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Nonlinear model order reduction for hyperbolic conservation laws by means of diffeomorphic transformations of space-time domains

Model Reduction and Surrogate Modeling (MORE) 2022

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Outline

Motivation: Transport dominated parametrized problems

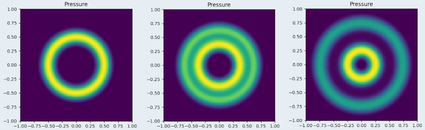
Problems and difficulties

- 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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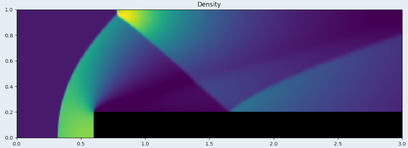

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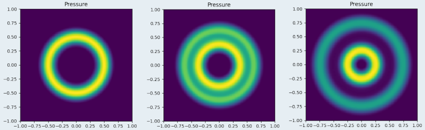

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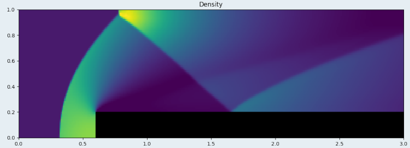


Simple example: Burgers' equation in 1d

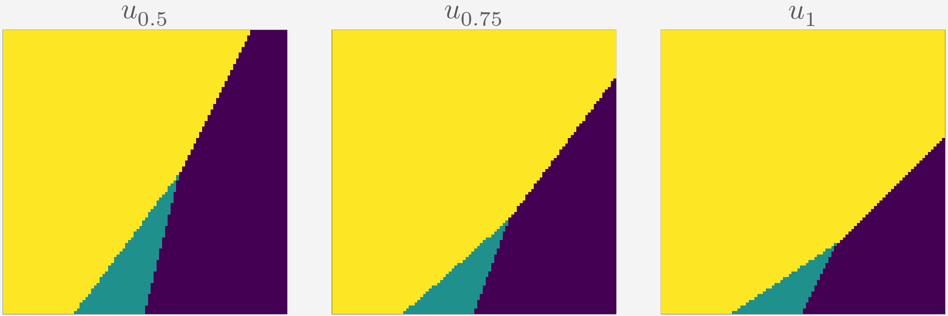
Consider the parametrized equation

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

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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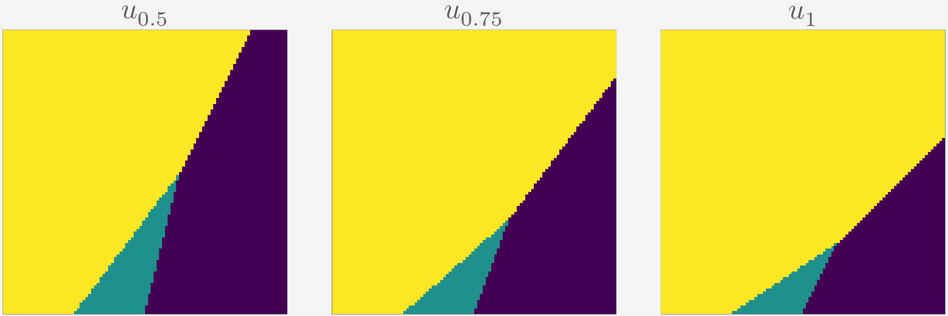

$\longrightarrow$ **Transform underlying space-time domain to match snapshots?**

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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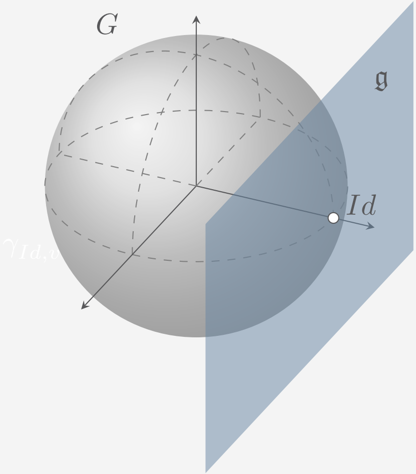
Lie groups and Lie algebras

Lie group

A group G such that group multiplication and inversion are smooth maps, i.e. G is a manifold.

