Nonlinear model order reduction for parametrized transport-dominated PDEs using registration-based methods

Young Mathematicians in Model Order Reduction (YMMOR) 2023

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Outline

Introduction and motivation

Basics from image registration

Model order reduction in the space of (smooth) vector fields

Numerical experiments

Outlook

Motivation: Transport dominated parametrized problems

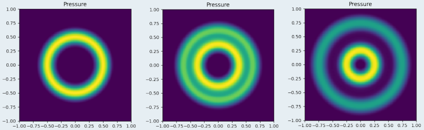
Problems and difficulties

- Slowly decaying Kolmogorov N-width of the solution manifold [Ohlberger/Rave'16, Greif/Urban'19]
- Parameter dependent shock evolution and topology
- Complex shock interactions

Linear methods are not sufficient!

Examples

- Acoustics equations:



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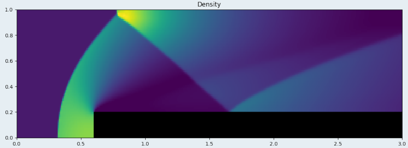

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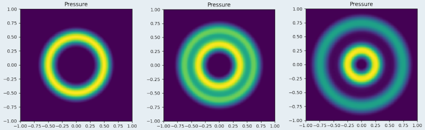

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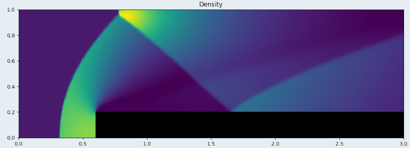


Simple example: Burgers' equation in 1d

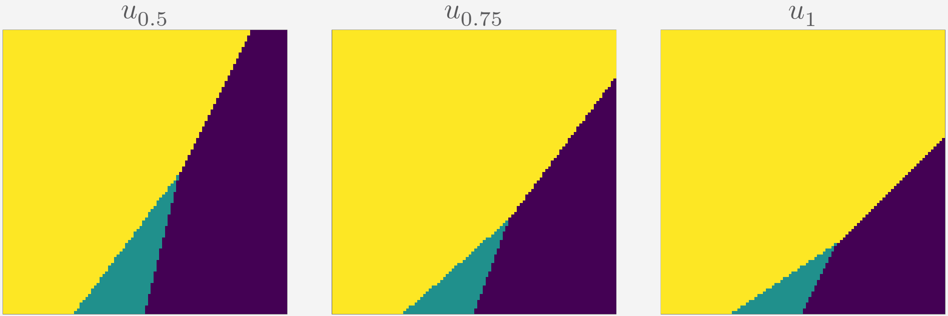
Consider the parametrized equation

$$\partial_t u_\mu(t,x) + \frac{\mu}{2}\partial_x u_\mu(t,x)^2 = 0, \qquad (t,x) \in [0,1]\times[0,1],$$
$$u_\mu(0,x) = u_0(x), \qquad x \in [0,1],$$

with piecewise constant initial condition

$$u_0(x) = \begin{cases} 2, & \text{if } x \leq 1/4, \\ 1, & \text{if } 1/4 < x \leq 1/2, \\ 0, & \text{if } 1/2 < x. \end{cases}$$

How do solutions for different parameters look like?



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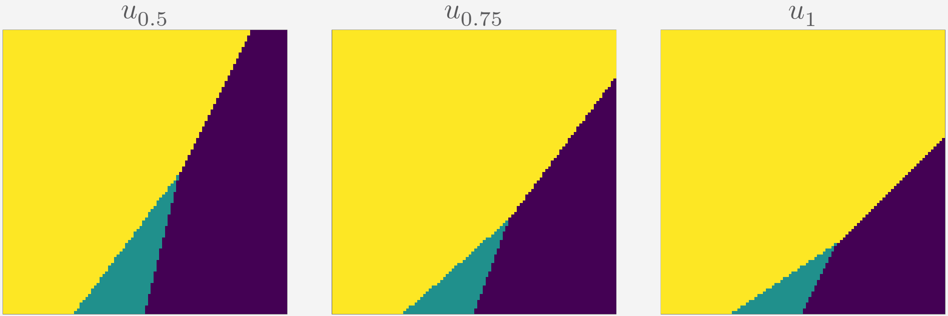

$\longrightarrow$ **Transform underlying space-time domain to match snapshots?**

Transformations of space-time domains to align shocks and discontinuities

- Shock interaction already incorporated in space-time solutions (no need to treat them separately).
- Diffeomorphic transformations (that can be represented in a reduced space, see below) of the underlying space-time domain to match snapshots to each other.
- Choose a (fixed) reference snapshot that can be transformed into all other solutions.
- Apply ideas and concepts from (medical) image registration.

