y_j, \tilde{u}_i \rangle y_j}_{=YY'\tilde{u}_i} = \frac{1}{2} \sum_{j=1}^l (\lambda_{ji} + \lambda_{ij}) \tilde{u}_i.$$



# POD as best-approximation

Together with the remaining first-order optimality conditions

$$\frac{\partial}{\partial \lambda_{ij}} \mathcal{L}(\tilde{U}, \Lambda) = \delta_{ij} - \langle \tilde{u}_i, \tilde{u}_j \rangle = 0,$$

we get  $\lambda_{ij} = \lambda_{ii} \delta_{ij}$  which implies

$$YY^t \tilde{u}_i = \lambda_{ii} \tilde{u}_i.$$

Hence,  $\tilde{U}^* = U$  and  $\Lambda^* = \text{diag}(\sigma_1^2, \dots, \sigma_l^2)$  solves the optimization problem and

$$\max_{(\tilde{u}_1, \dots, \tilde{u}_l)} \sum_{j=1}^n \sum_{i=1}^l |\langle y_j, \tilde{u}_i \rangle|^2 = \sum_{i=1}^l \sigma_i^2.$$



# Approximation of $\mathcal{L}^2(\Omega)$

Let  $\Omega := (a, b) \subseteq \mathbb{R}^1$ ,  $m \in \mathbb{N}$ ,  $h := \frac{b-a}{m-1}$ ,  $x := (x_1, \dots, x_m) \in \mathbb{R}^m$ ,  $x_i := (i-1)h \in \bar{\Omega}$ .

We approximate the infinite-dimensional Lebesgue space

$$\mathcal{L}^2(\Omega) := \{\varphi : \Omega \rightarrow \mathbb{R} \mid \langle \varphi, \varphi \rangle_{\mathcal{L}^2} < \infty\}, \quad \langle \varphi, \psi \rangle_{\mathcal{L}^2} := \int_{\Omega} \varphi(x)\psi(x) \, dx$$

by  $\varphi \mapsto \varphi_h := \varphi(x) \in \mathbb{R}^m$ ,

$$\mathcal{L}_h^2(\Omega) := \mathbb{R}^m, \quad \langle \varphi_h, \psi_h \rangle_{\mathcal{L}_h^2} := \frac{h}{2}\varphi_h^1\psi_h^1 + \sum_{i=2}^{m-1} h\varphi_h^i\psi_h^i + \frac{h}{2}\varphi_h^m\psi_h^m,$$

the trapezoidal rule for numerical integration.

Let  $W := \text{diag}(\frac{h}{2}, h, \dots, h, \frac{h}{2}) \in \mathbb{R}^{m \times m}$  (symmetric & positive definite). Then  $\langle \cdot, \cdot \rangle_{\mathcal{L}_h^2}$  can be considered as the weighted  $\mathbb{R}^m$ -scalar product

$$\langle \varphi_h, \psi_h \rangle_{\mathcal{L}_h^2} = \langle \varphi_h, W\psi_h \rangle \approx \langle \varphi, \psi \rangle_{\mathcal{L}^2}.$$



# The weighted POD method in $\mathbb{R}^m$

**THEOREM.** Let  $Y \in \mathbb{R}^{m \times n}$ ,  $\text{rank}(Y) = d$ , and  $W \in \mathbb{R}^{m \times m}$  symmetric & positive definite,  $\langle \cdot, \cdot \rangle_W := \langle \cdot, W \cdot \rangle$ .

Let  $\bar{Y} := \sqrt{W}Y$  and  $\bar{Y} = \bar{U}\Sigma\bar{V}^t$  the SVD of  $\bar{Y}$ .

Then the solution to the minimization problem

$$\left\{ \begin{array}{l} \min_{(\tilde{u}_1, \dots, \tilde{u}_l)} \sum_{j=1}^n \left\| y_j - \sum_{i=1}^l \langle y_j, \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 \\ \text{subject to } \langle \tilde{u}_i, \tilde{u}_j \rangle_W = \delta_{ij} \end{array} \right.$$

is given by  $u_i = \sqrt{W}^{-1} \tilde{u}_i$ .



