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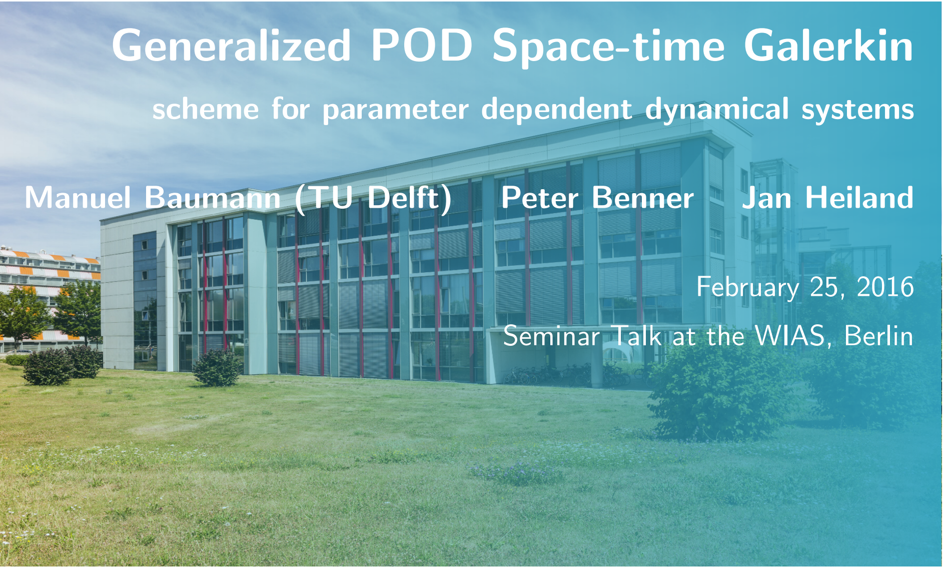

# Generalized POD Space-time Galerkin

## scheme for parameter dependent dynamical systems

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# Outline

## The Model Problem

We consider a parameter $\mu$-dependent PDE

$$\dot{\upsilon}(t,x) = \mathcal{F}(\upsilon(t,x);\mu), \quad \text{on } (0,T)\times\Omega, \quad \upsilon(0,\cdot) = \upsilon_0 \in \mathcal{Y},$$

and a finite element discretization with the *FEM* space

$$Y = \operatorname{span}\{\nu_1, \dots, \nu_q\}$$

given as

$$M_Y \dot{y}(t) = f(y(t);\mu) \quad \text{on } (0,T), \quad y(0) = y_0 \in \mathbb{R}^q,$$

where $M_Y$ is the mass matrix of $Y$.

# Generalized Measurements and POD modes

- Fix a $\mu = \mu_0$.
- Let $S = \operatorname{span}\{\psi_1, \dots, \psi_s\} \subset L^2(0, T)$ and
- consider the generalized measurement matrix:

$$X_{\mathrm{gmPOD}} := \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \vdots \\ \langle y_q, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix},$$

$$\text{cf.} \qquad X_{\mathrm{POD}} := \begin{bmatrix} y_1(t_1) & \dots & y_1(t_s) \\ \vdots & \ddots & \vdots \\ y_q(t_1) & \dots & y_q(t_s) \end{bmatrix}$$

– the snapshot matrix known from POD.

## Some observations

$$X_{\mathrm{gmPOD}} := \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \vdots \\ \langle y_q, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}$$

### Observation 1

The $L^2$-projection $y_S$ of the solution trajectory $y \in L^2(0,T) \cdot Y$ onto the space of measurements $S \cdot Y$ is given as

$$y_S = X_{\mathrm{gmPOD}} M_S^{-1} \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_s \end{bmatrix},$$

where $M_S$ is the mass matrix in $S$.