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Image registration

- *Main application:* Medical imaging to align images and to detect deviations from expected states.
- *Goal:* Given a “template image” $u_0\colon\Omega\to\mathbb{R}$ and a “target image” $u_1\colon\Omega\to\mathbb{R}$, find a transformation $\Phi\colon\Omega\to\Omega$, such that

$$u_0\circ\Phi^{-1}\approx u_1.$$

- In our approach:
  - Apply *diffeomorphism* $\Phi\in G$ from diffeomorphism group G as transformation.
  - Diffeomorphism induced by *vector field* $v\in\mathfrak{g}$ (see below).

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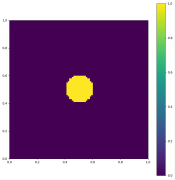
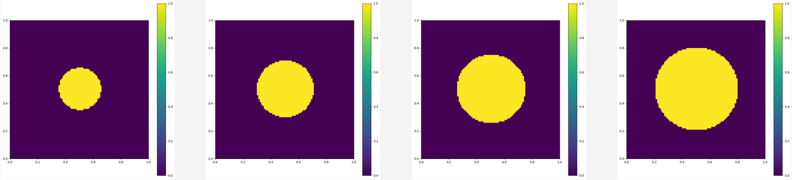
Simple example: Blowing up a circle

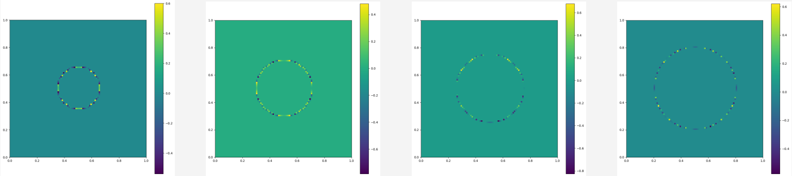
Template image



Target images



Differences between targets and transformed template



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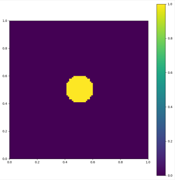
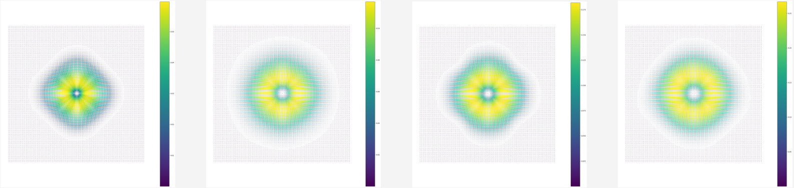
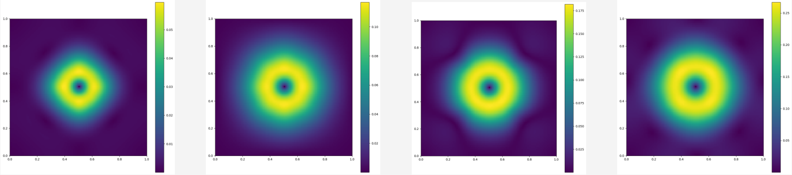


Vector fields inducing the diffeomorphism



Magnitude of vector fields inducing the diffeomorphism



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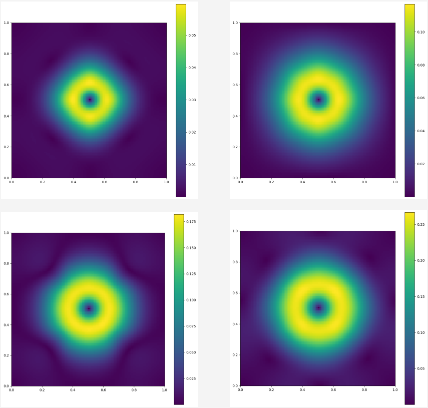

