MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Adaptivity concepts for POD reduced-order modeling

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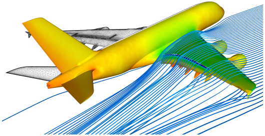
ICERM Mathematics of Reduced Order Models
17 February 2020

Modeling hierarchy (physics-based perspective)

Application	**Complex system**	 [1]
	↓ ↑	
Physics-based approach	**Mathematical model**	$$\begin{aligned} y_t + (y \cdot \nabla) y - \nu \Delta y + \nabla p &= f \\ \nabla \cdot y &= 0 \end{aligned}$$
	↓ ↓	
Offline phase	**High-fidelity discrete model**	$$\begin{aligned} M \frac{y_h^j - y_h^{j-1}}{\Delta t} + N(y_h^j) y_h^j - \nu A y_h^j + B^\mathsf{T} p_h^j &= f^j \\ B y_h^j &= 0 \end{aligned}$$
	↓ ↑	
Proper Orthogonal Decomposition (POD)	**Reduced-order model**	$$\begin{aligned} M_r \frac{y_r^j - y_r^{j-1}}{\Delta t} + N_r(y_r^j) y_r^j - \nu A_r y_r^j + B_r^\mathsf{T} p_r^j &= f_r^j \\ B_r y_r^j &= 0 \end{aligned}$$

[1] www.dlr.de, Numerical flow simulation on an Airbus A380

Challenge: input dependency of POD-MOR

Basic principle of POD-MOR:

High-fidelity model, dimension N

$$\begin{cases} \dot{y}(t) = f(t, y(t)) & t \in (0,T] \\ y(0) = y_0 \end{cases}$$

Low-order model, dimension $r \ll N$

$$\begin{cases} \dot{\eta}(t) = \Psi^{\mathsf{T}} f(t, \Psi\eta(t)) & t \in (0,T] \\ \eta(0) = \Psi^{\mathsf{T}} y_0 \end{cases}$$

Galerkin approximation: $y(t) \approx y_r(t) = \sum_{i=1}^{r} \eta_i(t)\psi_i = \Psi\eta(t)$

Construction of basis $\Psi = [\psi_1 \dots \psi_r]$ with POD:

- Collect snapshots by high-fidelity simulations or physical measurements[1]
- Identify embedded coherent structures

true solution → offline: high-fidelity snapshots → online: reduced-order model

POD-MOR is **input dependent**: ROM accuracy is limited by the snapshot information

[1] L. Sirovich. Turbulence and the dynamics of coherent structures I-III, Q. Appl. Math., 45(3):561-590, 1987

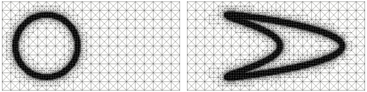
Agenda

Require 'good' snapshots: *Sufficiently good high-fidelity approximations of the true solution*

Goal: Use adaptive strategies in order to generate **good** snapshots **efficiently**

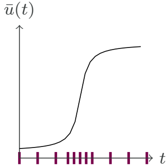
Space Adaptivity

- Combine POD with space-adapted snapshots
  $\rightarrow$ joint work with M. Hinze
- Conserve stability for incompressible flow
- Apply concept for optimal control

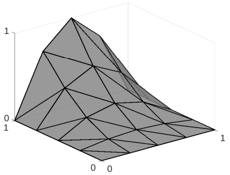


Time Adaptivity

- Snapshot location for POD-MOR in optimal control of linear systems
- Outlook to time adaptivity in MPC



Adaptivity concept

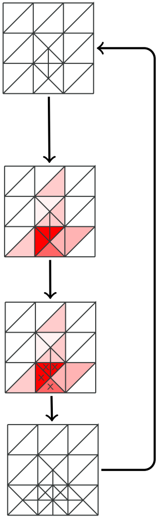


SOLVE

ESTIMATE — Residual based error indicator

MARK — Dörfler marking

REFINE — Mesh adaption



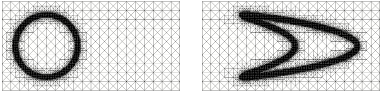
POD with space-adapted snapshots

POD-ROM procedure (discrete formulation):

- Snapshot sampling $Y = [y^1 \dots y^n] \in \mathbb{R}^{N \times n}$
- Compute POD modes $\{\psi_1, \dots, \psi_r\} \subset \mathbb{R}^N$
- Derive and solve POD-Galerkin model for $y_r(t) = \sum_{i=1}^r \eta_i(t)\psi_i$

static discretization

Challenge: Space-adaptive simulation

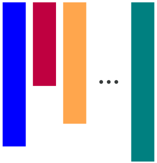


8235 $\qquad$ 15795

Degrees of freedom

Snapshots are vectors of different lengths

$Y \overset{?}{\neq} [y^1\ y^2\ y^3 \dots y^n] \overset{?}{\neq} \Psi\, \Sigma\, \Phi^{\mathsf{T}}$



Solution idea: Consider procedure from an ∞-dimensional perspective

POD with space-adapted snapshots

POD-ROM procedure (discrete formulation):

- Snapshot sampling $y^1 \in V^1, \ldots, y^n \in V^n$ with $V^1, \ldots, V^n \subset X$
- Compute POD modes $\{\psi_1, \ldots, \psi_r\} \subset X$
- Derive and solve POD-Galerkin model for $y_r(t) = \sum_{i=1}^{r} \eta_i(t)\psi_i$

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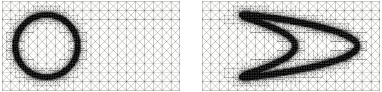

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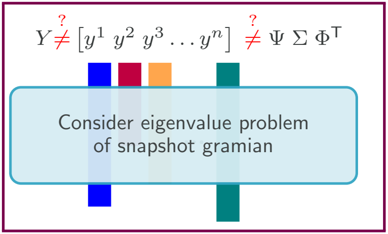


Solution idea: Consider procedure from an ∞-dimensional perspective

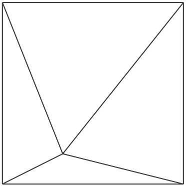
Literature on POD with space-adapted snapshots

- Fang, Pain, Navon, Piggott, Gorman, Allison, Goddard: *Reduced-order modelling of an adaptive mesh ocean model.* Int. J. Numer. Meth. Fluids, 59:827-851, 2008.
- Lass: *Reduced order modeling and parameter identification for coupled nonlinear PDE systems.* PhD thesis, Univ. Konstanz, 2014.
- Hinze, Krenciszek, Pinnau: *Proper Orthogonal Decomposition for Free Boundary Value Problems.* Hamb. Beitr. Angew. Math., 2014.
- Yano: *A minimum-residual mixed reduced basis method: Exact residual certification and simultaneous finite-element reduced-basis refinement.* ESAIM:M2AN, 50(1):163-185, 2016.
- Ali, Steih, Urban: *Reduced basis methods with adaptive snapshot computations.* Adv. Comput. Math., 43(2):257-294, 2017.
- Ullmann, Rotkvic, Lang: *POD-Galerkin reduced-order modeling with adaptive finite element snapshots.* J. Comput. Phys., 325:244-258, 2016.
- G., Hinze: *POD reduced-order modeling for evolution equations utilizing arbitrary finite element discretizations*, Adv. Comput. Math., 44(6):1941-1978, 2018.
- [...]