# Finite differences for the one-dimensional heat equation

Let  $T > 0$  and  $\Theta := (0, T)$ . We transform the one-dimensional heat equation

$$\begin{cases} \dot{y}(t, x) - \Delta y(t, x) &= f(t, x) & \text{on } \Theta \times \Omega \\ y_x(t, x) &= 0 & \text{on } \Theta \times \partial\Omega \\ y(0) &= y_0 & \text{on } \Omega \end{cases} \quad (\text{pde})$$

via

$$y(t, \cdot) \approx y_h(t) \in \mathbb{R}^m, \quad \Delta y(t, x_i) \approx \frac{y_h^{i-1}(t) - 2y_h^i(t) + y_h^{i+1}(t)}{h^2}$$

into a system of ordinary differential equations

$$\begin{cases} \dot{y}_h(t) - A_h y_h(t) &= f_h(t) & \text{on } \Theta \\ y_h(0) &= y_{0,h} \end{cases} \quad (\text{pde}_h)$$



# Finite differences for the one-dimensional heat equation

with

$$A_h = \frac{1}{h^2} \begin{pmatrix} -2 & 2 & & & & \\ 1 & -2 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & 1 & -2 & 1 & \\ & & & 2 & -2 & \end{pmatrix}$$

and

$$f_h(t) = \begin{pmatrix} f(t, x_1) \\ f(t, x_2) \\ \vdots \\ f(t, x_{m-1}) \\ f(t, x_m) \end{pmatrix}, \quad y_{0,h} = \begin{pmatrix} y_0(x_1) \\ y_0(x_2) \\ \vdots \\ y_0(x_{m-1}) \\ y_0(x_m) \end{pmatrix}.$$



# The continuous POD method

**THEOREM:** Let  $y_h \in C^1(\Theta, \mathbb{R}^m) \cap C^0(\bar{\Theta}, \mathbb{R}^m)$  the solution to (pde<sub>h</sub>).

Consider the operator  $\mathcal{Y}_h \in \mathcal{L}_b(\mathcal{L}^2(\Theta, \mathbb{R}), \mathbb{R}^m)$  and the corresponding adjoint operator  $\mathcal{Y}_h^* \in \mathcal{L}_b(\mathbb{R}^m, \mathcal{L}^2(\Theta, \mathbb{R}))$ , given by

$$\mathcal{Y}_h \varphi := \int_{\Theta} \varphi(t) y_h(t) \, dt \in \mathbb{R}^m, \quad \mathcal{Y}_h^* u := \langle u, y_h(\cdot) \rangle_W \in \mathcal{L}^2(\Theta, \mathbb{R}).$$

Let  $U^l = (u_1, \dots, u_l)$  a POD-basis of rank  $l$  to the operator  $\mathcal{Y}_h \mathcal{Y}_h^* : \mathbb{R}^m \rightarrow \mathbb{R}^m$ .

Then  $U^l$  solves the minimization problem

$$\left\{ \begin{array}{l} \min_{\tilde{u}_1, \dots, \tilde{u}_l} \int_{\Theta} \left\| y_h(t) - \sum_{i=1}^l \langle y_h(t), \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 dt \\ \text{subject to} \quad \langle \tilde{u}_i, \tilde{u}_j \rangle_W = \delta_{ij} \end{array} \right.$$



# The Reduced Order Model

To solve  $(\text{pde}_h)$  approximatively with little numerical effort, we make the **POD-Galerkin ansatz**

$$y^l(t) := \sum_{i=1}^l y_i^l(t) u_i \approx y_h(t).$$

The desired vector of the time-dependent coefficients,  $y^l(t) \in \mathbb{R}^m$ , is given as the solution to the **Reduced-Order Model (ROM)**

$$\begin{cases} \mathbf{M}(u) \dot{y}^l(t) - \mathbf{A}(u) y^l(t) &= \mathbf{F}(u)(t) & \text{on } \Theta \\ \mathbf{M}(u) y^l(0) &= y_0(u) \end{cases} \quad (\text{pde}_h^l)$$

where  $\mathbf{M}(u) := (\langle u_i, u_j \rangle_W) = \text{Id}(l)$ ,  $\mathbf{A}(u) := (\langle A_h u_i, u_j \rangle_W)$ ,  $\mathbf{F}(u) := (\langle f_h(t), u_i \rangle_W)$  and  $y_0(u) = (\langle y_{0,h}, u_i \rangle_W)$ .



