Universität Konstanz Fachbereich Mathematik und Statistik Prof. Dr. Stefan Volkwein Martin Gubisch, Oliver Lass 17.09.2013

Summerschool Reduced Basis Methods 2013 Solution Sheet



### PART A: POD FOR DYNAMICAL SYSTEMS

POD Galerkin ansatz. Consider the linear parabolic differential equation

$$M\dot{y}(t) + Ay(t) = f(t) + Bu(t), \qquad My(0) = y_{\circ}.$$

- 1. Find a linear and bounded operator  $S: U \to Y$  and  $\hat{y} \in Y$  such that  $y = Su + \hat{y}$ .
- 2. Complete line 7 and implement the function Rom in the algorithm

# Algorithm 1 (PodGalerkin)

**Require:**  $M, A, f, y_{\circ}, B, u, \Delta t, \ell_{\max}$ . 1: Solve  $\hat{y} = \text{State}(M, A, f, y_{\circ}, \Delta t)$ 2: Solve  $y_1 = \text{State}(M, A, Bu, 0, \Delta t)$  and  $y_2 = \text{State}(M, A, f + Bu, y_{\circ}, \Delta t)$ 3: Solve  $\Psi_1 = \text{Pod}(\Delta t, M, y_1, \ell_{\max})$  and  $\Psi_2 = \text{Pod}(\Delta t, M, y_2, \ell_{\max})$ 4: **for**  $\ell = 1, ..., \ell_{\max}$  **do** 5: Determine  $[M_1^{\ell}, A_1^{\ell}, B_1^{\ell}] = \text{Rom}(\Psi_1^{\ell}, M, A, B)$  and  $[M_2^{\ell}, A_2^{\ell}, B_2^{\ell}, f_2^{\ell}, y_{\circ 2}^{\ell}] = \text{Rom}(\Psi_2^{\ell}, M, A, B, f, y_{\circ})$ 6: Compute  $x_1^{\ell} = \text{State}(M_1^{\ell}, A_1^{\ell}, B_1^{\ell}u, 0, \Delta t)$  and  $x_2^{\ell} = \text{State}(M_2^{\ell}, A_2^{\ell}, f_2^{\ell} + B_2^{\ell}u, y_{\circ 2}^{\ell}, \Delta t)$ 7: Determine the corresponding high-dimensional states  $y_1^{\ell} = ..., y_2^{\ell} = ...$ 8: Compute  $e_1^{\ell} = ||y_2 - y_1^{\ell}||_Y$  and  $e_2^{\ell} = ||y_2 - y_2^{\ell}||_Y$ 

3. Visualize  $e_1, e_2$  and the first few Pod elements of  $\Psi_1, \Psi_2$ .

## Solutions.

1. We consider the homogeneous controlled and the inhomogeneous uncontrolled pdes

$$M\dot{y}(t) + Ay(t) = Bu(t) \& My(0) = 0, \qquad M\dot{y}(t) + Ay(t) = f(t) \& My(0) = y_0.$$

then S is the linear, bounded solution operator to the first problem and  $\hat{y}$  is the solution to the second one.

2. Let N be the dimension of the high-dimensional system and n be the number of control components, i.e.  $M, A \in \mathbb{R}^{N \times N}$  and  $B \in \mathbb{R}^{N \times n}$ . The function Rom assembles the system matrices of the reduced order model. For this purpose, the high-dimensional pde is transformed onto the space spanned by the POD basis elements which is provided by multiplication from the left with  $(\Psi^{\ell})^{\mathrm{T}} \in \mathbb{R}^{\ell \times N}$ ; further, the solution vector  $y(t) \in \mathbb{R}^{N}$  is replaced by its expansion in the POD basis,  $\sum x_i(t)\psi_i^{\ell} = \Psi^{\ell} \cdot x(t)$  where  $x(t) \in \mathbb{R}^{\ell}$ . The reduced pde is

$$M^{\ell} \dot{x}(t) + A^{\ell} x(t) = f^{\ell}(t) + B^{\ell} u(t), \qquad M^{\ell} x(0) = y_{0}^{\ell}$$

where  $M^{\ell}, A^{\ell}, B^{\ell}, f^{\ell}, y^{\ell}_{\circ}$  are calculated by the function ROM which is an implementation of