# Generalized Measurements and POD modes

$$X_{\text{gmPOD}} := \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \vdots \\ \langle y_q, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}$$

## Observation 2

The projector $P_{\hat{k}}$ that minimizes

$$\int_0^T \|y_S(t) - P_{\hat{k}} y_S(t)\|_Y^2 \, \mathrm{d}s$$

over all rank-$\hat{k}$ projectors is given as $P_{\hat{k}} = V_{\hat{k}} V_{\hat{k}}^{\mathsf{T}}$, where $V_{\hat{k}} \in \mathbb{R}^{q,\hat{k}}$ is the matrix of the $\hat{k}$ leading left singular vectors of

$$M_Y^{\frac{1}{2}} X_{\text{gmPOD}} M_S^{-\frac{1}{2}}.$$

# Generalized Measurements and POD modes

$$X_{\mathrm{gmPOD}} := \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \vdots \\ \langle y_q, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}$$

## Observation 3

The generalized orthogonal POD basis $\{\hat{\nu}_1, \dots, \hat{\nu}_{\hat{k}}\} \subset Y$ for the spatial discretization is obtained as

$$\begin{bmatrix} \hat{\nu}_1 \\ \vdots \\ \hat{\nu}_{\hat{k}} \end{bmatrix} = V_{\hat{k}}^{\mathsf{T}} M_Y^{-\frac{1}{2}} \begin{bmatrix} \nu_1 \\ \vdots \\ \nu_q \end{bmatrix}.$$

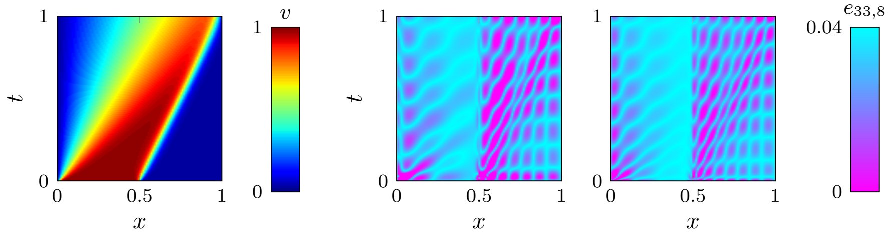
# Generalized Measurements and POD modes

## Numerical Example

This works reasonably well - for the test examples a spatial discretization of the nonlinear Burgers' equation,

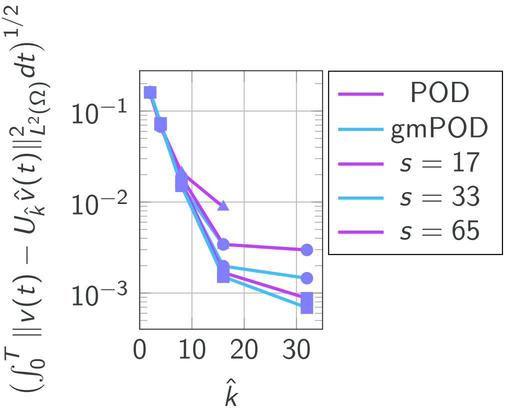
$$\partial_t z(t,x) + \partial_x\Big(\frac{1}{2} z(t,x)^2 - \mu \partial_x z(t,x)\Big) = 0,$$

with the spatial coordinate $x \in (0,1)$, the time variable $t \in (0,1]$, the viscosity parameter $\mu = 0.01$ completed by zero Dirichlet boundary conditions and a step function as initial condition.



# Generalized Measurements and POD modes

## POD vs gmPOD



## Also, we observe that

POD is literally...

> ...use measurements/snapshots over time
> to compress the spatial component of the evolution.

This can be turned around into ...

> ...use measurements in the space
> to compress the temporal component of the evolution.

$$S = \operatorname{span}\{\psi_1, \dots, \psi_s\} \subset L^2(0,T), \quad X_{\mathrm{gmPOD}} = \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \vdots \\ \langle y_q, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}$$

## Lemma ([Baumann et al. 2015])

*An POD optimal reduced basis* $\{\hat\psi_1, \cdots, \hat\psi_{\hat s}\} \subset S$ *for the time discretization can be obtained via an SVD of*

$$M_S^{-\frac{1}{2}} X_{\mathrm{gmPOD}}^{\mathsf{T}} M_Y^{\frac{1}{2}}$$

*and setting*

$$\begin{bmatrix} \hat\psi_1 \\ \vdots \\ \hat\psi_{\hat s} \end{bmatrix} = U_{\hat s}^{\mathsf{T}} M_S^{-\frac{1}{2}} \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_s \end{bmatrix},$$

*where* $U_{\hat s}$ *is the matrix of the* $\hat s$ *leading left singular vectors.*

# Space-Time-Parameter POD

For parametrized problems or problems with an input. . .