# Error analysis for continuous ROM

There exists some  $C > 0$  such that

$$\int_{\Theta} \|y_h(t) - y^l(t)\|_W^2 dt \leq C \sum_{i=l+1}^d \lambda_i + C \sum_{i=l+1}^m \int_{\Theta} |\langle \dot{y}_h(t), u_i \rangle_W|^2 dt.$$



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To avoid the last term, a POD basis which also respects the time derivative of  $y$  can be determined as the solution to

$$\left\{ \begin{array}{l} \min_{\tilde{u}_1, \dots, \tilde{u}_l} \int_{\Theta} \left\| y(t) - \sum_{i=1}^l \langle y(t), \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 dt + \int_{\Theta} \left\| \dot{y}(t) - \sum_{i=1}^l \langle \dot{y}(t), \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 dt \\ \text{subject to } \langle \tilde{u}_i, \tilde{u}_j \rangle_W = \delta_{ij} \end{array} \right.$$



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which is given as the set of eigenvectors to the  $l$  largest eigenvalues of  $\mathcal{Y}_h \mathcal{Y}_h^* + \dot{\mathcal{Y}}_h \dot{\mathcal{Y}}_h^*$ ,

$$\dot{\mathcal{Y}}_h \varphi := \int_{\Theta} \varphi(t) \dot{y}_h(t) dt \in \mathbb{R}^m, \quad \dot{\mathcal{Y}}_h^* u := \langle u, \dot{y}_h(\cdot) \rangle_W \in \mathcal{L}^2(\Theta, \mathbb{R}).$$



# Time discretization for the heat equation

Let  $n \in \mathbb{N}$ ,  $k := \frac{T}{n-1}$ ,  $t_j := (j-1)k \in \Theta$  and  $Y_j \approx y_h(t_j)$ .

We transform (pde<sub>h</sub>) via

$$y_h(\cdot) \approx Y \in \mathbb{R}^{m \times n}, \quad \dot{y}_h(t_j) \approx \frac{Y_j - Y_{j-1}}{k}$$

into a linear system of equations,

$$\begin{cases} \frac{Y_j - Y_{j-1}}{k} - A_h Y_j & = F \\ Y_1 & = Y_0 \end{cases} \quad (\text{pde}_{h,k})$$

where  $F = (f_h(t_j))$  and  $Y_0 = y_{0,h}$ .

Hence, we have  $y(t_j, x_i) \approx y_{h,i}(t_j) \approx Y_{ij}$ .



# The discrete POD method

**THEOREM:** Let  $\alpha = (\frac{k}{2}, k, \dots, k, \frac{k}{2}) \in \mathbb{R}^n$  the corresponding trapezoidal weights.

Let  $U^l = (u_1, \dots, u_l)$  a POD basis to the operator

$$\bar{Y} \text{diag}(\alpha) \bar{Y}^t : u \mapsto \sum_{j=1}^n \alpha_j \langle Y_j, u \rangle_W Y_j \approx \int_{\Theta} \langle y_h(t), u \rangle_W y_h(t) dt = \mathcal{Y}_h \mathcal{Y}_h^* u.$$

Then  $U^l$  solves the minimization problem

$$\left\{ \begin{array}{l} \min_{(\tilde{u}_1, \dots, \tilde{u}_l)} \sum_{j=1}^n \alpha_j \left\| Y_j - \sum_{i=1}^l \langle Y_j, \tilde{u}_i \rangle_W \tilde{u}_i \right\|_W^2 \\ \text{subject to } \langle \tilde{u}_i, \tilde{u}_j \rangle_W = \delta_{ij} \end{array} \right.$$

In general we have  $\| \bar{Y} \text{diag}(\alpha) \bar{Y}^t - \mathcal{Y}_h \mathcal{Y}_h^* \|_{\mathcal{L}_b(\mathbb{R}^m, \mathbb{R}^m)} \xrightarrow{n \rightarrow \infty} 0$ .



# The homogenous one-dimensional heat equation

Let  $\Omega = (0, 2)$ ,  $\Theta = (0, 3)$ ,  $m = 2500$  the number of time discretization points and  $n = 7500$  the number of spatial gridpoints.

$y \in \mathbb{R}^{m \times n}$ ,  $y_{ij} \approx y(t_i, x_j)$  denotes the approximative solution to

$$\begin{cases} \dot{y}(t, x) - \Delta y(t, x) = 0 & \text{on } \Theta \times \Omega \\ y(t, x) = 0 & \text{on } \Theta \times \partial\Omega \\ y(0, x) = y_0(x) := -x^2 + 2x & \text{on } \Omega \end{cases}$$

calculated by central differences for  $\Delta$  and the implicit Euler method for  $\frac{d}{dt}$  in **4.45 sec.**