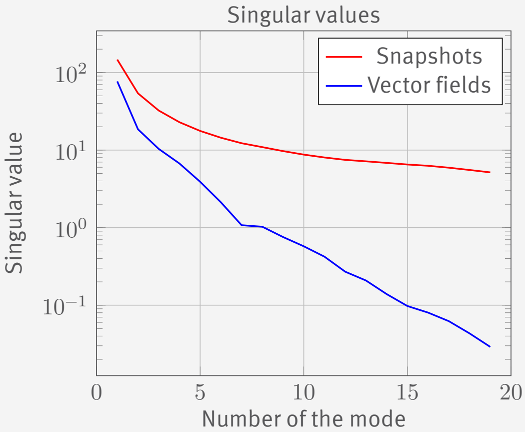

Geodesics in the diffeomorphism group

- Euler-Poincaré differential equation to determine time-dependent velocity field $v_t : \Omega \to \mathbb{R}^d$, $\Omega \subset \mathbb{R}^d$, as

$$\frac{\partial v_t}{\partial t} = -K\left[(Dv_t)^T \cdot Lv_t + D(Lv_t) \cdot v_t + Lv_t \cdot \operatorname{div} v_t\right], \qquad \boxed{v_0 = v \in \mathfrak{g},}$$

where L is a differential operator of the form $L = (Id - \alpha\Delta)^s$ with inverse $K = L^{-1}$.

- Diffeomorphism $\phi_t : \Omega \to \Omega$, given as flow of velocity field v_t, i.e.

$$\frac{\partial \phi_t}{\partial t} = v_t \circ \phi_t, \qquad \phi_0 = Id.$$

- Knowledge of v sufficient to compute $\Phi(v) := \phi_1$!
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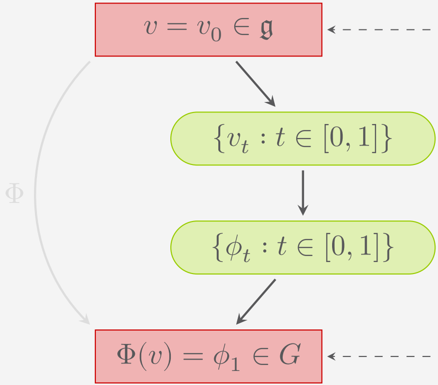

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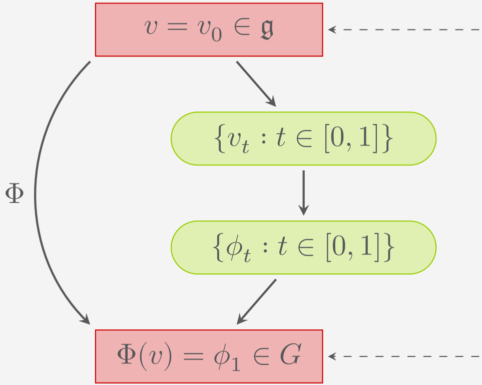

Hilbert space of vector fields

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Nonlinear diffeomorphism group

Computing the vector field

How to compute good choice of $v \in \mathfrak{g}$ given a “template image” $u_0 : \Omega \to \mathbb{R}$ and a “target image” $u_1 : \Omega \to \mathbb{R}$?

Minimize energy

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(Linear) Model order reduction in the space of smooth vector fields

- Smooth vector fields $\mathfrak{g}$ form a **Hilbert space** with inner product

$$\langle v, w\rangle_{\mathfrak{g}} := (Lv, w)_{L^2(\Omega)} = (v, Lw)_{L^2(\Omega)}.$$

- We can apply well-known linear model order reduction methods in $\mathfrak{g}$, like **POD** [Wang/Xing/Kirby/Zhang'19] or **Greedy algorithms**!

- Motivation of the approach: Due to the smoothness of the vector fields in $\mathfrak{g}$, we expect a faster decay of the Kolmogorov N-width in the space of vector fields. (Hard to tackle theoretically though.)