Consider eigenvalue problem of snapshot Gramian

$$\mathcal{K} : \mathbb{R}^n \to \mathbb{R}^n, \quad \mathcal{K}_{ij} = (\sqrt{\alpha_i \alpha_j}(y^i, y^j)_X)$$
$$\mathcal{K}\phi_i = \lambda_i \phi_i, \quad i = 1, \dots, r$$

→ Advantage: great flexibility concerning discretization
→ (might get computationally involved)



- Collision detection
- Mesh intersection
- Integrate over boundary

[1] POD in Hilbert spaces: K. Kunisch, S. Volkwein. Galerkin POD for a general equation in fluid dynamics, SIAM J. Numer. Anal., 40(2):492-515, 2002

POD: ∞-dimensional perspective[1]

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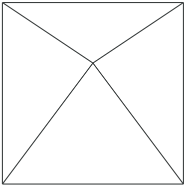

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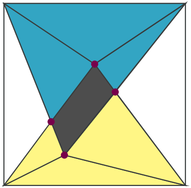

- Collision detection
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POD Galerkin ansatz:

$$y_r(t) = \sum_{i=1}^{r} \eta_i(t)\psi_i = \sum_{i=1}^{r} \eta_i(t) \frac{1}{\sqrt{\lambda_i}} \mathcal{Y}\phi_i \quad \text{for all } t \in [0, T]$$

Evolution problem:

$$\begin{cases} \frac{d}{dt}(y(t), v) = \langle f(t, y(t)), v \rangle & \forall v \in V \\ (y(0), v) = (y_0, v) & \forall v \in V \end{cases}$$

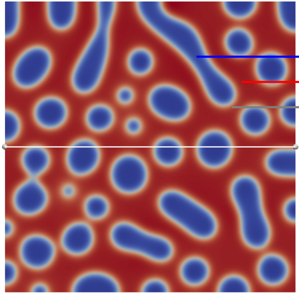
ROM:

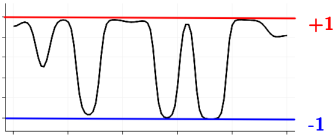
$$\begin{cases} \Lambda \Phi^{\mathsf{T}} \mathcal{K} \Phi \Lambda \, \dot{\eta}(t) = \Lambda F(t, \eta(t)) \\ \Lambda \Phi^{\mathsf{T}} \mathcal{K} \Phi \Lambda \, \eta(0) = \Lambda \bar{\eta}_0 \end{cases}$$

$$\Lambda = \text{diag}(1/\sqrt{\lambda_1}, \ldots, 1/\sqrt{\lambda_r}), \; \Phi = [\phi_1 \cdots \phi_r]$$

[1] POD in Hilbert spaces: K. Kunisch, S. Volkwein. Galerkin POD for a general equation in fluid dynamics, SIAM J. Numer. Anal., 40(2):492-515, 2002

Numerical example: Cahn-Hilliard model[1]





Modeling:

- introduce phase field variable $\varphi \in [-1, 1]$
  - $\varphi = -1$ pure phase
  - $\varphi = +1$ pure phase
  - $\varphi \in (-1, 1)$ interface
- diffuse interface approach
  $\oplus$ topology changes can be handled naturally
- interface thickness $\sim \varepsilon$

Ginzburg-Landau energy:

$$\mathcal{E}(\varphi) = \frac{\varepsilon}{2} \int_\Omega |\nabla \varphi|^2 dx + \frac{1}{\varepsilon} \int_\Omega \mathcal{F}(\varphi) dx$$

$$\text{s.t. } \int_\Omega \varphi dx = c_{vol}$$

- Equilibrium state: minimize $\mathcal{E}$ s.t. mass conservation

[1] J. W. Cahn, J. E. Hilliard. Free energy of a nonuniform system. I. Interfacial free energy. The Journal of chemical physics, 28:258-267, 1958

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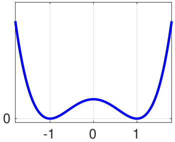

Double-well free energy
$\mathcal{F}(\varphi) = \frac{1}{4}(1-\varphi^2)^2$

- introduce chemical potential μ as first variation of $\mathcal{E}$ w.r.t. φ

Cahn-Hilliard

φ phase field
μ chemical potential

$$\begin{cases} \varphi_t + y\cdot\nabla\varphi - \text{div}(b\nabla\mu) = 0 & \text{in } (0,T]\times\Omega \\ -\varepsilon\Delta\varphi + \frac{1}{\varepsilon}\mathcal{F}'(\varphi) = \mu & \text{in } (0,T]\times\Omega \\ \partial_n\varphi = \partial_n\mu = 0 & \text{on } [0,T]\times\partial\Omega \\ \varphi(0,\cdot) = \varphi_0 & \text{in } \Omega \end{cases}$$

b mobility
y velocity
ε interface parameter
φ_0 initial value

$t = 0$ $\quad$ $t = T/2$ $\quad$ $t = T$

Numerical example: Cahn-Hilliard model

Ginzburg-Landau energy:

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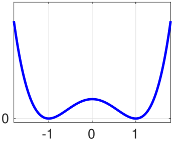

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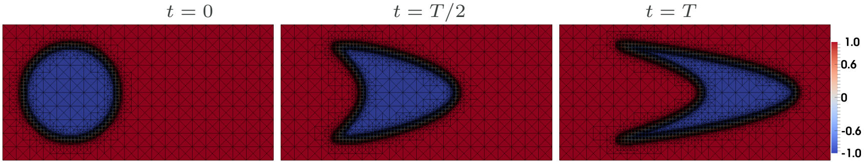
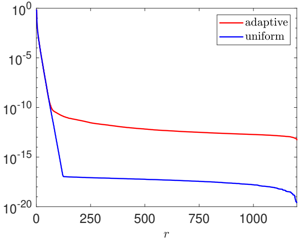
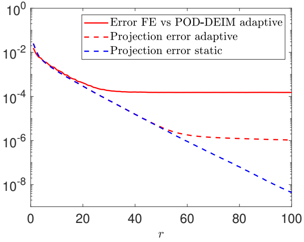


