Nonlinear Model Order Reduction for Optimal Control of Burgers' Equation

- Master thesis -

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Table of Contents

Nonlinear dynamical systems

Consider the nonlinear dynamical system

$$\begin{aligned} \dot{\mathbf{y}}(t) &= A\mathbf{y}(t) + \mathbf{F}(t, \mathbf{y}(t)), \quad \mathbf{y}(t) \in \mathbb{R}^N \\ \mathbf{y}(0) &= \mathbf{y}_0 \end{aligned} \tag{1}$$

- arises in many applications, e.g. mechanical systems, fluid dynamics, neuron modeling, ...
- the matrix A represents the linear dynamical behavior and the function $\mathbf{F}$ represents the nonlinear part
- often large dimension of (1) leads to *huge* computational work

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The idea of model order reduction

Approximate the state via

$$\mathbf{y}(t) \approx U_\ell \tilde{\mathbf{y}}(t), \quad U_\ell \in \mathbb{R}^{N\times \ell}, \tilde{\mathbf{y}} \in \mathbb{R}^{\ell},$$

where the matrix U_ℓ consists of orthonormal columns, the so-called *principal components* of $\mathbf{y}$, and $\ell \ll N$.

Galerkin projection of the original full-order system leads to a reduced $\ell \times \ell$ system of equations:

$$U_\ell^T (U_\ell \dot{\tilde{\mathbf{y}}} - A U_\ell \tilde{\mathbf{y}} - \mathbf{F}(t, U_\ell \tilde{\mathbf{y}})) = 0$$
$$\Rightarrow \quad \dot{\tilde{\mathbf{y}}} = \underbrace{U_\ell^T A U_\ell}_{=:\tilde{A}} \tilde{\mathbf{y}} + U_\ell^T \mathbf{F}(t, U_\ell \tilde{\mathbf{y}})$$

Two questions are left...

Considering the reduced model

$$\dot{\tilde{\mathbf{y}}}(t) = \tilde{A}\tilde{\mathbf{y}}(t) + U_\ell^T \mathbf{F}(t, U_\ell \tilde{\mathbf{y}}(t))$$

two questions are left:

1. How to obtain the matrix U_ℓ of principal components ?
2. Note that $U_\ell \tilde{\mathbf{y}}(t) \in \mathbb{R}^N$ is still large. How do we evaluate $\mathbf{F}(t, U_\ell \tilde{\mathbf{y}}(t))$ efficiently ?

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The Proper Orthogonal Decomposition (POD)

During the numerical simulation, build up the matrix

$$Y := [\mathbf{y}(t_1), ..., \mathbf{y}(t_{n_s})] \in \mathbb{R}^{N \times n_s},$$

with n_s being the number of snapshots.

Perform a Singular Value Decomposition (SVD)

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

and let $U_\ell := \texttt{U(:,1:l)}$ consist of those left singular vectors of Y that correspond to the ℓ largest singular values in Σ.

The Discrete Empirical Interpolation Method (DEIM)

Consider the nonlinearity

$$\mathbf{N} := \underbrace{U_\ell^T}_{\ell \times N} \underbrace{\mathbf{F}(t, U_\ell \tilde{\mathbf{y}}(t))}_{N \times 1}$$

The approximation

$$\mathbf{F} \approx W\mathbf{c}, \quad W \in \mathbb{R}^{N \times m}, \mathbf{c} \in \mathbb{R}^m$$

is over determined. Therefore, find projection $\mathcal{P}$ such that:

$$\begin{aligned} \mathcal{P}^T\mathbf{F} = (\mathcal{P}^T W)\mathbf{c} \quad &\Rightarrow \quad \mathbf{F} \approx W\mathbf{c} = W(\mathcal{P}^T W)^{-1}\mathcal{P}^T\mathbf{F} \\ &\Rightarrow \quad \mathbf{N} \approx U_\ell^T W \underbrace{(\mathcal{P}^T W)}_{m \times m}{}^{-1}\mathcal{P}^T\mathbf{F}(t, U_\ell \tilde{\mathbf{y}}(t)) \end{aligned}$$

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Algorithm 1 The DEIM algorithm [Chaturantabut, Sorensen, 2010]

INPUT: $\{\mathbf{w}_i\}_{i=1}^m \subset \mathbb{R}^N$ linear independent
OUTPUT: $\vec{\wp} = [\wp_1, ..., \wp_m]^T \in \mathbb{R}^m,\ \mathcal{P} \in \mathbb{R}^{N \times m}$
$[|\rho|, \wp_1] = \max\{|\mathbf{w}_1|\}$
$W = [\mathbf{w}_1], \mathcal{P} = [\mathbf{e}_{\wp_1}], \vec{\wp} = [\wp_1]$
for $i = 2$ to m **do**
    Solve $(\mathcal{P}^T W)\mathbf{c} = \mathcal{P}^T \mathbf{w}_i$ for $\mathbf{c}$
    $\mathbf{r} = \mathbf{w}_i - W\mathbf{c}$
    $[|\rho|, \wp_i] = \max\{|\mathbf{r}|\}$
    $W \leftarrow [W\ \mathbf{w}_i], \mathcal{P} \leftarrow [\mathcal{P}\ \mathbf{e}_{\wp_i}], \vec{\wp} \leftarrow \begin{bmatrix} \vec{\wp} \\ \wp_i \end{bmatrix}$
end for

The product $\mathcal{P}^T\mathbf{F}$ is a selection of entries

Let $m = 3$. Suppose the DEIM-algorithm has chosen indices $\wp_1, \ldots, \wp_m$ such that:

$$\mathcal{P}^T\mathbf{F} = \begin{bmatrix} 0 & \ldots & \overset{\wp_1}{\downarrow} 1 & \ldots & 0 \\ 0 & 1 & \ldots & \ldots & 0 \\ 0 & \ldots & 0 & \underset{\wp_m}{\uparrow} 1 & 0 \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_N \end{bmatrix} = \begin{bmatrix} F_{\wp_1} \\ F_{\wp_2} \\ F_{\wp_m} \end{bmatrix}$$

Therefore, suppose $\mathbf{F}(\cdot)$ acts pointwise, we obtain:

$$\begin{aligned} \mathbf{N} &\approx U_\ell^T W (\mathcal{P}^T W)^{-1} \mathcal{P}^T \mathbf{F}(t, U_\ell \tilde{\mathbf{y}}(t)) \\ &= \underbrace{U_\ell^T W (\mathcal{P}^T W)^{-1}}_{\ell \times m} \underbrace{\mathbf{F}(t, \mathcal{P}^T U_\ell \tilde{\mathbf{y}}(t))}_{m \times 1} \end{aligned}$$

The nonlinear 1D Burgers' model

$$
\begin{aligned}
y_t + \left(\frac{1}{2}y^2 - \nu y_x\right)_x &= f, \quad (x,t) \in (0,L)\times(0,T),\\
y(t,0) = y(t,L) &= 0, \quad t \in (0,T),\\
y(0,x) &= y_0(x), \quad x \in (0,L).
\end{aligned}
$$

FEM-discretization in space leads to:

$$
\begin{aligned}
M\dot{\mathbf{y}}(t) &= -\frac{1}{2}B\mathbf{y}^2(t) - \nu C\mathbf{y}(t) + \mathbf{f}, \quad t > 0\\
\mathbf{y}(0) &= \mathbf{y}_0
\end{aligned}
$$

POD-DEIM for Burgers' equation

Suppose, Φ_ℓ is an M-orthogonal POD basis.