. . . use measurements over time *and over a parameter domain*
to compress the spatial component of the evolution

A discretization of the parameter domain with $p$ degrees of freedom adds another dimension to the generalized measurement matrix turning it into a tensor $\mathbf{X} \in \mathbb{R}^{q \times s \times p}$.

$$\begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \dots & \dots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \ddots & \vdots \\ \langle y_n, \psi_1 \rangle_{\mathcal{S}} & \dots & \dots & \langle y_n, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}_{\mu=\mu_0}$$

$$\begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & & \\ \vdots & & \\ \langle y_n, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_n, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}_{\mu=\mu_1}$$

$$\begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & & \\ \vdots & & \\ \langle y_n, \psi_1 \rangle_{\mathcal{S}} & \dots & \langle y_n, \psi_s \rangle_{\mathcal{S}} \end{bmatrix}_{\mu=\mu_2}$$

## Truncated Higher Order SVD [De Lathauwer et al. 2000]

- There is a HOSVD:

$$\mathbf{X} = \mathbf{C} \times_1 U^{(\psi)} \times_2 U^{(\nu)} \times_3 U^{(\mu)},$$

  - with the *core tensor* $\mathbf{C} \in \mathbb{R}^{q \times s \times p}$,
  - with unitary matrices $U^{(\psi)} \in \mathbb{R}^{s \times s}$, $U^{(\nu)} \in \mathbb{R}^{q \times q}$, and $U^{(\mu)} \in \mathbb{R}^{p \times p}$,
  - and with $\times_1$, $\times_2$, and $\times_3$ denoting tensor-matrix multiplications.
- To compute the HOSVD:
  - define a *matrix unfolding* $\tilde{\mathbf{X}}^{(\psi)} \in \mathbb{R}^{s \times qp}$ of the tensor $\tilde{\mathbf{X}}$ via putting all elements belonging to $\psi_1, \psi_2 \ldots \psi_s$ into one respective row.
  - Similarly, define the unfoldings $\mathbf{Y}^{(\nu)} \in \mathbb{R}^{q \times ps}$ and $\mathbf{Y}^{(\mu)} \in \mathbb{R}^{p \times sq}$.

## Truncated Higher Order SVD [De Lathauwer et al. 2000]

- From the unfoldings, compute $U^{(\psi)}$, $U^{(\nu)}$ and $U^{(\mu)}$
  - by means of three SVDs like $\mathbf{Y}^{(\psi)} = U^{(\psi)}\Sigma^{(\psi)}(W^{(\psi)})^\mathsf{T}$
  - with $\Sigma^{(\psi)}$ diagonal with entries $\sigma_1^{(\psi)} \geq \sigma_2^{(\psi)} \geq \dots \sigma_s^{(\psi)} \geq 0$
- From these SVDs, derive an approximation $\hat{\mathbf{X}} \in \mathbb{R}^{q\times s\times p}$ of $\mathbf{X}$ by discarding the smallest $n$-mode singular values.

Then, it holds that

$$\|\mathbf{X} - \hat{\mathbf{X}}\|_F^2 \leq \sum_{i=\hat{s}+1}^{s} \sigma_i^{(\psi)} + \sum_{k=\hat{q}+1}^{q} \sigma_k^{(\nu)} + \sum_{l=\hat{p}+1}^{p} \sigma_l^{(\mu)}.$$

# Space-Time-Parameter POD

Thus, optimal bases are obtained via a *higher-order SVD*, i.e. via SVDs of tensor unfoldings with respect to the space dimension

$$\mathbf{X}^{(\nu)} := \left| \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \cdots & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & \ddots & \vdots \\ \langle y_q, \psi_1 \rangle_{\mathcal{S}} & \cdots & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix} \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \cdot & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & . & \vdots \\ \langle y_q, \psi_1 \rangle_{\mathcal{S}} & \cdot & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix} \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \cdot & \langle y_1, \psi_s \rangle_{\mathcal{S}} \\ \vdots & . & \vdots \\ \langle y_q, \psi_1 \rangle_{\mathcal{S}} & \cdot & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix} \right|,$$