Numerics: POD-MOR with space-adapted snapshots

Eigenvalues for φ snapshots



Relative $L^2(0,T;\Omega)$-error in φ



Speed up

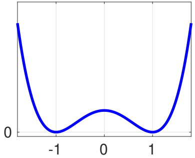
CPU times	
Static FE solution	8.5 h
Adaptive FE solution	1.8 h
ROM construction	12 min
ROM solution	12 min
ROM-DEIM solution	0.2 s

Speed up (Static FE solution vs. Adaptive FE solution): 4.7

Speed up (Adaptive FE solution vs. ROM-DEIM solution): 32000

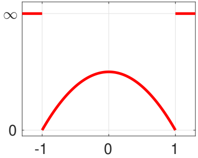
$r = 30$

Relative error
$1.75 \cdot 10^{-04}$
$1.84 \cdot 10^{-04}$



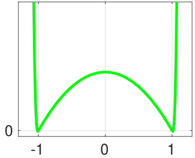
double-well

$\frac{1}{4}(1-\varphi^2)^2$



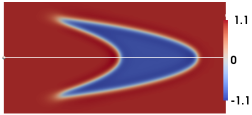
double-obstacle

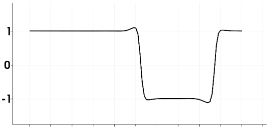
$I_{[-1,1]}(\varphi) - \frac{1}{2}\varphi^2$



Moreau-Yosida relaxation

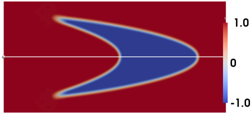
$\frac{1}{2}(1-\varphi^2) + \frac{s}{r}(\max(\varphi-1,0)^r$
$+ \min(\varphi+1,0)^r)$

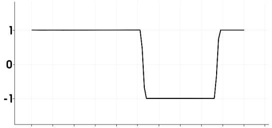


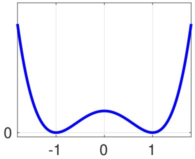


- non-smooth
- variational inequality

FE solution







double-well

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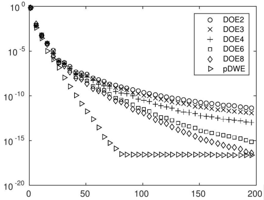
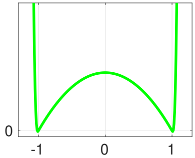
Eigenvalues for φ snapshots



[1]



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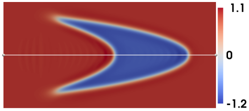
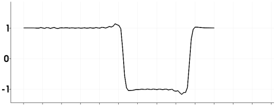
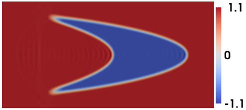
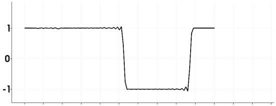




POD-ROM solution

$\leftarrow r = 30 \qquad r = 40 \rightarrow$





[1] J. O. Alff. Modellordnungsreduktion für das Cahn-Hilliard System, Bachelors' thesis, University Hamburg, 2015

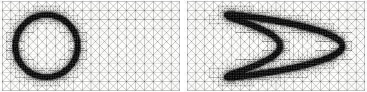
Agenda

Require 'good' snapshots: *Sufficiently good high-fidelity approximations of the true solution*

Goal: Use adaptive strategies in order to generate **good** snapshots for **efficiently**

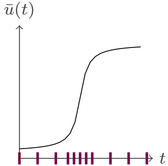
Space Adaptivity

- Combine POD with space-adapted snapshots
- Conserve stability for incompressible flow
  $\rightarrow$ joint work with M. Hinze, J. Lang, S. Ullmann
- Apply concept for optimal control



Time Adaptivity

- Snapshot location for POD-MOR in optimal control of linear systems
- Outlook to time adaptivity in MPC



POD-MOR for incompressible flow

Navier-Stokes (fully discrete form) $\forall v \in V_h^j,\ q \in Q_h^j$

$$\begin{cases} \frac{1}{\Delta t}(y_h^j - y_h^{j-1}, v) + ((y_h^j \cdot \nabla) y_h^j, v) + Re^{-1}(\nabla y_h^j, \nabla v) + b(v, p_h^j) & = & \langle f(t^j), v\rangle \\ b(y_h^j, q) & = & 0 \end{cases}$$

Notation: $b(v,q) = -(q, \nabla \cdot v)$

Navier-Stokes (POD-ROM) $\forall v \in V_r,\ q \in Q_r$

$$\begin{cases} \frac{1}{\Delta t}(y_r^j - y_r^{j-1}, v) + ((y_r^j \cdot \nabla) y_r^j, v) + Re^{-1}(\nabla y_r^j, \nabla v) + b(v, p_r^j) = \langle f(t^j), v\rangle \\ b(y_r^j, q) = 0 \end{cases}$$

- **Stability** is not guaranteed for all pairs (V_r, Q_r)
- Two solution concepts[1]:
  - (i) **Velocity ROM**[2]: projection onto weak divergence-free space
  - (ii) **Velocity-pressure ROM**[3,4]: enrich the velocity POD space with stabilizers

[1] C. G., M. Hinze, J. Lang, S. Ullmann, 2019, POD model order reduction with space-adapted snapshots for incompressible flows, Adv. Comp. Math. 45:2401-2428, 2019

[2] L. Sirovich, Turbulence and the dynamics of coherent structures, I-II, Q. Appl. Math.,45(3):561-590, 1987

[3] G. Rozza, K. Veroy, On the stability of the reduced basis method for the Stokes equations in parametrized domains, Comput. Methods Appl. Eng, 196(7):1244-1260, 2007

[4] F. Ballarin, A. Manzoni, A. Quarteroni, G. Rozza, Supremizer stabilization of POD-Galerkin approximation of parametrized steady incompressible Navier-Stokes equations, Int. J. Numer. Meth. Eng, 102(5):1136-1161, 2015

Static case:

- $b(y_h^j, q) = 0 \quad \forall q \in Q_h \qquad \Rightarrow$ POD basis is weakly divergence-free by construction
- POD-ROM: $V_r = \text{span}\{\psi_1, \ldots, \psi_r\}$

$$\begin{cases} \frac{1}{\Delta t}(y_r^j - y_r^{j-1}, v) + ((y_r^j \cdot \nabla) y_r^j, v) + Re^{-1}(\nabla y_r^j, \nabla v) + \cancel{b(v, p_r^j)} & = \langle f(t^j), v \rangle \quad \forall v \in V_r \\ \cancel{b(y_r^j, q)} & \cancel{= 0} \quad \forall q \in Q_h \end{cases}$$

Adaptive case:

- **In general:** $b(y_h^j, q) \neq 0$ for $q \in Q_h^i$ if $i \neq j$

Problem 1 (Optimal projection)

For given $u \in X$, find $\tilde{u} \in \tilde{V}$ which solves

$$\min_{v \in \tilde{V}} \frac{1}{2} \|v - u\|_X^2 \quad \text{s.t.} \quad b(v, q) = 0 \quad \forall q \in \tilde{Q}$$