The POD reduced Burgers' equation

$$\overbrace{\Phi_\ell^T M \Phi_\ell}^{=I_\ell} \dot{\tilde{y}}(t) = -\frac{1}{2}\Phi_\ell^T B(\Phi_\ell \tilde{\mathbf{y}}(t))^2 - \nu \Phi_\ell^T C \Phi_\ell \tilde{\mathbf{y}}(t)$$

$$\Rightarrow \quad \dot{\tilde{y}}(t) = -\frac{1}{2} B_\ell(\Phi_\ell \tilde{\mathbf{y}}(t))^2 - \nu C_\ell \tilde{\mathbf{y}}(t)$$

Next, obtain W via a truncated SVD of $[\mathbf{y}^2(t_1), \ldots, \mathbf{y}^2(t_{n_s})]$ and apply DEIM to the columns of W.

The POD-DEIM reduced Burgers' equation

$$\dot{\tilde{y}}(t) = -\frac{1}{2}\tilde{B}(\tilde{F}\tilde{\mathbf{y}}(t))^2 - \nu \tilde{C}\tilde{\mathbf{y}}(t),$$

with $\tilde{B} = \Phi_\ell^T B W (\mathcal{P}^T W)^{-1} \in \mathbb{R}^{\ell \times m}$, $\tilde{F} = \mathcal{P}^T \Phi_\ell \in \mathbb{R}^{m \times \ell}$, and $\tilde{C} = C_\ell \in \mathbb{R}^{\ell \times \ell}$.