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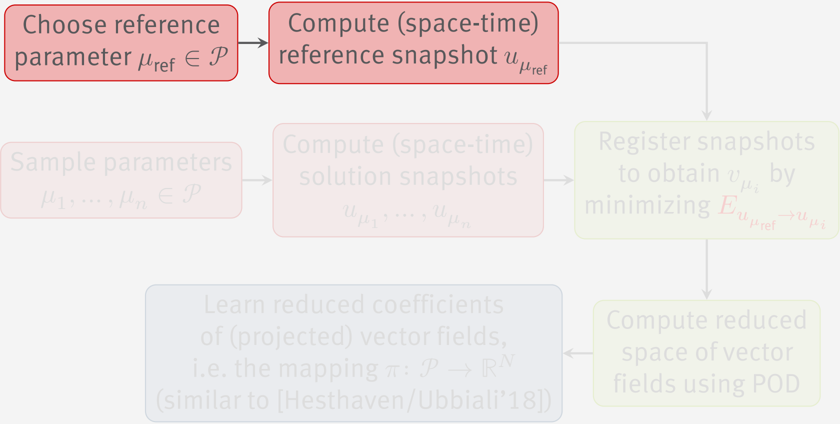

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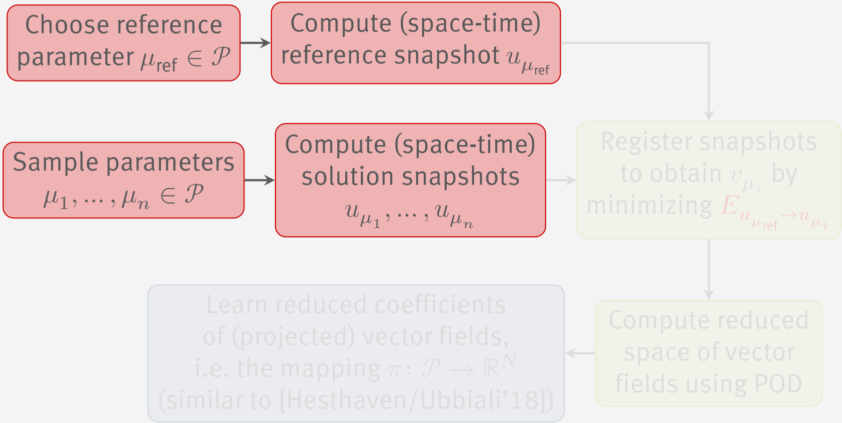

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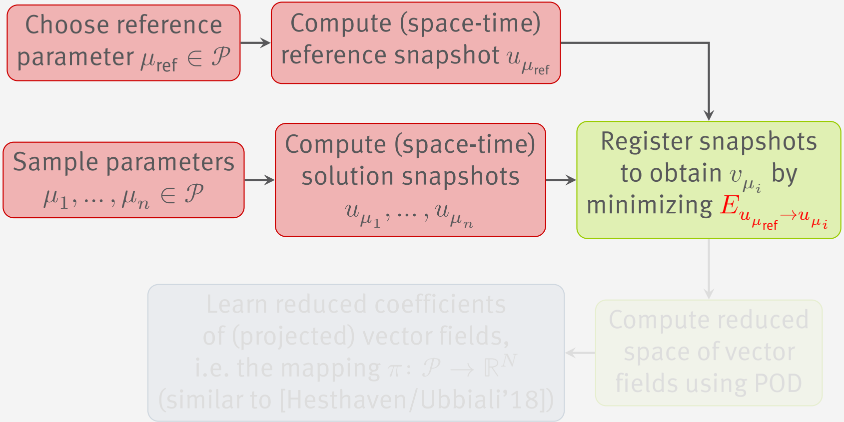

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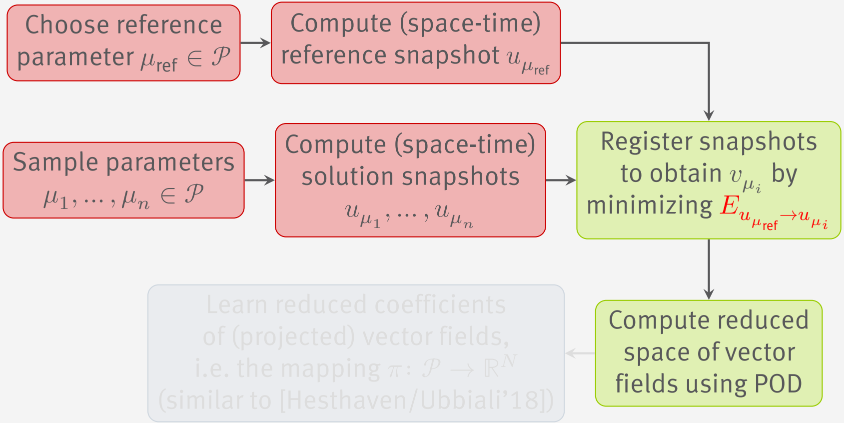