and with respect to the time dimension

$$\mathbf{X}^{(\psi)} := \left| \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \cdots & \langle y_q, \psi_1 \rangle_{\mathcal{S}} \\ \vdots & \ddots & \vdots \\ \langle y_1, \psi_s \rangle_{\mathcal{S}} & \cdots & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix} \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \cdot & \langle y_q, \psi_1 \rangle_{\mathcal{S}} \\ \vdots & . & \vdots \\ \langle y_1, \psi_s \rangle_{\mathcal{S}} & \cdot & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix} \begin{bmatrix} \langle y_1, \psi_1 \rangle_{\mathcal{S}} & \cdot & \langle y_q, \psi_1 \rangle_{\mathcal{S}} \\ \vdots & . & \vdots \\ \langle y_1, \psi_s \rangle_{\mathcal{S}} & \cdot & \langle y_q, \psi_s \rangle_{\mathcal{S}} \end{bmatrix} \right|,$$

which, as above, lead to optimized bases $\{\hat{\nu}_1, \dots, \hat{\nu}_{\hat{k}}\} \subset Y$ and $\{\hat{\psi}_1, \cdots, \hat{\psi}_{\hat{s}}\} \subset S$ in space and time and which are also optimal for the considered parameter samplings [De Lathauwer et al. 2000].

## Numerical Example

Consider again

$$\partial_t z(t,x) + \partial_x\left(\frac{1}{2}z(t,x)^2 - \mu\partial_x z(t,x)\right) = 0,$$

- spatial coordinate $x \in (0,1)$, time variable $t \in (0,1]$,
- completed by zero Dirichlet boundary conditions, a step function as initial condition,
- choose the discrete spaces $S$ and $Y$,
- simulate and compute $\mathbf{X}$ for training parameters

$$\mu = \{10^{-2}, 3\cdot 10^{-3}, 10^{-3}\},$$

- use optimized space and time bases for a space-time Galerkin discretization.

## Full order and reduced system

The discrete spaces

- $Y$ – piecewise linear finite elements on an equidistant grid of $q = 130$ nodes.
- $S \subset L^2(0,1)$ – span of $s = 65$ equidistantly distributed linear hat functions.

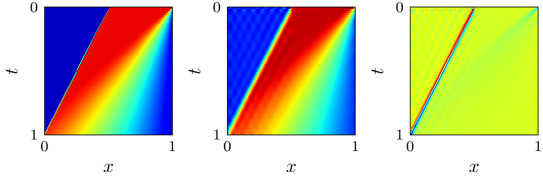



Figure : Burger setup for $\mu = 3 \cdot 10^{-3}$: The full solution, the reduced solution, and the space-time $L^2$ approximation error.

## Space vs. Time Resolution

- Set the overall number of POD modes to $K := \hat{q} + \hat{s}$ and
- consider varying ratios of space and time resolutions

$$\hat{q} = f \cdot K \quad \text{and} \quad \hat{s} = (1 - f) \cdot K, \quad \text{for } f \in [0.2, 0.8]$$

- and the approximation error over varying parameter $\mu$

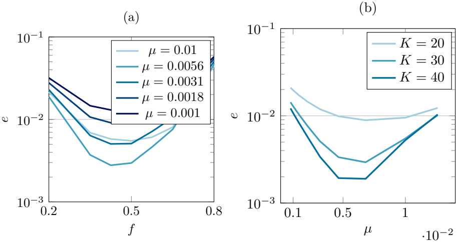



Figure : (a) the error for various numbers of $f$. (b): the error in the reduced model over the parameter range for various $K$.

## Conclusion

- POD on the base of generalized measurements
  - more flexibility in the data assimilation
  - outperforms standard POD in some cases
  - ? special measurement functions for special problems
  - ? inherent averaging is beneficial for noisy data
  - ? analytical framework to be exploited for error estimates
- Space-time-parameter Galerkin POD
  - well backed by theory
  - it works reasonably well
  - more tensor directions can be added
  - not competitive in forward problems
  - however...

### Application in Optimal Control

Consider a finite time optimal control problem

$$\mathcal{J}(z,u) := \int_0^T \mathcal{K}(z,u)\,\mathrm{d}t \to \min_u \quad \text{subject to} \quad \dot z = \mathcal{F}(z,u), \quad z(0) = z_0.$$

The first order optimality conditions contain the adjoint equation

$$-\dot\lambda = \mathcal{F}_{;z}(z,u)'\lambda - \mathcal{K}_{;z}(z,u), \quad \lambda(T) = 0,$$

so that the optimality system is global in time.
For the solution, space-time-parameter may be a good choice

- sample the input space as tensor direction
- sample both primal and dual variables
- apply space-time Galerkin with the optimized bases

# Thank you for your attention!

I am always open for discussion

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