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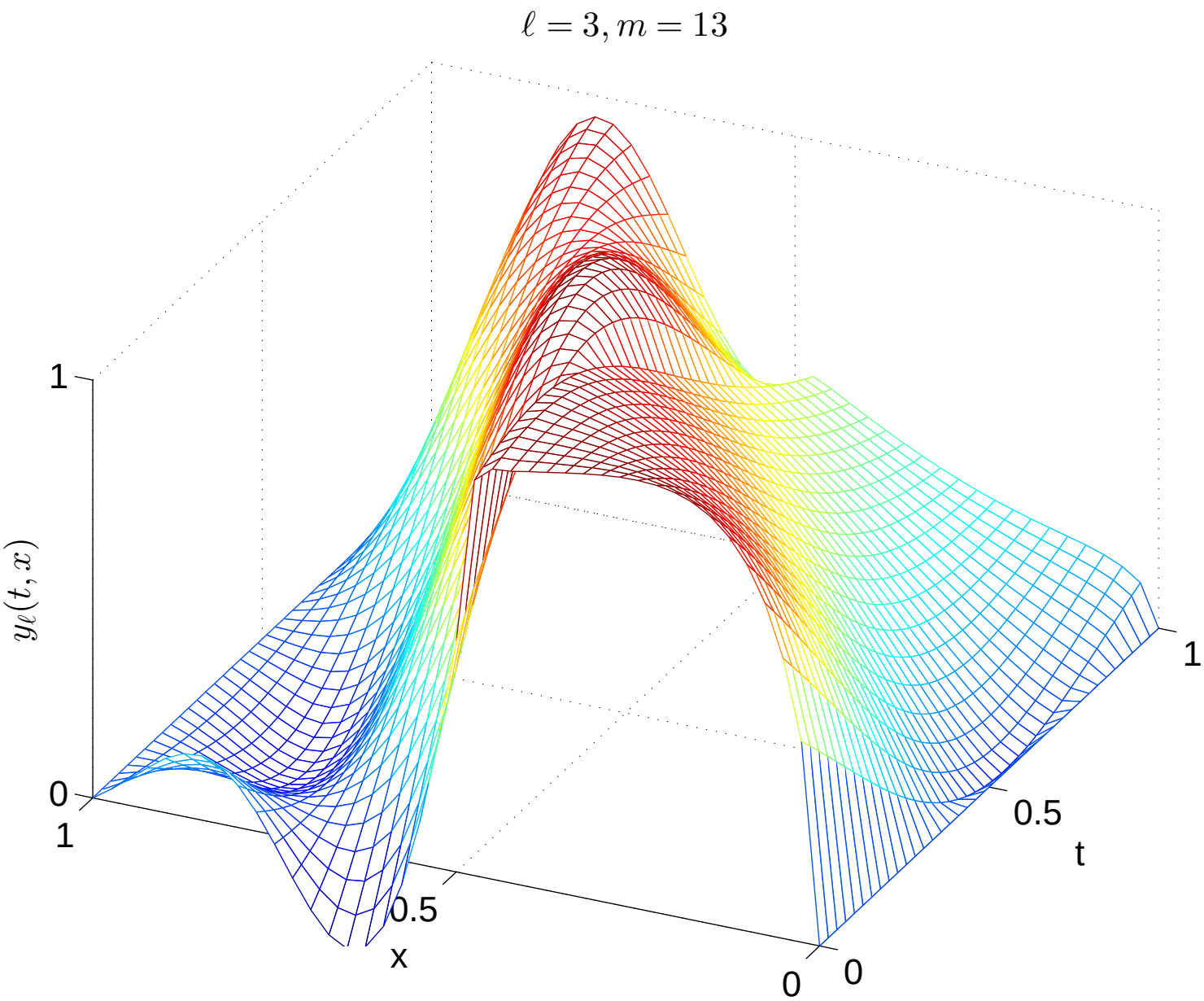
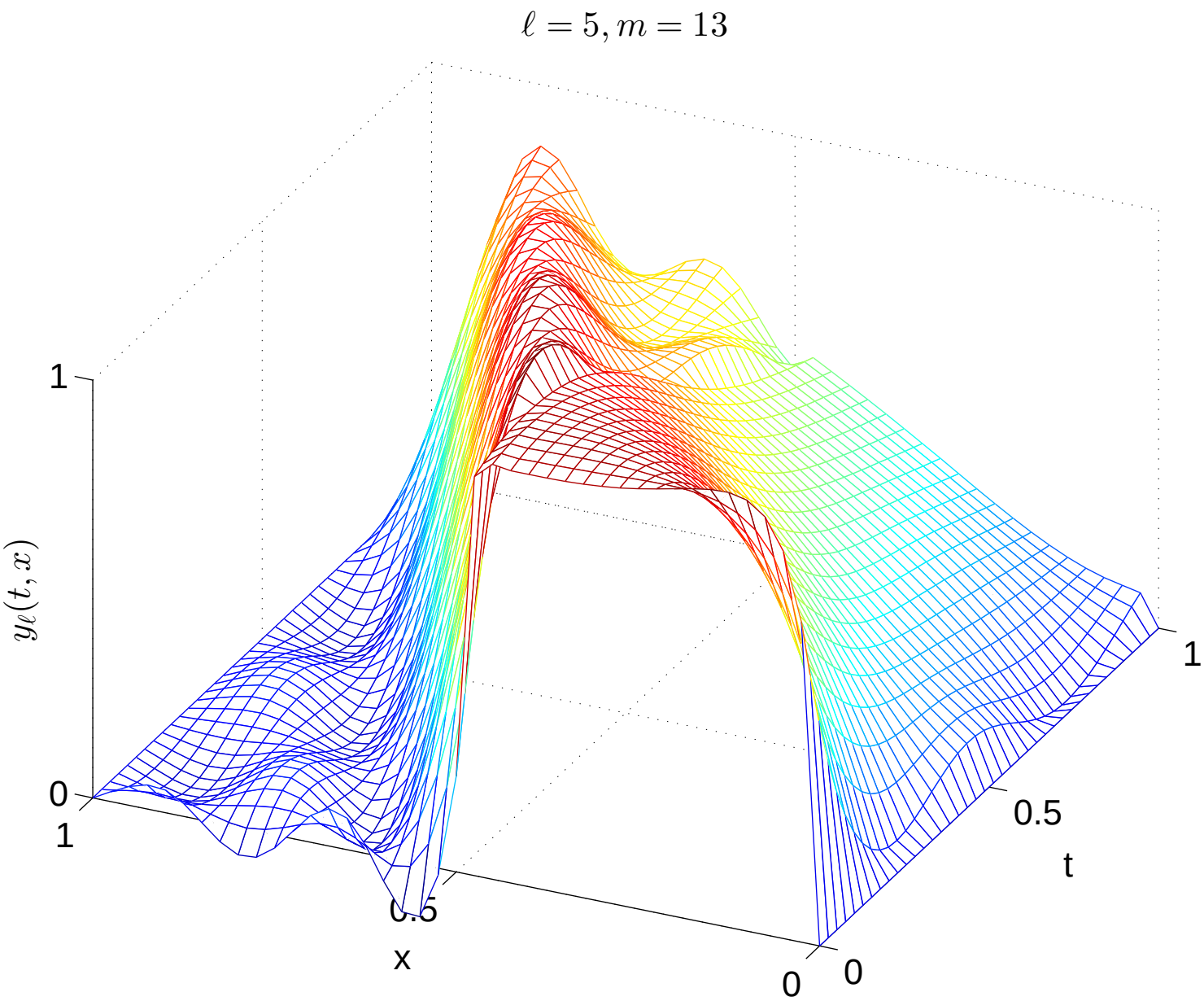