Problem 2 (Leray / Stokes problem)

For given $u \in X$, find $\tilde{u} \in \tilde{V}$ and $\lambda \in \tilde{Q}$ such that

$$\begin{aligned} (\tilde{u}, w)_X + b(w, \lambda) &= (u, w)_X \qquad \forall w \in \tilde{V} \\ b(\tilde{u}, q) &= 0 \qquad \forall q \in \tilde{Q} \end{aligned}$$

Stable velocity-pressure ROM

- Compute POD basis for velocity $\{\psi_1, \ldots, \psi_{r_y}\}$ and
  POD basis for pressure $\{\phi_1, \ldots, \phi_{r_p}\} =: Q_r$
- Enrich reduced velocity space by supremizers:

$$V_r := \text{span}\{\psi_1, \ldots, \psi_{r_y}, \bar{\psi}_1, \ldots, \bar{\psi}_{r_p}\}$$

Supremizer computation

For given $q \in L^2_0(\Omega)$ find $\mathbb{T}q \in \tilde{V}$ such that

$$(\mathbb{T}q, v)_{H^1_0(\Omega)} = b(v, q) \quad \forall v \in \tilde{V}$$

Choose: $\bar{\psi}_i := \mathbb{T}\phi_i$ for $i = 1, \ldots r_p$

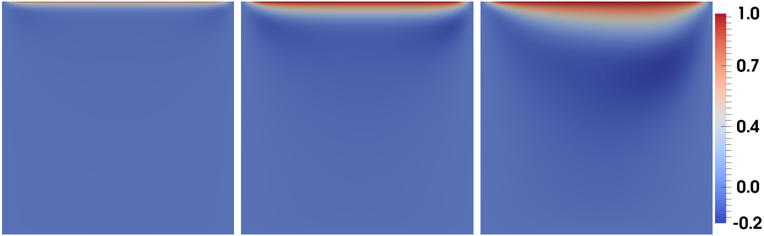
Inf-sup stability constraint for the ROM:

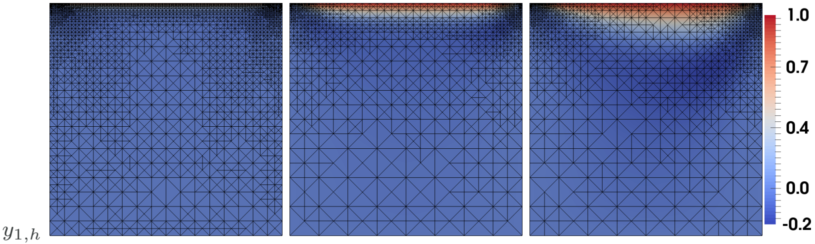
$$\beta_r := \inf_{\substack{q \in Q_r \\ q \neq 0}} \sup_{\substack{v \in V_r \\ v \neq 0}} \frac{b(v, q)}{\|v\|_{H^1_0(\Omega)} \|q\|_{L^2(\Omega)}} > 0$$

Follows from inf-sup stability of the FEM

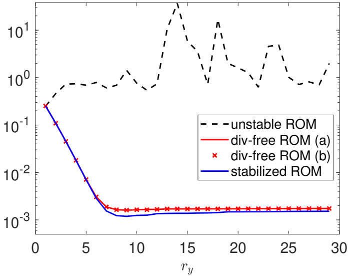
Numerical example: lid-driven cavity flow

$y_{1,h}$





Relative velocity error



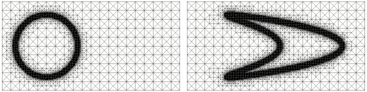
CPU times $r = 8$	div-free ROM	stabilized ROM
FE solution	125.66 s	125.66 s
Velocity POD	1.73 s	1.73 s
Pressure POD	–	0.05 s
Div-free proj	5.54 s	–
Supremizers	–	0.31 s
ROM solution	0.009 s	0.03 s
Speed up	13962	4188

Require 'good' snapshots: *Sufficiently good high-fidelity approximations of the true solution*

Goal: Use adaptive strategies in order to generate **good** snapshots **efficiently**

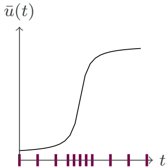
Space Adaptivity

- Combine POD with space-adapted snapshots
- Conserve stability for incompressible flow
- Apply concept for optimal control
  $\rightarrow$ joint work with J. O. Alff, M. Hinze, N. Scharmacher



Time Adaptivity

- Snapshot location for POD-MOR in optimal control of linear systems
- Outlook to time adaptivity in MPC



Optimal control of Cahn-Hilliard[1]

(P) $\min \hat{J}(u) = J(\varphi, u)$ **s.t.** $e(\varphi, u) = 0$ **and** $u \in U_{ad}$

$$J(\varphi, u) = \frac{\beta}{2}\|\varphi(T) - \varphi_d\|^2_{L^2(\Omega)} + \frac{\gamma}{2}\|u\|^2_U$$

$$\begin{cases} \varphi_t - \Delta\mu &= u & \text{in } (0,T)\times\Omega, \\ -\varepsilon\Delta\varphi + \frac{1}{\varepsilon}\mathcal{F}'(\varphi) &= \mu & \text{in } (0,T)\times\Omega, \\ \partial_n\varphi = \partial_n\mu &= 0 & \text{in } (0,T)\times\partial\Omega, \\ \varphi(0) &= \varphi_0 & \text{in } \Omega. \end{cases}$$

Find a locally optimal solution to (P):

$$\langle \hat{J}'(\bar{u}), u - \bar{u}\rangle_{U',U} \geq 0 \qquad \forall u \in U_{ad}$$

is equivalent to

$$\int_0^T \int_\Omega (\gamma\bar{u} + \bar{p})(u - \bar{u})\, dxdt \geq 0 \qquad \forall u \in U_{ad},$$

where $\bar{p}$ is a solution to the adjoint equations

$$\begin{cases} -p_t - \varepsilon\Delta q + \frac{1}{\varepsilon}\mathcal{F}''(\bar{\varphi})q &= 0 & \text{in } (0,T)\times\Omega, \\ -q - \Delta p &= 0 & \text{in } (0,T)\times\Omega, \\ \partial_n p = \partial_n q &= 0 & \text{in } (0,T)\times\partial\Omega, \\ p(T) &= -\beta(\bar{\varphi}(T) - \varphi_d) & \text{in } \Omega, \end{cases}$$

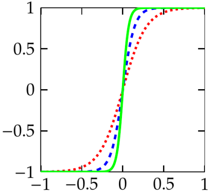
where $\bar{\varphi}$ is the solution to the state equations associated with an optimal control $\bar{u}$.