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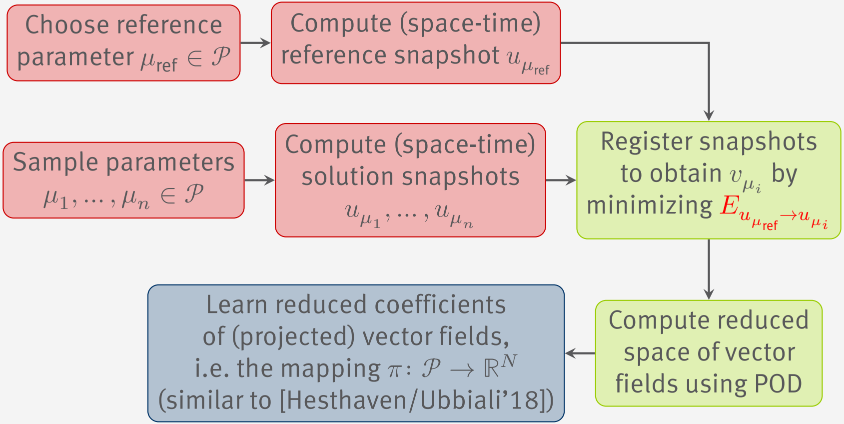

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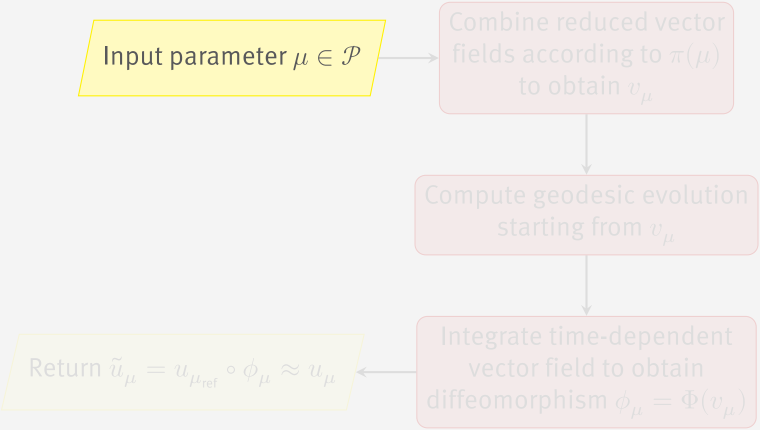

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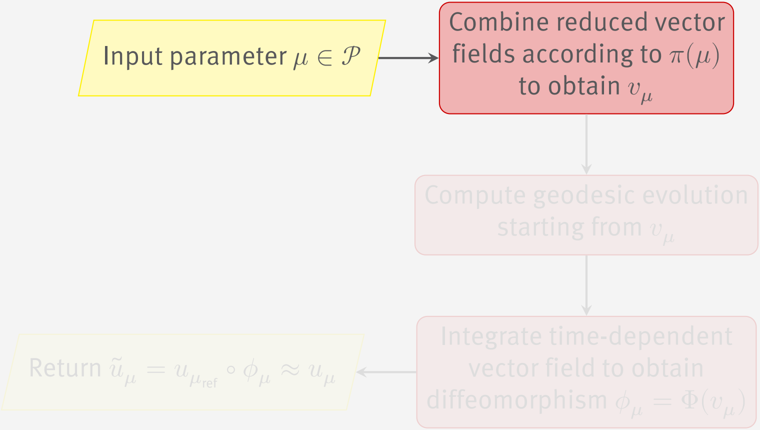