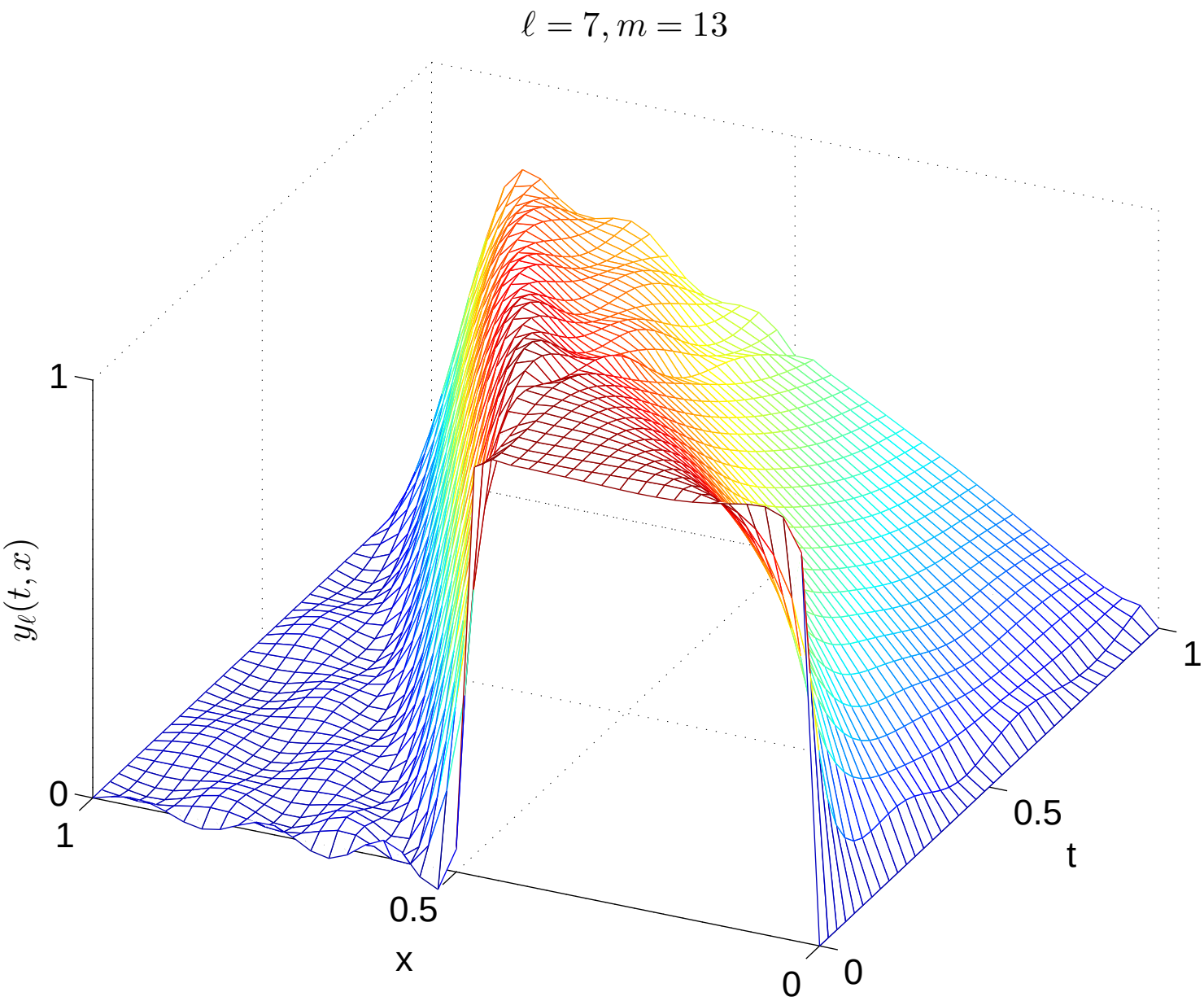
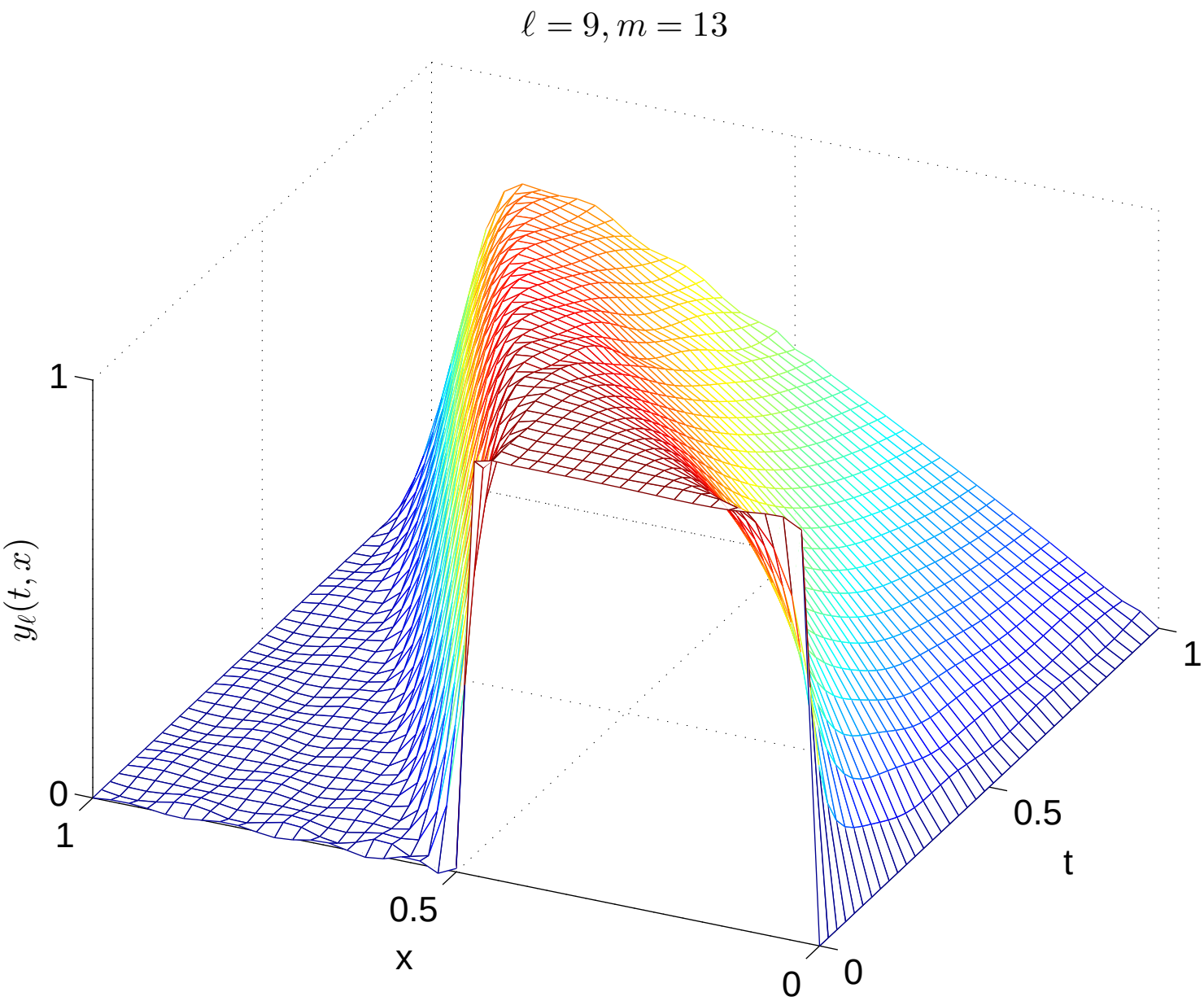
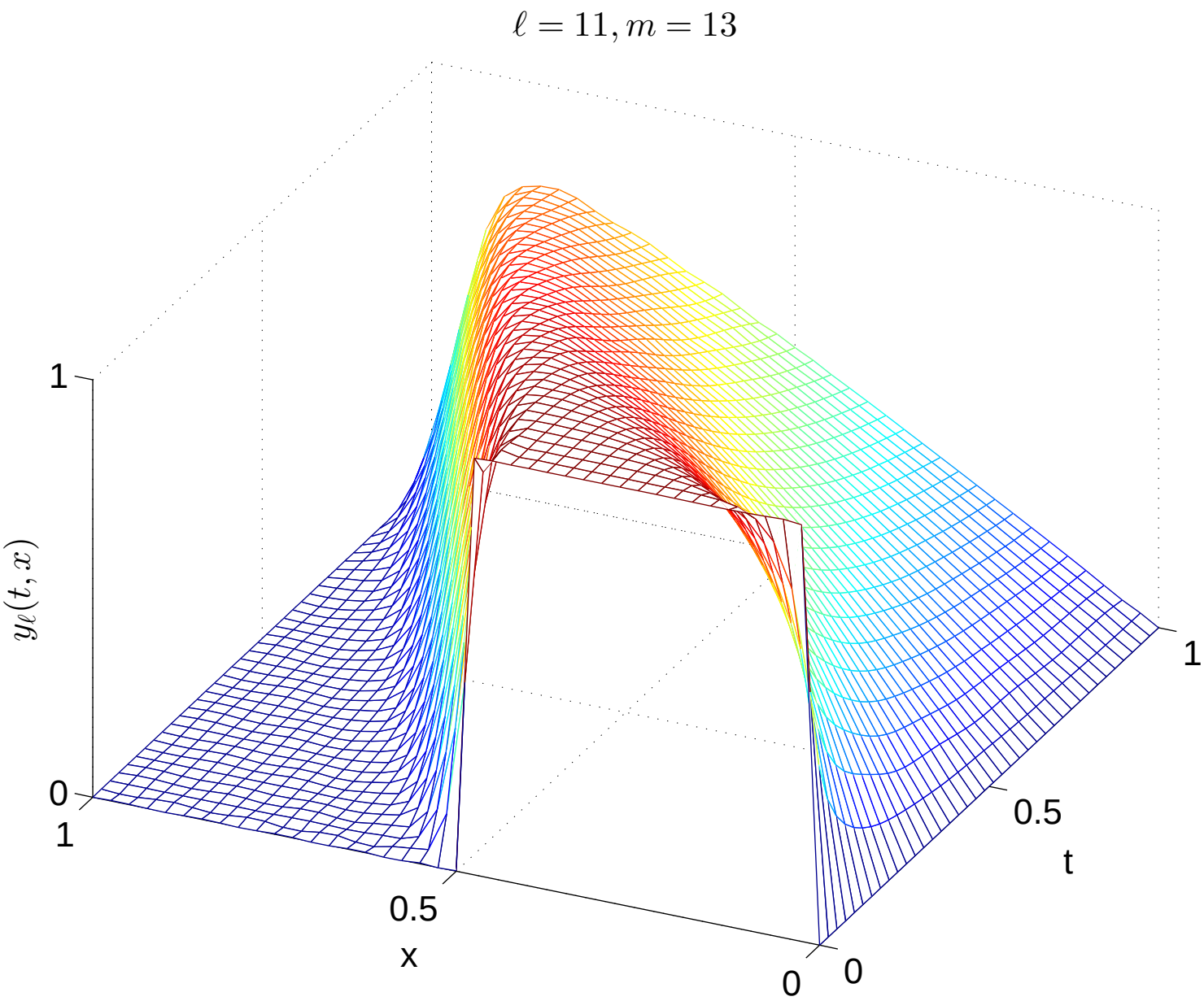