[1] M. Hintermüller, D. Wegner. Distributed optimal control of the Cahn-Hilliard system including the case of a double-obstacle homogeneous free energy density. SIAM J. Control Optim. 50:388-418, 2012

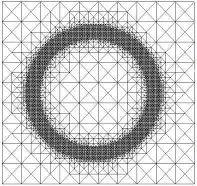
Optimization goal: circle $\rightarrow$ rounded square[1]

φ_0

φ_d



interface profile
$\varepsilon = \mathbf{0.2}, \mathbf{0.1}, \mathbf{0.05}$



adaptive mesh

Computational times

- uniform mesh: double-well $\mathcal{F}$: $\sim \mathbf{13}h$, Moreau-Yosida rel. $\mathcal{F}$: $\sim \mathbf{18}h$
- adaptive mesh: double-well $\mathcal{F}$: $\sim \mathbf{3.5}h$, Moreau-Yosida rel. $\mathcal{F}$: $\sim \mathbf{3}h$

$\rightarrow$ Apply POD-MOR in order to speed up computations

- TR-POD with adaptivity: double-well $\mathcal{F}$: $\sim$ **10**min, Moreau-Yosida rel. $\mathcal{F}$: $\sim$ **37**min

[1] J. O. Alff: Trust Region POD for Optimal Control of Cahn-Hilliard Systems, Master's Thesis, University Hamburg, 2018

TR-POD using uniform spatial meshes

k	$\hat{J}_h(u^k)$	$\hat{J}_r(u^k)$	$\|\hat{J}_h'(u^k)\|$	$\|\hat{J}_r'(u^k)\|$	r
0	0.3064	0.3065	0.1216	0.1239	2
1	0.1971	0.1974	0.0972	0.0989	2
2	0.0535	0.0542	0.0464	0.0471	2
3	0.0143		0.0107		

Table: TR-POD iteration history (double well $\mathcal{F}$)

k	$\hat{J}_h(u^k)$	$\hat{J}_r(u^k)$	$\|\hat{J}_h'(u^k)\|$	$\|\hat{J}_r'(u^k)\|$	r
0	0.4573	0.4573	0.1770	0.1789	4
1	0.3182	0.3083	0.1284	0.1250	4
2	0.1190	0.1205	0.0810	0.0833	8
3	0.0328	0.0327	0.0277	0.0268	25
4	0.0209	0.0209	0.0153	0.0151	25
5	0.0185		0.0095		

Table: TR-POD iteration history (relaxed double obstacle $\mathcal{F}$)

TR-POD using adaptive spatial meshes

k	$\hat{J}_h(u^k)$	$\hat{J}_r(u^k)$	$\|\hat{J}_h'(u^k)\|$	$\|\hat{J}_r'(u^k)\|$	r
0	0.3069	0.3070	0.1217	0.1241	2
1	0.1973	0.1977	0.0972	0.0990	2
2	0.0535	0.0542	0.0464	0.0472	2
3	0.0143		0.0107		

Table: TR-POD iteration history (double well $\mathcal{F}$)

k	$\hat{J}_h(u^k)$	$\hat{J}_r(u^k)$	$\|\hat{J}_h'(u^k)\|$	$\|\hat{J}_r'(u^k)\|$	r
0	0.4592	0.4593	0.1769	0.1788	4
1	0.3190	0.3088	0.1287	0.1258	4
2	0.1200	0.1212	0.0808	0.0872	8
3	0.0333	0.0341	0.0272	0.0269	13
4	0.0205	0.0205	0.0136	0.0140	17
5	0.0188		0.0107		

Table: TR-POD iteration history (relaxed double obstacle $\mathcal{F}$)

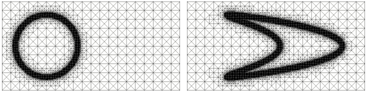
Agenda

Require 'good' snapshots: *Sufficiently good high-fidelity approximations of the true solution*

Goal: Use adaptive strategies in order to generate **good** snapshots **efficiently**

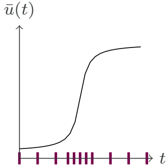
Space Adaptivity

- Combine POD with space-adapted snapshots
- Conserve stability for incompressible flow
- Apply concept for optimal control



Time Adaptivity

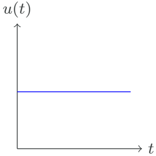
- Snapshot location for POD-MOR in optimal control of linear systems
  $\rightarrow$ joint work with A. Alla, M. Hinze
- Outlook to time adaptivity in MPC



Snapshot location in POD-MOR for optimal control

Open-loop control problem

Input y_0, y_d, f → $\min_{y,u} J(y,u)$ s.t. $e(y,u) = 0$ → Output $\bar{y}, \bar{u}$



Challenge:

- What are suitable time instances for snapshot locations?
- What is a suitable input control for snapshot generation?

Open-loop control problem

Input y_0, y_d, f → $\min_{y,u} J(y,u)$ s.t. $e(y,u) = 0$ → Output $\bar{y}, \bar{u}$

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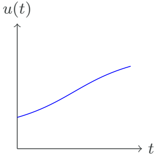
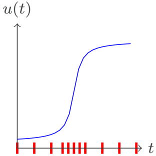


Snapshot location in POD-MOR for optimal control

Open-loop control problem

Input y_0, y_d, f → $\min_{y,u} J(y,u)$ s.t. $e(y,u) = 0$ → Output $\bar{y}, \bar{u}$



Challenge:

- What are suitable time instances for snapshot locations?
- What is a suitable input control for snapshot generation?

Solution idea:

- Reformulate optimality system as a space-time elliptic equation
- Apply concepts of a-posteriori error estimation in time for two-point boundary value problem

Literature on snapshot location strategies

- Kunisch, Volkwein. *Optimal snapshot location for computing POD basis functions.* ESAIM:M2AN, 44(3):509-529, 2010.
- Siade, Putti, Yeh. *Snapshot selection for groundwater model reduction using proper orthogonal decomposition.* Water Resources Research 46(8), 2010.
- Hoppe, Liu. *Snapshot location by error equilibration in proper orthogonal decomposition for linear and semilinear parabolic partial differential equations.* Journal of Numerical Mathematics 22(1):1-32, 2014.
- Nigro, Anndif, Teixeira, Pimenta, Wriggers. *An adaptive model order reduction by proper snapshot selection for nonlinear dynamical problems.* Computational Mechanics 57(4):537-554, 2016.
- Alla, G., Hinze. *A residual based snapshot location strategy for POD in distributed optimal control of linear parabolic equations.* IFAC-PapersOnLine, 49(8):13-18 2016.
- Oxberry, Kostova-Vassilevska, Arrighi, Chand. *Limited-memory adaptive snapshot selection for proper orthogonal decomposition.* International Journal for Numerical Methods in Engineering, 109(2):198-217, 2017.
- Alla, G., Hinze. *A-posteriori snapshot location for POD in optimal control of linear parabolic equations.* ESAIM:M2AN, 52(5):1847-1873, 2018.
- *[...]*