The calculation of the first 10 pod elements takes **19.88 sec.**

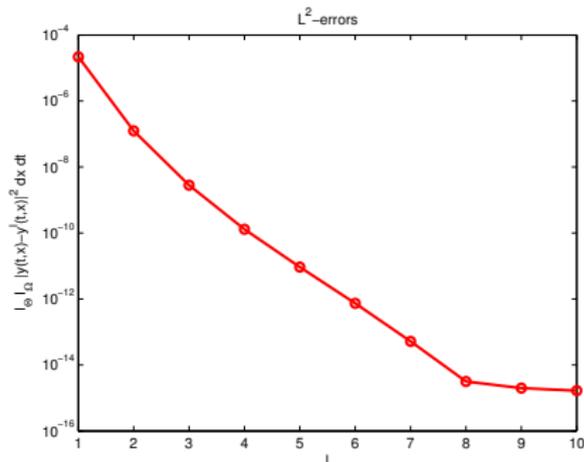
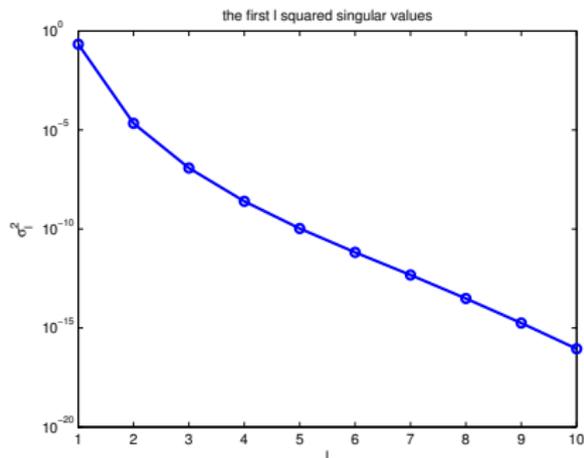


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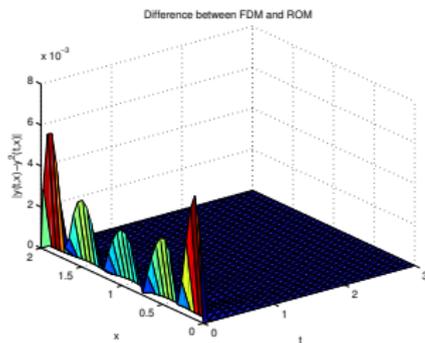
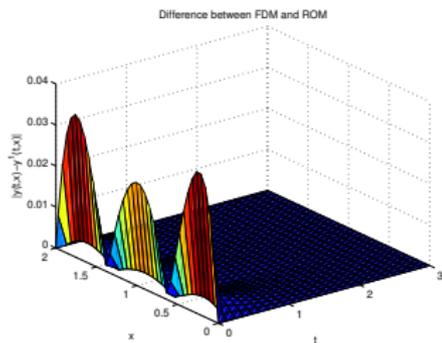
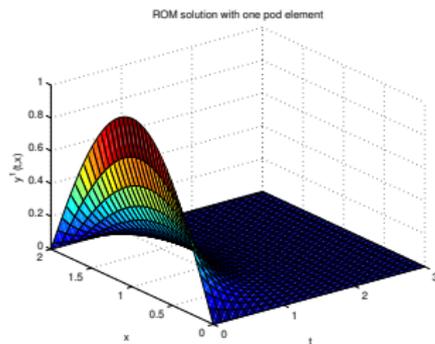
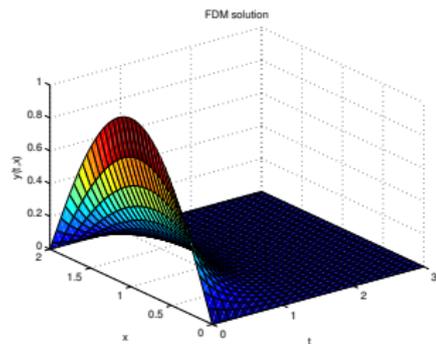
l	eigval.	time absol. / relat.	L <sup>2</sup> error	inform.
1	2.16e-01	0.51sec / 11.66%	2.17e-05	96.52%
2	2.16e-05	0.50sec / 11.25%	1.25e-07	99.39%
3	1.20e-07	0.55sec / 12.49%	2.80e-09	99.83%
4	2.51e-09	0.58sec / 13.06%	1.29e-10	99.94%
5	1.05e-10	0.59sec / 13.47%	9.23e-12	99.98%
6	6.63e-12	0.58sec / 13.06%	7.38e-13	99.99%
7	4.74e-13	0.58sec / 13.04%	5.17e-14	99.99%
8	3.10e-14	0.59sec / 13.31%	3.15e-15	99.99%
9	1.77e-15	0.58sec / 13.10%	1.98e-15	99.99%
10	8.81e-17	0.60sec / 13.61%	1.65e-15	99.99%