$\ell = 3, m = 13$
$y_\ell(t, x)$
1
0
1
x
0.5
0
0
0.5
t
1


$\ell = 5, m = 13$
$y_\ell(t, x)$
1
0
1
x
0.5
0
0
t
0.5
1

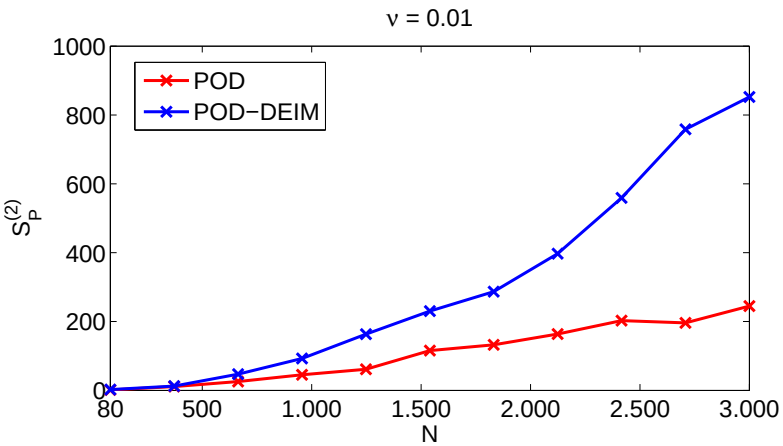

$\ell = 7, m = 13$
$y_\ell(t, x)$
1
0
1
0.5
x
0
0
0.5
t
1

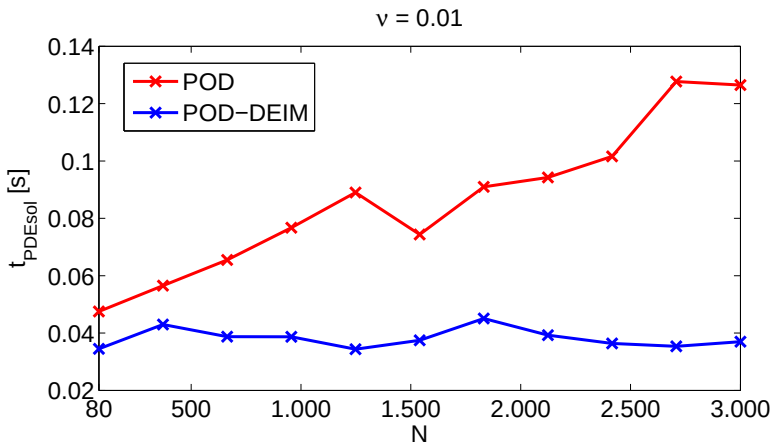

$\ell = 9, m = 13$
1
0
$y_\ell(t,x)$
1
0.5
x
0
0
0.5
t
1


$\ell = 11, m = 13$
$y_\ell(t, x)$
1
0
1
x
0.5
0
0
t
0.5
1

Computational Speedup

	$\nu = 0.01$			$\nu = 0.001$			$\nu = 0.0001$		
	Full	POD	DEIM	Full	POD	DEIM	Full	POD	DEIM
$N/\ell/m$	80	11	(11, 13)	200	35	(35, 40)	800	40	(40, 55)
$t_{setup}[s]$	-	0.003	0.011	-	0.009	0.021	-	0.0729	0.182
$t_{PDEsol}[s]$	0.068	0.047	0.040	0.232	0.12	0.055	4.416	0.276	0.085
$\bar{e}[10^{-4}]$	-	6.13	6.46	-	6.12	6.85	-	7.43	7.66
$S_P^{(1)}$	-	1.35	1.34	-	1.74	3.03	-	12.54	16.52
$S_P^{(2)}$	-	1.44	1.71	-	1.88	4.21	-	15.85	51.85





PDE-constrained optimization

Minimize

$$\min_u \mathcal{J}(y(u), u),$$

where y is the solution to a nonlinear, possibly time-dependent partial differential equation,

$$c(y, u) = 0.$$

- $\mathcal{J}$ is called objective function,
- in order to evaluate $\mathcal{J}$, we need to solve $c(y, u) = 0$ for $y(u)$,
- first-order and second-order optimization algorithms.

A second-order optimization algorithm

Minimize $\mathcal{J}(y(\cdot),\cdot)$ over u taking information of the first and second derivative into account.

- Choose u_0 and $k = 0$
- Repeat until convergence
  - Solve the PDE-constraint $c(y_k, u_k) = 0$ for y_k
  - Solve the Newton equation $\nabla^2 \mathcal{J}(y_k, u_k)s_k = -\nabla \mathcal{J}(y_k, u_k)$ via the **truncated CG-method**
  - Obtain $\alpha^* = \operatorname{argmin}_{\alpha \in \mathbb{R}_+} \mathcal{J}(y(u_k + \alpha s_k), u_k + \alpha s_k)$ via **Armijo line search**
  - Calculate new control $u_{k+1} = u_k + \alpha^* s_k$
  - Stop if $\|\nabla \mathcal{J}(y_k, u_k)\|$ is small or $\mathcal{J}(y_k, u_k)$ does not change anymore
  - $k = k + 1$

Gradient computation via adjoints

Consider the Lagrangian function

$$\mathcal{L}(y, u, \lambda) = \mathcal{J}(y, u) + \lambda^T c(y, u)$$

and **impose** the zero-gradient condition $\nabla_y \mathcal{L}(y, u, \lambda) = 0$.