Problem setting and optimality system

$$\min_{y,u} J(\varphi, u) = \frac{1}{2}\|y - y_d\|^2_{L^2(0,T;\Omega)} + \frac{\alpha}{2}\|u\|^2_U$$

$$\begin{cases} y_t - \Delta y = \mathcal{B}u & \text{in } Q = (0,T] \times \Omega \\ y = 0 & \text{on } \Sigma = [0,T] \times \partial\Omega \\ y(0,\cdot) = y_0 & \text{in } \Omega \end{cases}$$

$u \in U_{ad} = \{u \in U \mid u_a(t) \leq u(t) \leq u_b(t) \text{ in } \mathbb{R}^m \text{ a.e. in } [0,T]\}$

Notation: $\mathcal{B}u = \sum_{i=1}^m u_i \chi_i$
$\chi_i \in H^{-1}(\Omega)$
$U = L^2(0,T;\mathbb{R}^m)$

Optimality system

$$\begin{cases} \text{(SE):} & y_t - \Delta y = \mathcal{B}u \text{ in } Q, \quad y = 0 \text{ on } \Sigma, \quad y(0) = y_0 \text{ in } \Omega \\ \text{(AE):} & -p_t - \Delta p = y - y_d \text{ in } Q, \quad p = 0 \text{ on } \Sigma, \quad p(T) = 0 \text{ in } \Omega \\ \text{(PF):} & u(t) = \mathbb{P}_{[u_a,u_b]}\{-\frac{1}{\alpha}(\mathcal{B}^* p)(t)\} \text{ f.a.a. } t \in [0,T] \end{cases}$$

Reformulation to an elliptic system

Optimality system

$$
\begin{cases}
\text{(SE):} & y_t - \Delta y = \mathcal{B}u \ \text{ in } Q, \quad y = 0 \text{ on } \Sigma, \quad y(0) = y_0 \text{ in } \Omega \\
\text{(AE):} & -p_t - \Delta p = y - y_d \ \text{ in } Q, \quad p = 0 \text{ on } \Sigma, \quad p(T) = 0 \ \text{ in } \Omega \\
\text{(PF):} & u(t) = \mathbb{P}_{[u_a,u_b]}\{-\frac{1}{\alpha}(\mathcal{B}^* p)(t)\} \ \text{ f.a.a. } t \in [0,T]
\end{cases}
$$

$y_0 \in H^1_0(\Omega), y_d \in L^2(Q) \Rightarrow p \in H^{2,1}(Q) := L^2(0,T; H^2(\Omega) \cap H^1_0(\Omega)) \cap H^1(0,T; L^2(\Omega))$
$y_d \in H^{2,1}(Q)$

Reformulation: The optimal adjoint state p fulfills:

$$
\text{(ES)} \begin{cases}
-p_{tt} + \Delta^2 p - \mathcal{B}\mathbb{P}_{[u_a,u_b]}\left(-\frac{1}{\alpha}\mathcal{B}^* p\right) = -(y_d)_t + \Delta y_d & \text{in } Q \\
p = 0 & \text{on } \Sigma \\
\Delta p = y_d & \text{on } \Sigma \\
(p_t + \Delta p)(0,\cdot) = y_d(0,\cdot) - y_0 & \text{in } \Omega \\
p(T,\cdot) = 0 & \text{in } \Omega
\end{cases}
$$

Second-order in time fourth-order in space elliptic problem

Temporal residual type a-posteriori error estimate[1]

Time discretization: $0 = t_0 < \ldots < t_n = T, \quad \Delta t_j = t_j - t_{j-1}, \quad I_j = [t_{j-1}, t_j]$

$$V_k = \{v \in H^{2,1}(0,T;\Omega) : v|_{I_j} \in \mathbb{P}_1(I_j)\}, \bar{V}_k = V_k \cap H_0^{2,1}(0,T;\Omega)$$

Theorem [Alla, G., Hinze]

Let $p \in H_0^{2,1}(0,T;\Omega)$ be the weak solution to (ES) and $p_k \in \bar{V}_k$ be the time-discrete approximation. Then, we obtain the a-posteriori error estimation

$$\|p - p_k\|^2_{H^{2,1}(0,T;\Omega)} \leq c\, \eta^2_{ad},$$

where $c > 0$ and

$$\eta^2_{ad} = \sum_{j=1}^{n} \Delta t_j^2 \int_{I_j} \left\| -(y_d)_t + \Delta y_d + (p_k)_{tt} + \mathcal{B}\, \mathbb{P}_{U_{ad}} \left\{ -\frac{1}{\alpha} \mathcal{B}^* p_k \right\} - \Delta^2 p_k \right\|^2_{L^2(\Omega)}$$
$$+ \sum_{j=1}^{n} \int_{I_j} \|y_d - \Delta p_k\|^2_{L^2(\partial\Omega)}.$$

[1] *In the spirit of* W. Gong, M. Hinze, Z. Zhou. Space-time finite element approximation of parabolic optimal control. J. Numer. Math., 20(2):111-146, 2012

Adaptive snapshot location strategy

Algorithm 1: Adaptive snapshot location for optimal control problems

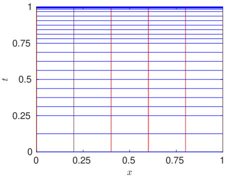
1: Solve (ES) adaptively in time with coarse spatial resolution h^+
$\rightarrow$ Obtain time grid $\mathcal{T}$ + approximation of the optimal adjoint state p_{h^+}

2: Set $u_{h^+} = \mathbb{P}_{[u_a, u_b]}\left\{-\frac{1}{\alpha}\mathcal{B}^* p_{h^+}\right\}$

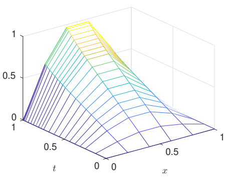
⊕ **Time grid is related to optimal control**

⊕ **Use approximation of optimal control as input for snapshot generation**

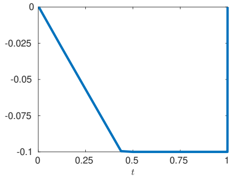
$\rightarrow$ Run usual POD offline phase: generate snapshots on $\mathcal{T}$ with fine spatial resolution h^* and input control u_{h^+}