Algorithm 2 (ReducedOrderModel)

 $\begin{array}{l} \hline \mathbf{Require:} \ \Psi^{\ell}, M, A, B, f, y_{\circ}, y_{\Omega}, y_{\Omega}. \\ 1: \ M^{\ell} = (\Psi^{\ell})^{\mathrm{T}} M \Psi^{\ell} \in \mathbb{R}^{\ell \times \ell}, \ A^{\ell} = (\Psi^{\ell})^{\mathrm{T}} A \Psi^{\ell} \in \mathbb{R}^{\ell \times \ell}, \ B^{\ell} = (\Psi^{\ell})^{\mathrm{T}} B \in \mathbb{R}^{\ell \times n}. \\ 2: \ \text{if nargout} \geq 5 \ \text{then} \\ 3: \ f^{\ell}(t) = (\Psi^{\ell})^{\mathrm{T}} f(t) \in \mathbb{R}^{\ell}, \ y_{\circ}^{\ell} = (\Psi^{\ell})^{\mathrm{T}} y_{\circ} \in \mathbb{R}^{\ell} \\ 4: \ \text{end if} \\ 5: \ \text{if nargout} \geq 7 \ \text{then} \\ 6: \ y_{Q}^{\ell}(t) = (\Psi^{\ell})^{\mathrm{T}} y_{Q}(t) \in \mathbb{R}^{\ell}, \ y_{\Omega}^{\ell} = (\Psi^{\ell})^{\mathrm{T}} y_{\Omega} \in \mathbb{R}^{\ell}. \\ 7: \ \text{end if} \end{array}$ 

Notice: The coefficients for  $y_Q, y_\Omega$  are required later.

The full solutions  $y_1^\ell(t), y_2^\ell(t) \in \mathbb{R}^N$  are reconstructed by  $y_1^\ell(t) = \Psi_1^\ell \cdot x_1(t) + \hat{y}(t)$  and  $y_2^\ell(t) = \Psi_2^\ell \cdot x_2(t)$ .

3. We have a look at the inhomogeneous, controlled state solution  $y_2 = y_1 + \hat{y}$ , at the errors between the highdimensional FE model and the low-dimensional POD model and at the shape of the POD basis elements of the two ansatzes.



**Fig.** 1: The state solution with discontinuous initialization. As typical for linear parabolic equations, the initial value is smoothend imediately.



Fig. 2: The state errors caused by the model reduction. As one sees, the modified ansatz where just the snapshots of the homogeneous solution component  $y_1 = Su$  are used for the POD basis creation leads to significantly better results than the classical ansatz where the snapshots of  $y_2 = Su + \hat{y}$  generate the POD basis.



Fig. 3: The first POD basis elements  $\psi_1^l$  of the homogeneous ansatz (left) and  $\psi_2^l$  of the inhomogeneous one (right). As one sees, the rows  $\psi_2^l$  of  $\Psi_2$  include jumps at the positions where  $y_{\circ}$  is discontinuous to be able to reconstruct the initial value which is not required for the homogeneous ansatz.



Fig. 4: The reconstruction of the initial value,  $\Psi^{\ell} y_0^{\ell}$  for different POD basis ranks  $\ell$  with the modified ansatz (left) and the classical one (right). The approximation with the inhomogeneous basis  $\Psi_2$  works quite well where with  $\Psi_1$ , it is neither required nor possible to build up  $y_{\circ}$  accurately.