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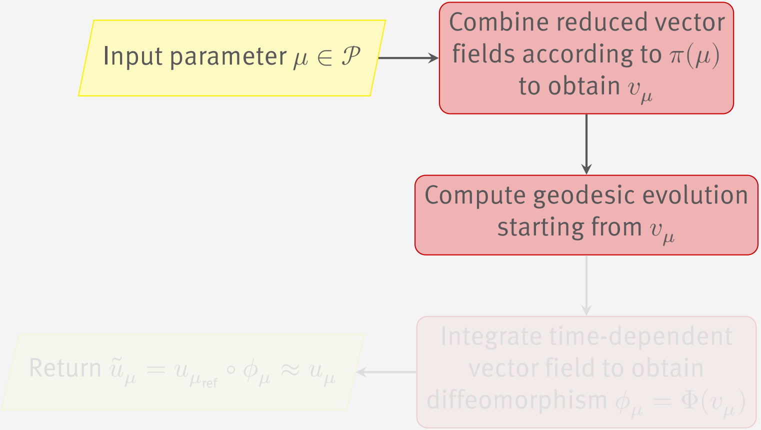

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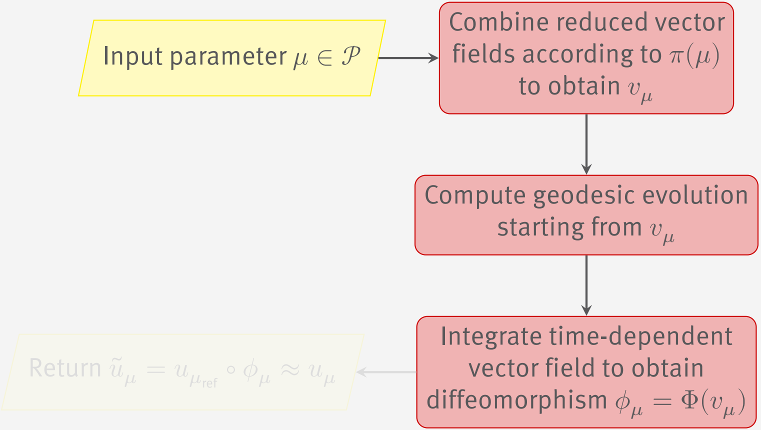

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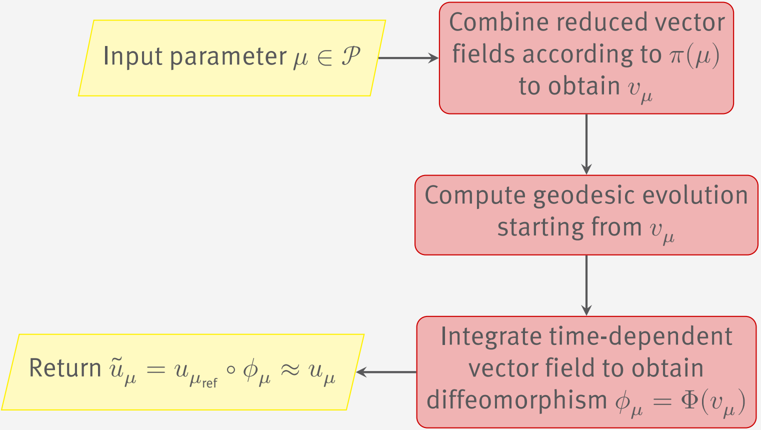

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Numerical results – Burgers' equation with two shocks

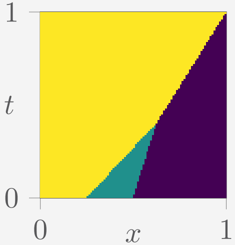
$$\partial_t u_\mu + \mu \partial_x u_\mu^2 = 0, \qquad (t,x) \in [0,T] \times \Omega,$$
$$u_\mu(0) = u_0, \qquad x \in \Omega,$$

$$u_0(x) = \begin{cases} 2, & \text{if } x \leq 1/4, \\ 1, & \text{if } 1/4 < x \leq 1/2, \\ 0, & \text{if } 1/2 < x. \end{cases}$$

Parameter domain	$\mathcal{P} = [0.25, 1.5]$
Discretization	$N_x = N_t = 100$
Reference parameter	$\mu_{\text{ref}} = 0.625$
Num. of training samples	$n \in \{20, 50\}$