Time grid $\mathcal{T}$

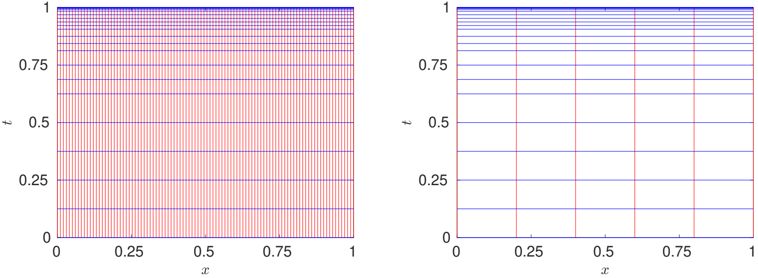


p_{h^+}

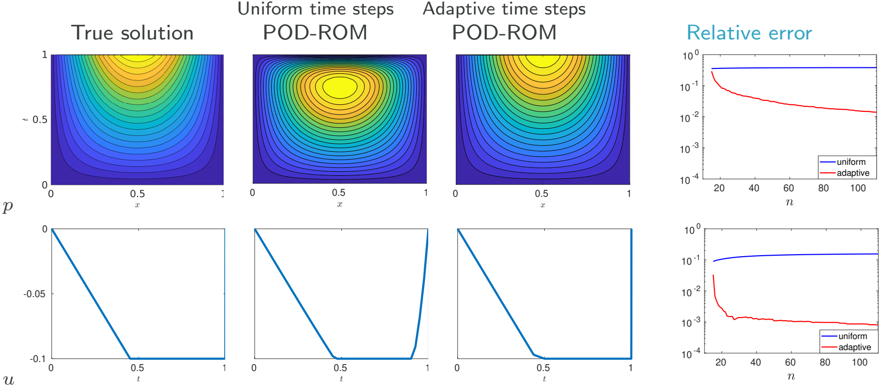


u_{h^+}

Assume: Spatial and temporal discretization decouple



Numerics: snapshot location for optimal control



CPU times	Uniform, ROM	Adaptive, ROM
n	7550	40
err_u	$1.2 \cdot 10^{-03}$	$1.2 \cdot 10^{-03}$
Optimal control solution	0.58 s	0.02 s
Snapshot generation	0.18 s	0.002 s
POD basis	6.34 s	0.09 s
Time-adaptive grid	–	0.48 s

State-oriented adaptivity in time

Time grid: $t_s = t_0 < t_1 < \cdots < t_n = t_e$ with $\Delta t_j = t_j - t_{j-1}$ and $I_j = [t_{j-1}, t_j]$

Time-discrete space (continuous in space):

$$V_k = \{v \in H^{2,1}(t_s, t_e; \Omega) : v|_{I_j} \in \mathbb{P}_1(I_j)\},\ \bar{V_k} = V_k \cap H_0^{2,1}(t_s, t_e; \Omega)$$

Temporal residual type a-posteriori error estimate

Let y and y_k denote the weak solution to the elliptic equation and the time-discrete approximation, respectively. Then,

$$\|y - y_k\|^2_{H^{2,1}(t_s,t_e;\Omega)} \leq c\eta^2$$

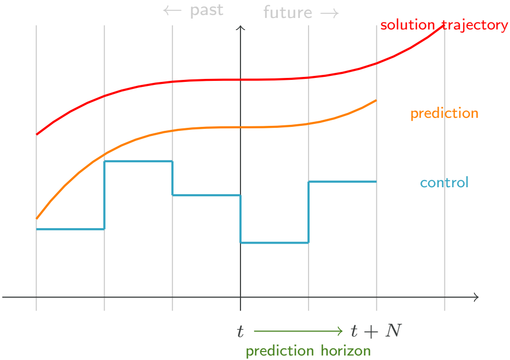
where $\eta^2 = \sum_{j=1}^{n} \Delta t_j^2 \int_{I_j} \|\frac{1}{\alpha} y_d + (y_k)_{tt} - \frac{1}{\alpha} y_k - \Delta^2 y_k\|^2_{L^2(\Omega)} + \sum_{j=1}^{n} \int_{I_j} \|\Delta y_k\|^2_{L^2(\partial\Omega)}.$

$\Rightarrow$ The resulting adaptive time grid is related to the **optimal state** solution

$\hookrightarrow$ exploit concept for design of prediction horizon in MPC.

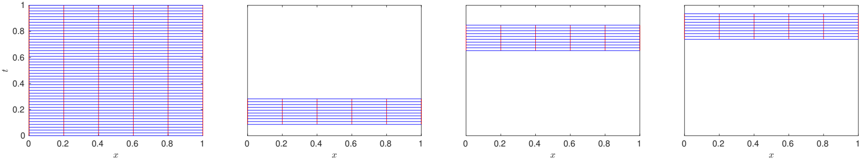
[1] W. Gong, M. Hinze, Z. Zhou. Space-time finite element approximation of parabolic optimal control. J. Numer. Math., 20(2):111-146, 2012

Utilize the temporal error estimates for the elliptic system
in order to get **time adaptive grids for MPC**

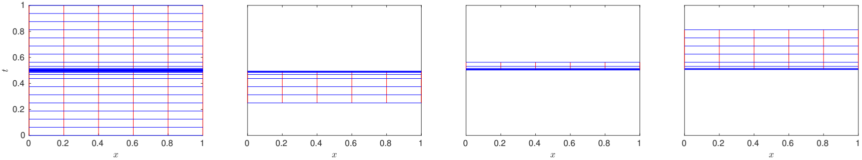


Concept 1: Offline Approach: Time adaptivity with adaptive time horizon length

Uniform



Adaptive



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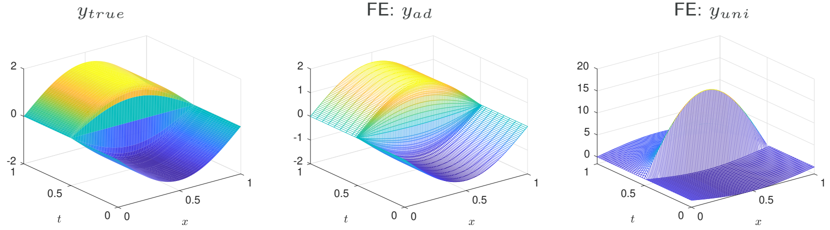
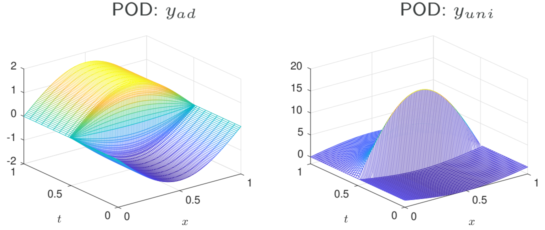
Time Adaptivity in MPC

Concept 1: Offline Approach: Time adaptivity with adaptive time horizon length



FE dimension: 100
POD dimension: 1
speed up factor: 5



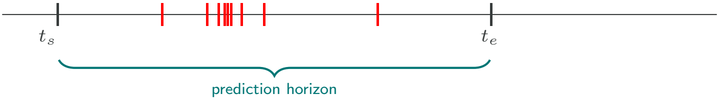
rel err $= 2.48 \cdot 10^{-2}$ rel err $= 2.59 \cdot 10^{0}$