We derive the *adjoint equation*:

$$c_y(y(u), u)^T \lambda = -\nabla_y \mathcal{J}(y(u), u)$$

Algorithm 2 Computing $\nabla \hat{\mathcal{J}}(u)$ via adjoints [Heinkenschloss, 2008]

1: For a given control u, solve $c(y, u) = 0$ for the state $y(u)$
2: Solve the adjoint equation $c_y(y(u), u)^T \lambda = -\nabla_y \mathcal{J}(y(u), u)$ for $\lambda(u)$
3: Compute $\nabla \hat{\mathcal{J}}(u) = \nabla_u \mathcal{J}(y(u), u) + c_u(y(u), u)^T \lambda(u)$

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First-order optimization algorithms

- Instead of solving $\nabla^2 \mathcal{J}(y_k, u_k)s_k = -\nabla \mathcal{J}(y_k, u_k)$, first-order methods approximate the Hessian via H_k and solve $H_k s_k = -\nabla \mathcal{J}(y_k, u_k)$,
- We have used Matlab implementations for the BFGS and the SPG method,
- Evaluation of $\mathcal{J}$ and gradient computation as seen before,
- SPG easily allows to include bounds on the control, i.e. $u_{lower} \leq u(t, x) \leq u_{upper}$ which is used in many applications

Optimal Control problem for Burgers' equation

Minimize

$$\min_u \frac{1}{2} \int_0^T \int_0^L [y(t,x) - z(t,x)]^2 + \omega u^2(t,x) \, dx \, dt, \tag{2}$$

where y is a solution to the nonlinear Burgers' equation

$$\begin{aligned} y_t + \left(\frac{1}{2}y^2 - \nu y_x\right)_x &= f + u, \quad (x,t) \in (0,L) \times (0,T), \\ y(t,0) = y(t,L) &= 0, \quad t \in (0,T), \\ y(0,x) &= y_0(x), \quad x \in (0,L). \end{aligned} \tag{3}$$

- u is the control that determines y
- z is the desired state

Control goal

We want to control the solution of Burgers' equation in such a way that it stays in the desired state $z(t, \cdot) = y_0, \forall t$:

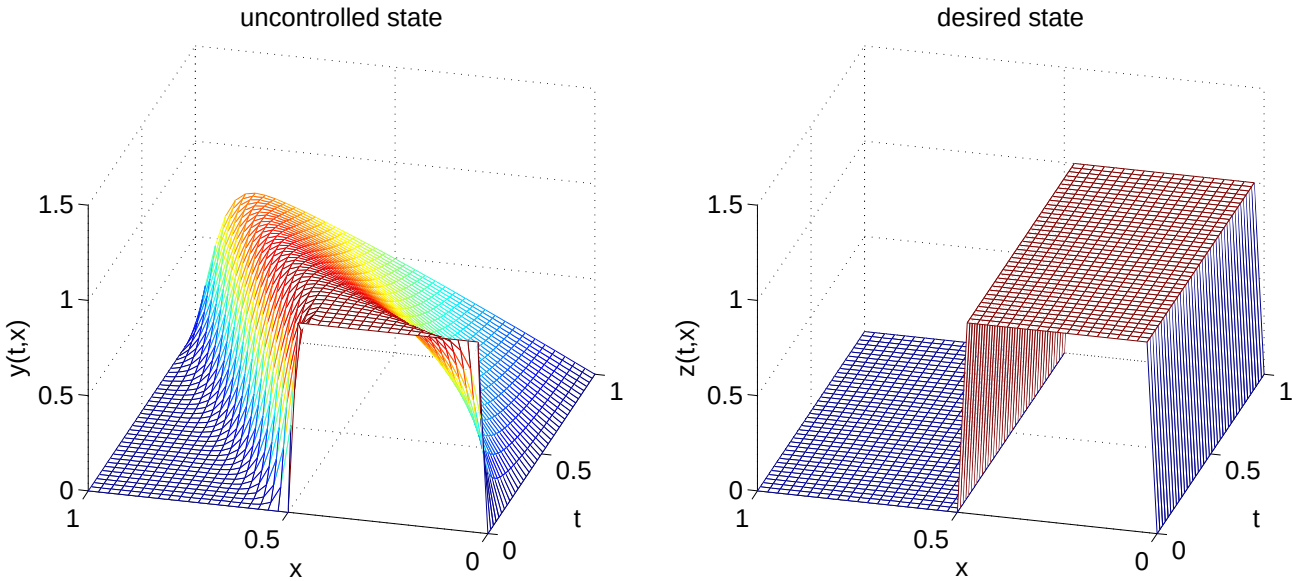


Figure: Uncontrolled and desired state for $\nu = 0.01$.

The full-order discretized optimal control problem

$$\min_u \mathcal{J}(y(u),u) \equiv \min_{\mathbf{u}_0,\dots,\mathbf{u}_{N_t}} \sum_{i=0}^{N_t} \delta t \left(\frac{1}{2}\mathbf{y}_i^T M \mathbf{y}_i - \mathbf{z}^T \mathbf{y}_i + \frac{\omega}{2}\mathbf{u}_i^T M \mathbf{u}_i \right),$$

where $\mathbf{y}_i$ is the solution of the full-order Burgers' equation

$$c(y,u) \equiv \frac{1}{\delta t} M \mathbf{y}_{i+1} - \frac{1}{\delta t} M \mathbf{y}_i + \frac{1}{2} B \mathbf{y}_{i+1}^2 + \nu C \mathbf{y}_{i+1} - \mathbf{f} - M \mathbf{u}_{i+1} = 0$$

The POD-DEIM reduced optimal control problem

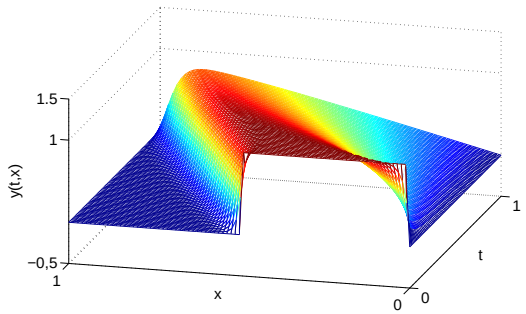
$$\min_u \tilde{\mathcal{J}}(\tilde{y}(u),u) \equiv \min_{\mathbf{u}_1,\dots,\mathbf{u}_{N_t}} \sum_{i=0}^{N_t} \delta t \left(\frac{1}{2}\tilde{\mathbf{y}}_i^T \tilde{\mathbf{y}}_i - \tilde{\mathbf{z}}^T \tilde{\mathbf{y}}_i + \frac{\omega}{2}\mathbf{u}_i^T M \mathbf{u}_i \right),$$

where $\tilde{\mathbf{y}}_i$ is the solution of the POD-DEIM reduced Burgers' equation