## PART B: OPTIMAL CONTROL OF PDES

Optimization problem. We consider the pde-constrained optimal control problem

$$\min J(y,u) = \frac{1}{2} \int_{0}^{T} \|y(t) - \vec{y}_{Q}(t)\|_{H}^{2} dt + \frac{1}{2} \|y(T) - \vec{y}_{\Omega}\|_{H}^{2} + \frac{\sigma}{2} \|u\|_{U}^{2}$$

subject to

$$M\dot{y}(t) + Ay(t) = f(t) + Bu(t) \& My(0) = y_{\circ}, \qquad u_a(t) \le u(t) \le u_b(t).$$

**Optimality system.** An optimal control-state pair  $(\bar{y}, \bar{u}) \in Y \times U$  is given by

$$M\dot{y}(t) + Ay(t) - f(t) - Bu(t) = 0, \qquad My(0) = y_{\circ},$$
  
$$-M\dot{p}(t) + Ap(t) + My(t) - y_{Q}(t) = 0, \qquad Mp(T) + My(T) - y_{\Omega}, = 0$$
  
$$u(t) - \mathbb{P}(\sigma^{-1}B^{*}p(t)) = 0$$

where  $\mathbb{P}(u) = \min(\max(u, u_a), u_b)$  is the canonical projection of U onto  $[u_a, u_b]$  and  $y_Q(t) = M\vec{y}_Q(t), y_\Omega = M\vec{y}_\Omega$ .

Lagrange calculus. The optimality system is derived by differentiating the Lagrange function

$$L(y, u, p) = \hat{J}(y, u) + \int_{0}^{1} \langle E(y, u)(t), p(t) \rangle_{L^{2}(V', V)} dt$$

with the modified objective functional  $\hat{J}: Y \times U \to \mathbb{R}$  and the constraints operator  $E: Y \times U \to \mathcal{L}^2(\Theta, \mathbb{R}^N)$ ,

$$\hat{J}(y,u) = \int_{0}^{T} \|y(T) - (\vec{y}_Q(t) - \hat{y}(t))\|_{H}^{2} dt + \|y(t) - (\vec{y}_\Omega(t) - \hat{y}(T))\|_{H}^{2} + \frac{\sigma}{2} \|u\|_{U}^{2},$$
  
$$E(y,u) = M\dot{y}(t) + Ay(t) - Bu(t).$$

Notice: The resulting variational inequality  $\forall \tilde{u} \in [u_a, u_b] : \langle \sigma u - B^* p, \tilde{u} - u \rangle_U \ge 0$  is equivalent to  $u = \mathbb{P}(\sigma^{-1}B^*p)$ .

- 4. Find a linear and bounded operator  $\tilde{S}: U \to Y$  and  $\hat{p} \in Y$  such that  $p = \tilde{S}u + \hat{p}$ .
- 5. Define a selfmapping F on U such that the optimal control  $\bar{u}$  is a fixpoint of F.
- 6. Formulate a condition of the regularisation parameter  $\sigma$  such that the corresponding Banach fixpoint iteration admits a unique solution.

## Solutions.

4. Consider the two initial value problems

$$\begin{split} -M\dot{p}(t) + Ap(t) &= -MSu(t) & \& \quad Mp(T) &= -MSu(T), \\ -M\dot{p}(t) + Ap(t) &= y_Q(t) - M\hat{y}(t) & \& \quad Mp(T) &= y_\Omega - M\hat{y}(T), \end{split}$$

then  $\hat{S}$  is the linear, bounded solution operator to the first one and  $\hat{p}$  is the solution of the second one.

- 5. Choose  $F(u) = \mathbb{P}(\sigma^{-1}(B^*\tilde{S}u + B^*\hat{p}))$ , then (y, u, p) solves the optimality system if and only if  $y = Su + \hat{y}$ ,  $p = \tilde{S}u + \hat{p}$  and F(u) = u.
- 6. We show that F is a contraction for suitable  $\sigma$ , i.e. that

$$\exists C \in (0,1) : \forall u, \tilde{u} \in U : \|F(u) - F(\tilde{u})\|_U \le C \|u - \tilde{u}\|_U.$$