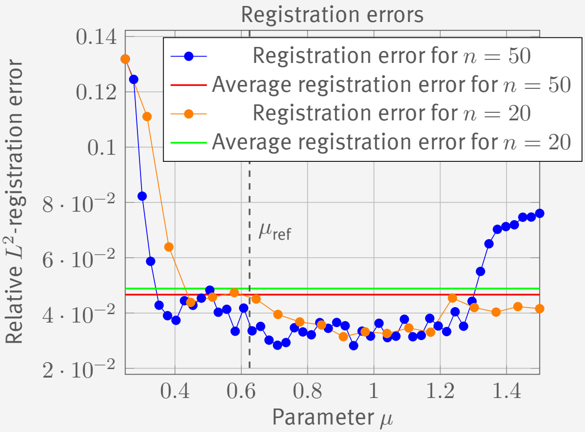
Test parameters	$\mu \in \{0.5, 0.75, 1.0, 1.25\}$

Reference solution $u_{\mu_{\text{ref}}} = u_{0.625}$



Geodesic shooting implementation: `https://github.com/HenKlei/geodesic-shooting`

Numerical results – Registration errors and singular values



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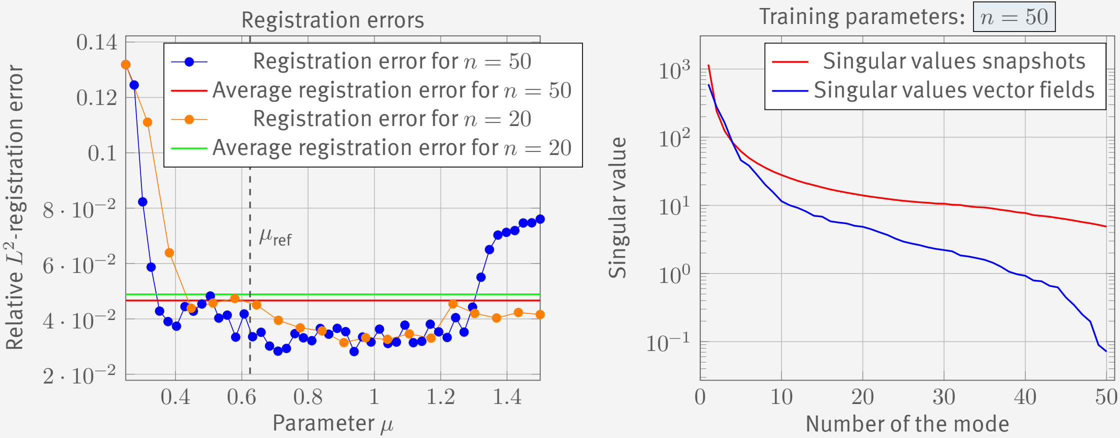
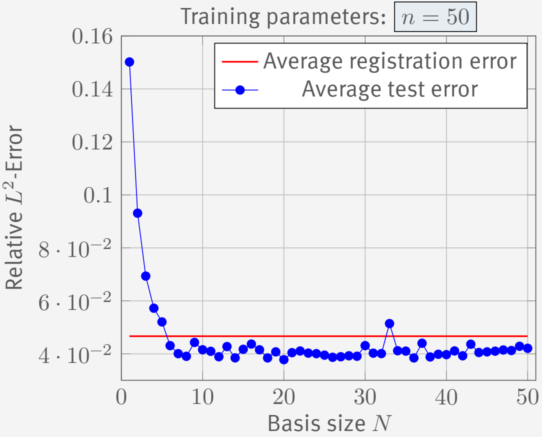