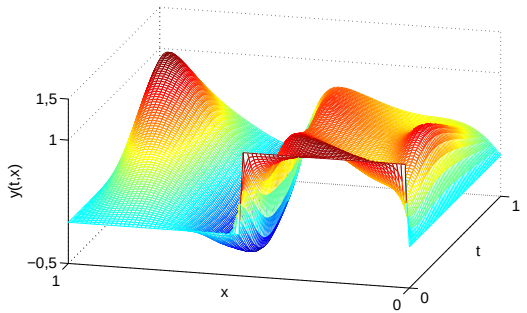
$$\tilde{c}(\tilde{y},u) \equiv \frac{1}{\delta t} \tilde{\mathbf{y}}_{i+1} - \frac{1}{\delta t} \tilde{\mathbf{y}}_i + \frac{1}{2} \tilde{B}(\tilde{F}\tilde{\mathbf{y}}_{i+1})^2 + \nu \tilde{C} \tilde{\mathbf{y}}_{i+1} - \tilde{\mathbf{f}} - \tilde{M} \mathbf{u}_{i+1} = 0$$

Numerical tests

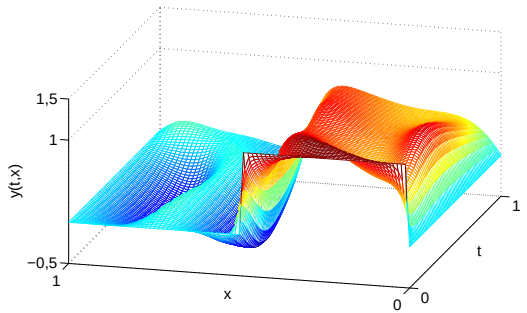
Newton-type method for the full-order Burgers' model:



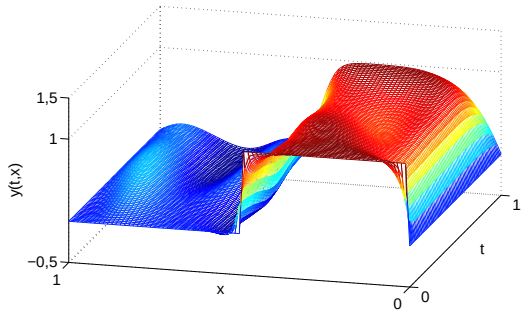
(a) $k = 0$ (uncontrolled)



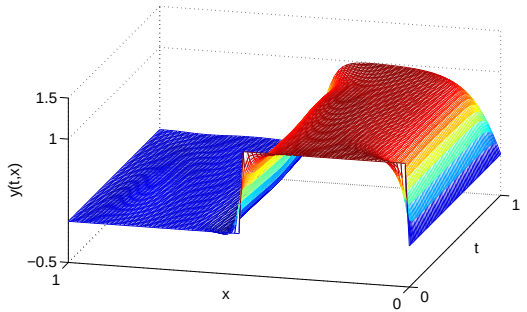
(b) $k = 1$



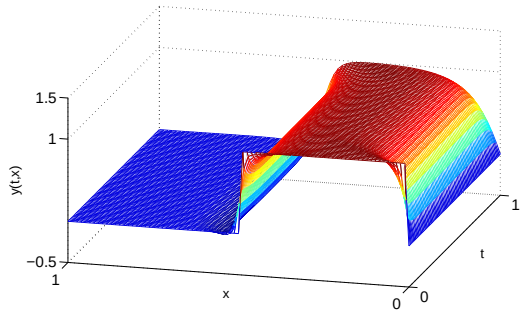
(c) $k = 2$



(d) $k = 3$

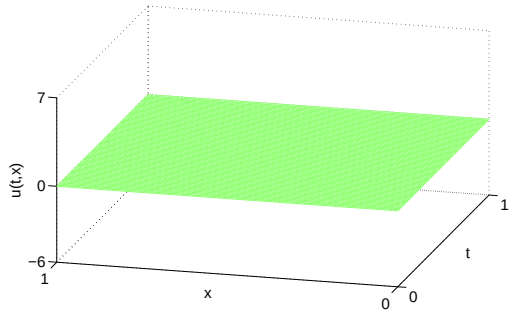


(e) $k = 4$

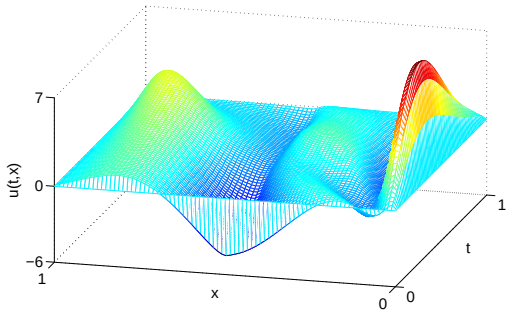


(f) $k = 5$

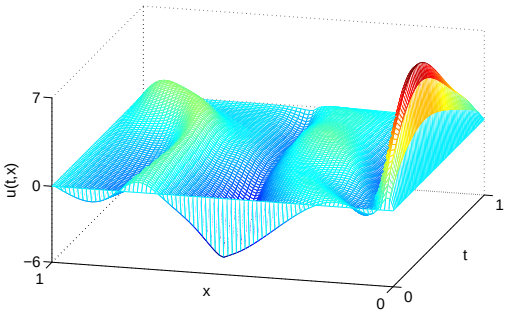
The corresponding optimal control at each iteration:



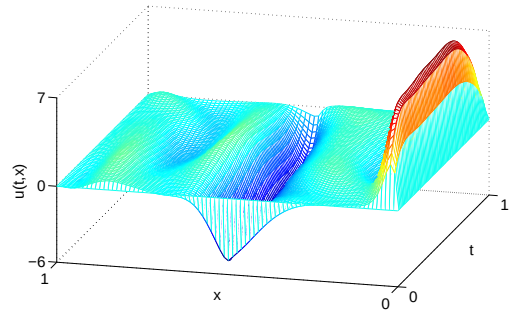
(g) $k = 0$ (initial)