Since  $\mathbb{P}$  is an orthogonal projector on the nonempty, closed, convex set  $[u_a, u_b]$ ,  $\mathbb{P}$  is Lipschitz continuous of order 1, i.e.  $\|\mathbb{P}(u) - \mathbb{P}(\tilde{u})\|_U \leq 1 \cdot \|u - \tilde{u}\|_U$  for all  $u, \tilde{u} \in U$ . Further, the operator  $B^*\tilde{S}$  is bounded. Hence:

$$||Fu - F\tilde{u}||_U \le \sigma^{-1} ||B^*\tilde{S}|| ||u - \tilde{u}||.$$

Choosing  $C = \sigma^{-1} \| B^* \tilde{S} \|$ , we get  $C \in (0, 1)$  for  $\sigma > \| B^* \tilde{S} \|$ .

## PART C: REDUCED ORDER MODELLUNG FOR OPTIMIZATION PROBLEMS

**Optimization algorithm.** We provide the following fixpoint strategy:

Algorithm 3 (SolverOptimizationProblem)

**Require:** initial control  $u_{\circ}$ , desired exactness  $\varepsilon$ , maximal iterations  $k_{\max}$ , inhomogeneous component  $B^*\hat{p}$ 1: Set  $k = 0, u = u_{\circ}$ 

2: repeat

3: Compute  $y_h = Su = \text{State}(M, A, Bu, 0, \Delta t)$ 

- 4: Compute  $p_h = \tilde{S}u = \texttt{fliplr}(\texttt{State}(M, A, -\texttt{fliplr}(My_h), -My(T), \Delta t))$
- 5: Evaluate  $u_{+} = \mathbb{P}(\sigma^{-1}(B^{\star}p_{h} + B^{\star}\hat{p}))$
- 6: **until**  $||u_+ u||_U < \varepsilon$  or  $k = k_{\max}$ .

7: Set  $u = u_+$  and k = k + 1

8: Return optimal control u.

Notice that the adjoint equation can be solved with the forward routine **State** as well by backwards transformation in time:

 $M\dot{q}(t) + Aq(t) = -M(Su)(T-t) \& Mq(0) = -M(Su)(T), \qquad p(t) = q(T-t).$ 

- 7. Design an algorithm which combines the model reduction via POD with the provided optimization strategy.
- 8. Visualize the errors between the suboptimal controls  $u^{\ell}$  and the optimal control u for  $\ell = 1, ..., 15$ .

### Solutions.

7. We have to calculate the inhomogeneous component  $B^{\star}\hat{p}$ , to solve the high-dimensional state equation to build up the snapshot matrix, to construct the reduced order system matrices and to execute the optimizer with the reduced objects as input parameters:

Algorithm 4 (ReducedOrderOptimization)

- 1: Calculate  $\hat{y}(t) = \texttt{State}(M, A, f, y_{\circ}, \Delta t)$ .
- 2: Calculate  $\hat{p}(t) = \texttt{fliplr}(\texttt{State}(M, A, \texttt{fliplr}(y_Q M\hat{y}), y_\Omega M\hat{y}(T), \Delta t)) \in \mathbb{R}^N$ .
- 3: Construct inhomogeneous component  $(B^*\hat{p})(t) \in \mathbb{R}^n$ .
- 4: Execute optimizer  $\bar{u}(t) = \text{Solver}(u_{\circ}, \epsilon, k_{\max}, M, A, B, \Delta t, \sigma, u_a, u_b, B^{\star}\hat{p}) \in \mathbb{R}^n$ .
- 5: Calculate snapshots  $y(t) = \text{State}(M, A, Bu_{\circ}, 0, \Delta t) \in \mathbb{R}^{N}$ .
- 6: Determine a rank- $\ell_{\max}$  POD basis  $\Psi = \operatorname{Pod}(\Delta t, M, y, \ell_{\max}) \in \mathbb{R}^{N \times \ell_{\max}}$ .
- 7: for  $\ell = 1, ..., \ell_{\max}$  do
- 8: Assemble reduced order model  $[M^{\ell}, A^{\ell}, B^{\ell}] = \operatorname{Rom}(\Psi^{\ell}, M, A, B) \in \mathbb{R}^{\ell \times \ell} \times \mathbb{R}^{\ell \times \ell} \times \mathbb{R}^{\ell \times n}$ .
- 9: Execute optimizer  $u^{\ell}(t) = \text{Solver}(u_{\circ}, \epsilon, k_{\max}, M^{\ell}, A^{\ell}, B^{\ell}, \Delta t, \sigma, u_a, u_b, B^{\star}\hat{p}) \in \mathbb{R}^n$ .
- 10: Compute control error  $e(\ell) = \|\bar{u} u^{\ell}\|_U$ .

```
11: end for
```