# The homogenous one-dimensional heat equation



# The homogenous one-dimensional heat equation



# The controlled one-dimensional heat equation

Consider the optimization problem

$$\min_{(y,u) \in Y \times U} J(y, u) = \frac{1}{2} \|y\|_{\mathcal{L}^2(\Theta \times \Omega)}^2 + \frac{1}{2} \|u\|_{\mathcal{L}^2(\Theta)}^2$$

subject to

$$\begin{cases} \dot{y}(t, x) - \Delta y(t, x) = f(t, x) + u(t)\chi(x) & \text{for } (t, x) \in \Theta \times \Omega \\ y(t, x) = 0 & \text{for } (t, x) \in \Theta \times \partial\Omega \\ y(0, x) = y_0(x) & \text{for } x \in \Omega \end{cases} \quad (\text{pde}_u)$$



# The controlled one-dimensional heat equation

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- $f \in \mathcal{L}^2(\Theta \times \Omega)$  and  $y_0, \chi \in \mathcal{L}^2(\Omega)$  are given data.
- The state-control pair  $(y, u) \in Y \times U$  is desired.
- $U = \mathcal{L}^2(\Theta)$  and  $Y = \mathcal{L}^2(\Theta, \mathcal{H}_0^1(\Omega)) \cap \mathcal{H}^1(\Theta, \mathcal{H}_0^1(\Omega)^*)$ .
- $(\text{pde}_u)$  admits an affine linear and bounded solution operator  $S : U \rightarrow Y$ .



# Optimality condition and numerical strategy

We consider the equivalent unconstrained optimization problem

$$\min_{u \in U} \hat{J}(u) = \frac{1}{2} \|Su\|_{\mathcal{L}^2(\Theta \times \Omega)}^2 + \frac{1}{2} \|u\|_{\mathcal{L}^2(\Theta)}^2.$$

which admits a unique solution  $u^* \in U$ .



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- The first-order optimality condition is

$$\nabla \hat{J}(u) = S^* Su + u = 0$$

where  $S^* : Y \rightarrow U$  can be considered as the adjoint operator of  $S$ .



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- Let  $u_n \in U$  some suboptimal control, then the direction that guarantees maximal local decay of  $\hat{J}$  in  $u_n$  is  $d_n = -\nabla \hat{J}(u_n)$  and there is some stepsize  $s_n > 0$  such that  $u_{n+1} = u_n + s_n d_n$  satisfies  $\hat{J}(u_{n+1}) \ll \hat{J}(u_n)$ .



# Optimality condition and numerical strategy

We consider the equivalent unconstrained optimization problem

$$\min_{u \in U} \hat{J}(u) = \frac{1}{2} \|Su\|_{\mathcal{L}^2(\Theta \times \Omega)}^2 + \frac{1}{2} \|u\|_{\mathcal{L}^2(\Theta)}^2.$$

which admits a unique solution  $u^* \in U$ .

- The first-order optimality condition is

$$\nabla \hat{J}(u) = S^* Su + u = 0$$

where  $S^* : Y \rightarrow U$  can be considered as the adjoint operator of  $S$ .

- Let  $u_n \in U$  some suboptimal control, then the direction that guarantees maximal local decay of  $\hat{J}$  in  $u_n$  is  $d_n = -\nabla \hat{J}(u_n)$  and there is some stepsize  $s_n > 0$  such that  $u_{n+1} = u_n + s_n d_n$  satisfies  $\hat{J}(u_{n+1}) \ll \hat{J}(u_n)$ .
- $\ll$  is interpreted in the sense that a sequence  $(u_n)_{n \in \mathbb{N}}$  created in this way converges at least linearly towards  $u^*$ .



# Application of model reduction with POD

- We can determine  $d_n = -(S^* S u_n + u_n)$  by solving (pde<sub>u</sub>) and the corresponding adjoint equation (pde<sub>Su</sub><sup>\*</sup>).



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- We can determine  $d_n = -(S^* S u_n + u_n)$  by solving  $(\text{pde}_u)$  and the corresponding adjoint equation  $(\text{pde}_{S^* u}^*)$ .
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- But: To check if  $\hat{J}(u_{n+1}) \ll \hat{J}(u_n)$  requires to calculate  $S(u_n + s_n d_n)$ , i.e. to solve  $(\text{pde}_u)$  again and again.



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- To accelerate the algorithm, we determine a rank- $l$  POD basis of  $y_n = S u_n$  and solve  $y(s_n) = S(u_n + s_n d_n)$  by the cheap POD-Galerkin ansatz.



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- To summarize: The effort of POD model order reduction is justified if the POD basis is used during an iteration that requires many evaluations of partial differential equations, i.e. if the same POD basis is used for multiple Galerkin ansätze.



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