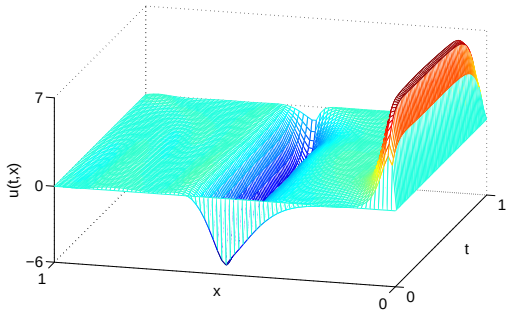
(h) $k = 1$



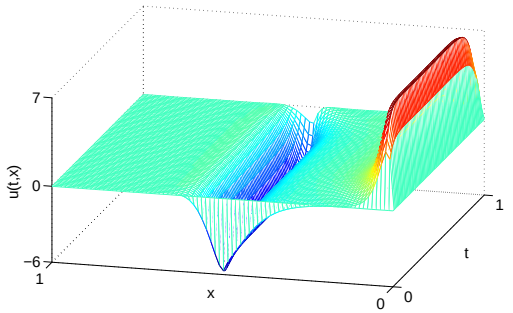
(i) $k = 2$



(j) $k = 3$



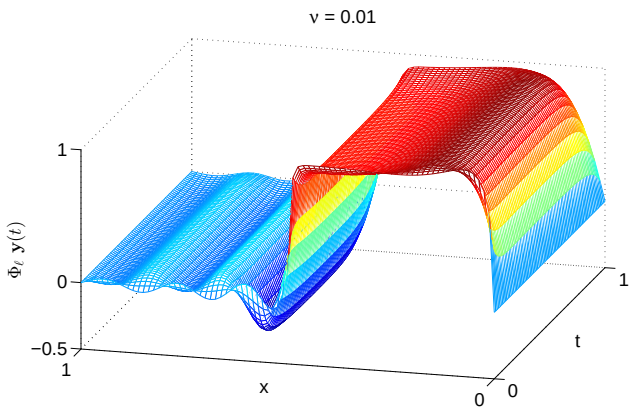
(k) $k = 4$



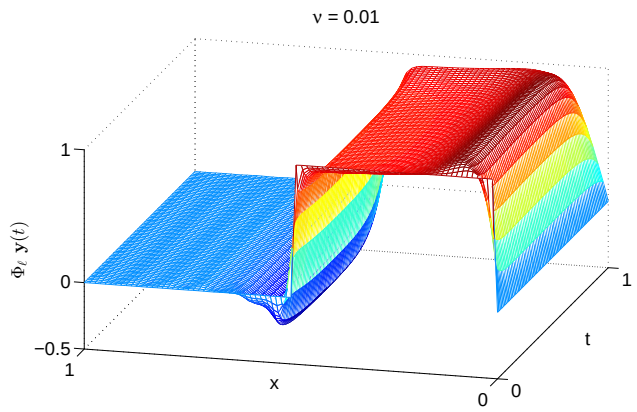
(l) $k = 5$

The following algorithm for POD-DEIM reduced optimal control has been developed:

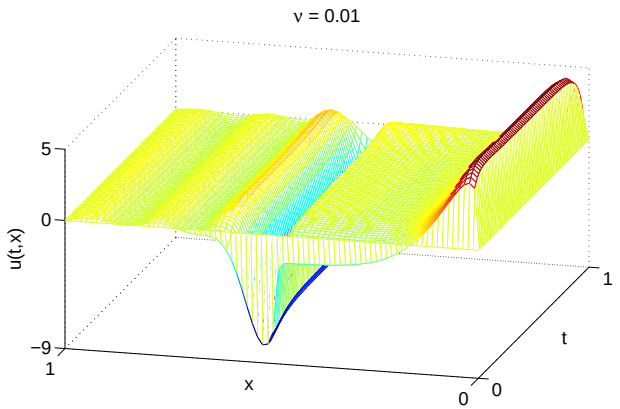
- Choose $u^{(0)}$ for the full-order model, $K = 0$
- Solve full-order Burgers' equation $c(y^{(0)}, u^{(0)}) = 0$ for $y^{(0)}$
- Choose POD-dimension ℓ and DEIM-dimension m
- Repeat until $\|y^{(K)} - z\|_{L_2(\Omega)} < tol$
  - Perform POD-DEIM algorithm using snapshots of $y^{(K)}$ $\hookrightarrow$ $\Phi_\ell, \mathcal{P}$
  - Solve $u^{(K+1)} = \operatorname{argmin}_u \tilde{\mathcal{J}}(\tilde{y}(u), u)$
  - Solve reduced Burgers' equation $\tilde{c}(\tilde{y}^{(K+1)}, u^{(K+1)}) = 0$ for $\tilde{y}^{(K+1)}$
  - Expand $y^{(K+1)} = \Phi_\ell \tilde{y}^{(K+1)}$
  - $K = K + 1$



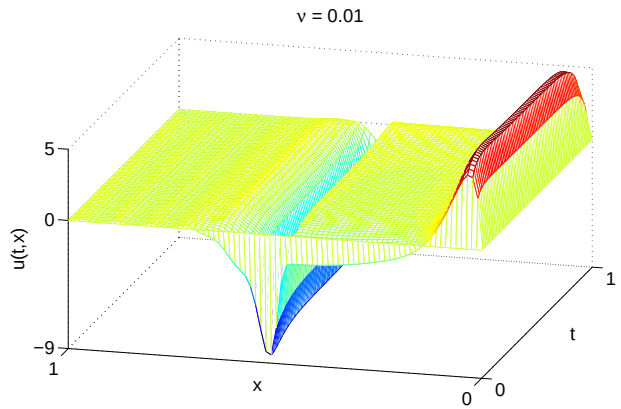
(m) $\ell = m = 7$



(n) $\ell = m = 15$



(o) $\ell = m = 7$



(p) $\ell = m = 15$

Computational benefit of the reduced optimization

Newton-type optimization for different values of ν:

	$\nu = 0.01$			$\nu = 0.001$			$\nu = 0.0001$		
	Full	POD	DEIM	Full	POD	DEIM	Full	POD	DEIM
$N/\ell/m$	80	9	(9, 25)	200	11	(11, 25)	800	15	(15, 25)
$t_{opt}[s]$	4.83	4.13	3.22	23.1	6.38	5.25	1,865.8	23.61	18.42
$\mathcal{J}(y^*, u^*)$	0.0241	0.0262	0.0233	0.0206	0.0198	0.0200	0.0202	0.0191	0.0233
$\bar{e}$	-	0.0097	0.0141	-	0.0194	0.0192	-	0.0255	0.0238
S_P	-	1.35	1.9	-	3.7	4.4	-	79.0	101.3

Further numerical tests have shown:

- For $\nu = 0.0001$ and $n_c = 3$ discrete control points in $[0, L]$, a speedup of ~ 20 for all three optimization methods has been obtained.
- For a bounded control $-2 \leq u(t, x) \leq 2$, optimization with SPG leads to a speedup of 8.8 using POD-DEIM and $\nu = 0.0001$.

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Overview and main results

- Optimal Control of Burgers' equation using POD-DEIM leads to a speedup of ~ 100 for small ν.
- For the reduced model, all derivatives need to be computed in terms of the reduced variable. This can be quite hard in practice.
- The accuracy of the reduced Burgers' model is of the same order when POD is extended by DEIM.

Future research questions

- Use the POD basis Φ_ℓ also for dimension reduction of the control, i.e.

$$\mathbf{u}(t) \approx \Phi_\ell \tilde{\mathbf{u}}(t) = \sum_{i=1}^{\ell} \varphi_i \tilde{u}_i(t)$$

- Extend Burgers' model to 2D/3D
- More elaborated choice of reduced dimensions ℓ and m

This Master project is supervised by Marielba Rojas and Martin van Gijzen.

Thank you for your attention!

Are there any questions or remarks?

https://github.com/ManuelMBaumann/MasterThesis

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Further information can be found in...

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