8. We visualize the optimal control functions  $\bar{u}_i$  first.



optimal controls

Fig. 5: The control bounds  $u_a = 0.25$  and  $u_b = 0.75$  are active for  $u_1, u_{10}$  and for the central components.

An efficient decay of the control errors can just be expected if the initial control guess  $u_{\circ}$  is already close to the optimal control  $\bar{u}$ . If this is not the case, the procedure may by repeated several times to construct a sequence  $(u_k^{\ell})_k$  with initialization  $u_{\circ 0}^{\ell} = u_{\circ}$  and  $u_{\circ k}^{\ell} = u_{k-1}^{\ell}$ , k = 2, ...



Fig. 6: The control errors with respect to the reduced control solutions  $u_1^{\ell}$ , calculated without a basis adaptivity strategy, and  $u_2^{\ell}$  where the POD basis is updated once by initialiting the snapshots with  $u_1^{\ell}$ . Indeed, the snapshots to  $u_1^{\ell}$  already numerically coincide with those to  $\bar{u}$ , i.e. a second basis update leads to no improvement in the error decay.

Further information, especially concerning the asymptotic behavior of the errors, decay rates, a priori error bounds and a posteriori error estimators, can be found in the literature.

# Literature

- Gubisch, M. & Volkwein, S.: POD reduced-order modelling for PDE constrained optimization. in preparation, 2013.
- [2] Hinze, M. & Rösch, A.: Discretization of Optimal Control Problems. Int. S. Num. Math., vol. 160: pp. 391–430, 2012.
- [3] Hinze, M. & Tröltzsch, F.: Discrete concepts versus error analysis in pde constrained optimization. GAMM-Mitt., vol. 33, no. 2: pp. 148–162, 2010.
- [4] Hinze, M. & Volkwein, S.: Error estimates for abstract linear-quadratic optimal control problems using proper orthogonal decomposition. Comput. Optim. Appl., vol. 39, no. 3: pp. 319–345, 2007.
- [5] Kunisch, K. & Volkwein, S.: Galerkin proper orthogonal decomposition methods for parabolic problems. Numer. Math., vol. 90, no. 1: pp. 117–148, 2001.
- [6] Kunisch, K. & Volkwein, S.: Optimal snapshot location for computing POD basis functions. ESAIM: M2AN, vol. 44: pp. 509–529, 2010.
- [7] Meidner, D. & Vexler, B.: A Priori Error Estimates for Space-Time Finite Element Discretization of Parabolic Optimal Control Problems Part II: Problems with Control Constraints. SIAM J. Contr. Optim., vol. 47, no. 3: pp. 1301–1329, 2008.
- [8] Tröltzsch, F.: Optimal Control of Partial Differential Equations. Theory, Methods and Applications, vol. 112. American Math. Society, Providence, 2010.
- [9] Tröltzsch, F. & Volkwein, S.: POD a-posteriori error estimates for linear-quadratic optimal control problems. Comp. Opt. Appl., vol. 44, no. 1: pp. 83–115, 2009.
- [10] Volkwein, S.: Proper Orthogonal Decomposition: Theory and Reduced-Order Modelling. Lecture Notes, University of Konstanz, 2012.