Concept 2: Online Approach: Time adaptivity with fixed horizon length

1. Fix a length for the prediction horizon

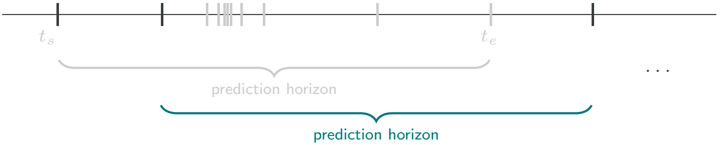
Concept 2: Online Approach: Time adaptivity with fixed horizon length

1. Fix a length for the prediction horizon
2. Compute an adaptive time grid within the prediction horizon



Concept 2: Online Approach: Time adaptivity with fixed horizon length

1. Fix a length for the prediction horizon
2. Compute an adaptive time grid within the prediction horizon
3. Solve the MPC subproblem and shift the horizon



Concept 2: Online Approach: Time adaptivity with fixed horizon length

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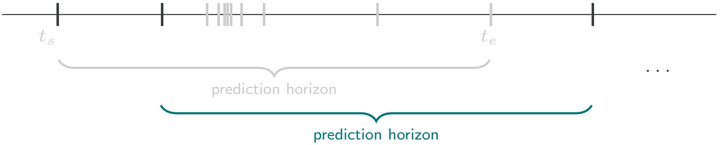
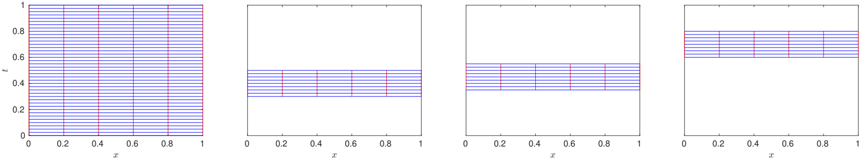


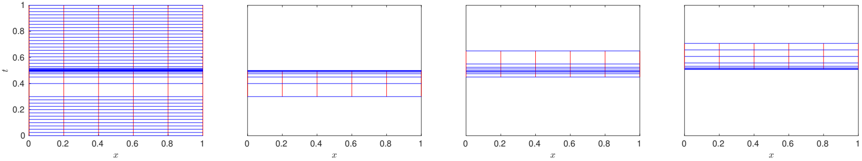
$\Rightarrow$ Each time horizon has the same length
but (possibly) different time discretizations

Concept 2: Online Approach: Time adaptivity with fixed horizon length

Uniform

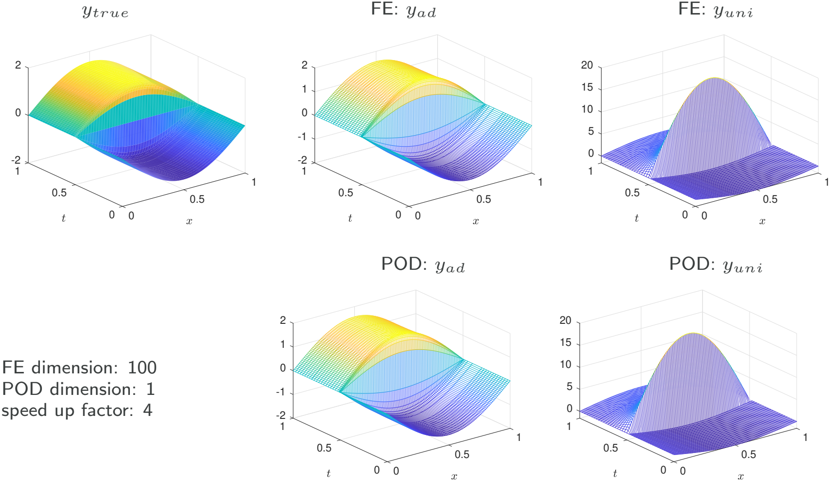


Adaptive



dof = 47

Concept 2: Online Approach: Time adaptivity with fixed horizon length



FE dimension: 100
POD dimension: 1
speed up factor: 4

rel err $= 5.26 \cdot 10^{-2}$

rel err $= 3.05 \cdot 10^{0}$

Conclusions: input dependency of POD-MOR

POD-MOR is **input dependent**: ROM accuracy is limited by the snapshot information

Require 'good' snapshots: *Sufficiently good high-fidelity approximations of the true solution*

Goal: Use adaptive strategies in order to generate **good** snapshots **efficiently**

Conclusions of Part I: adaptivity in space

- Combine POD and space-adapted snapshots using an explicit computation of the snapshot gramian $\Rightarrow$ allows broad spectrum of discretizations
- Achieve large computational speedup in POD offline phase with similar approximation quality in comparison to a uniform discretization
- Derive stable ROM for Navier-Stokes in the case of space-adapted snapshots
  (i) velocity-ROM
  (ii) velocity-pressure ROM
- Apply POD-MOR with space-adapted snapshots for optimal control in a trust-region POD framework

Current research steps:

(1) MOR for Cahn-Hilliard with double-obstacle energy (joint work with O. Burkovska)
(2) Enrich POD model with measurement data using data assimilation techniques

References:

- Gräßle, Hinze. *POD reduced-order modeling for evolution equations utilizing arbitrary finite element discretizations*. Adv. Comp. Math. 44(6):1941-1978, 2018
- Gräßle, Hinze, Scharmacher. *POD for optimal control of the Cahn-Hilliard system using spatially adapted snapshots*. Proceedings Enumath 703-711, 2019
- Gräßle, Hinze, Lang, Ullmann. *POD model order reduction with space-adapted snapshots for incompressible flows*. Adv. Comp. Math. 45:2401-2428, 2019

Conclusions of Part II: adaptivity in time

- Snapshot location strategy for POD in optimal control
- Exploit reformulation of the optimality system into an elliptic equation
- Apply residual based a-posteriori error estimates in time

Current research steps:

(1) Utilize time-adaptive strategies in POD based MPC (joint work with A. Alla, M. Hinze)
(2) Derive a-posteriori error estimates for a fully space-time adaptive approach

References:

- Alla, Gräßle, Hinze. *A residual based snapshot location strategy for POD in distributed optimal control of linear parabolic equations.* IFAC-PapersOnLine 49(8):13-18, 2016.
- Alla, Gräßle, Hinze. *A-posteriori snapshot location for POD in optimal control of linear parabolic equations.* ESAIM:M2AN, 52(5):1847-1873, 2018.

GAMM Juniors' Summer School on Applied Mathematics and Mechanics

Learning Models from Data

Magdeburg, July 27-31, 2020

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J. Nathan Kutz (U Washington)
Benjamin Peherstorfer (New York U)
Feliks Nüske (U Paderborn)

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https://www.mpi-magdeburg.mpg.de/csc/events/samm20

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