Numerical results – Errors on the test set



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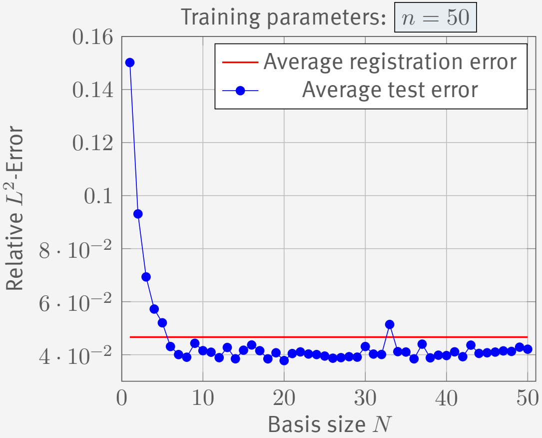
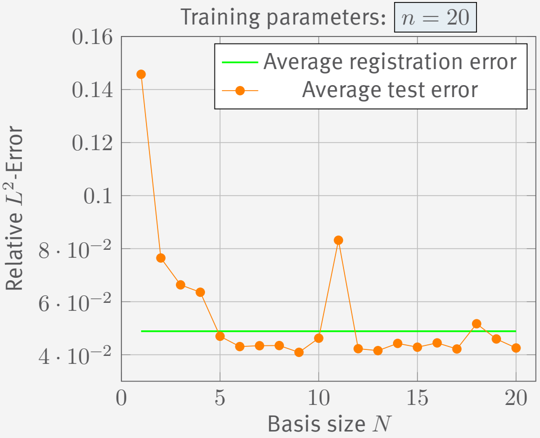
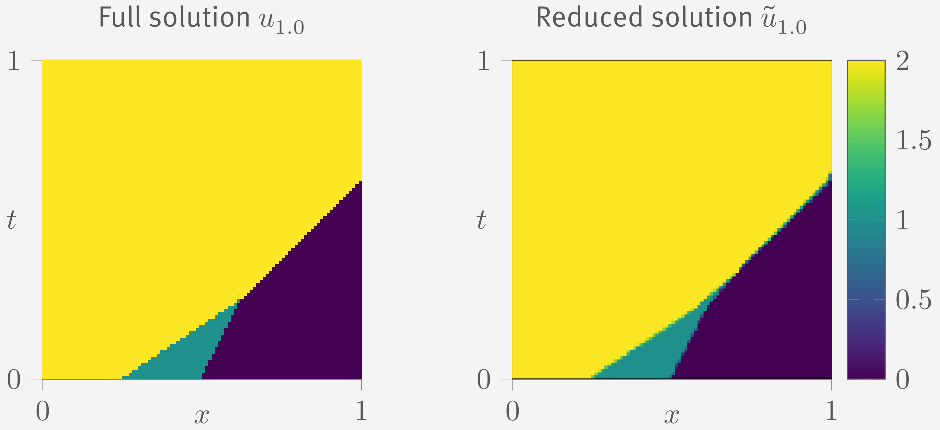




Numerical results – Reduced basis of size $N = 10$



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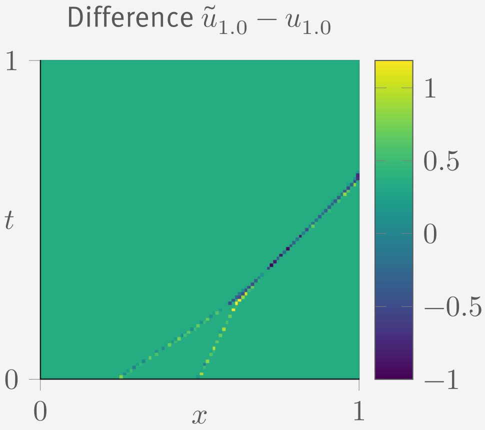

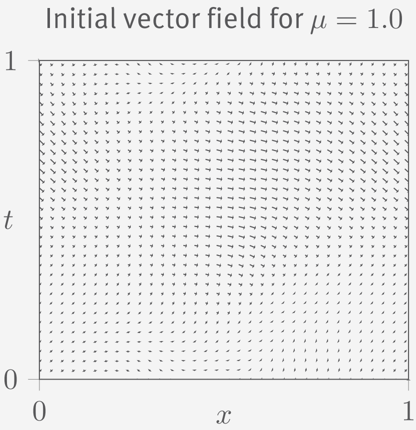

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Outlook and further research perspectives

- Examples in higher space dimensions (registration becomes harder).
- Greedy procedure instead of POD to extract vector fields.
- Residual minimization during online phase instead of learning the coefficients.
- Localize the approach to be able to tackle the evolution of complex shock fronts in higher dimensions.

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Thank you for your attention!

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