Lie algebra

The tangent space $\mathfrak{g} = T_{Id}G$ to a Lie group G at the identity element $Id \in G$.



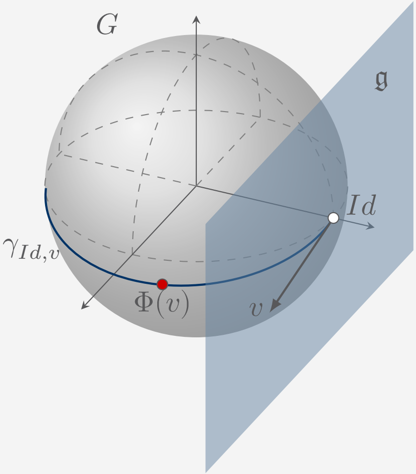
Lie groups and Lie algebras

Geodesic curve

Smooth curve $\gamma_{p,v}\colon I \to G$, I an open interval, $\gamma_{p,v}(0) = p \in G$, $\gamma'_{p,v}(0) = v \in T_p G$, that (locally) minimizes lengths.

Unit time geodesic

Following geodesic from the identity in direction $v \in \mathfrak{g}$ for unit time defines a mapping $\Phi\colon \mathfrak{g} \to G$, $\Phi(v) = \gamma_{Id,v}(1)$.



Lie groups and Lie algebras in image registration

- Diffeomorphism group G on $\mathbb{R}^n$ forms a Lie group.
- Lie algebra $\mathfrak{g}$ is the space of smooth vector fields.
- Diffeomorphism group acts on underlying space by transforming it.

- Attention: Diffeomorphism group is infinite dimensional! (Theory is much harder in general, e.g. exponential map and geodesics do not coincide.)

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Geodesics in the diffeomorphism group

- Euler-Poincaré differential equation to determine time-dependent velocity field $v_t\colon\Omega\to\mathbb{R}^d$, $\Omega\subset\mathbb{R}^d$, 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 $\phi_t\colon\Omega\to\Omega$, 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 $\Phi(v):=\phi_1$!
$\longrightarrow$ Main idea of **geodesic shooting** [Miller/Trouvé/Younes'06].

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Ideas and concepts from image registration

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

$$E_{u_0 \to u_1}(v) := \underbrace{(Lv, v)_{L^2(\Omega)}}_{\text{Regularization term}} + \frac{1}{\sigma^2} \underbrace{\|u_0 \circ \Phi(v)^{-1} - u_1\|_{L^2(\Omega)}^2}_{\text{Mismatch measurement}}$$

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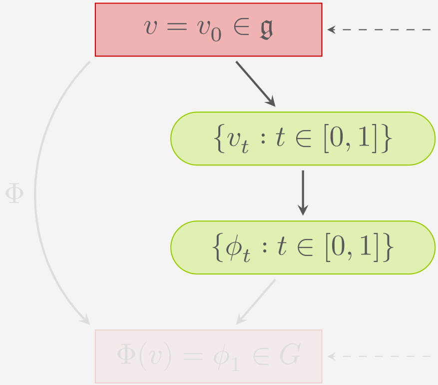

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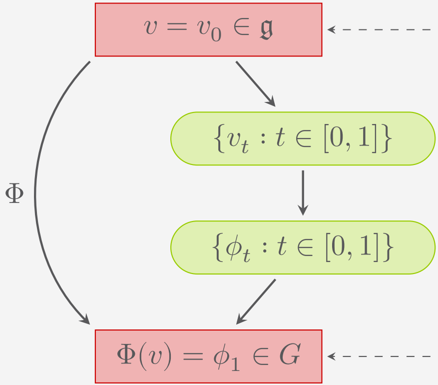

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(Linear) Model order reduction in the Lie algebra

- Lie algebra of smooth vector fields $\mathfrak{g}$ forms 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 Lie algebra. (Hard to tackle theoretically though.)

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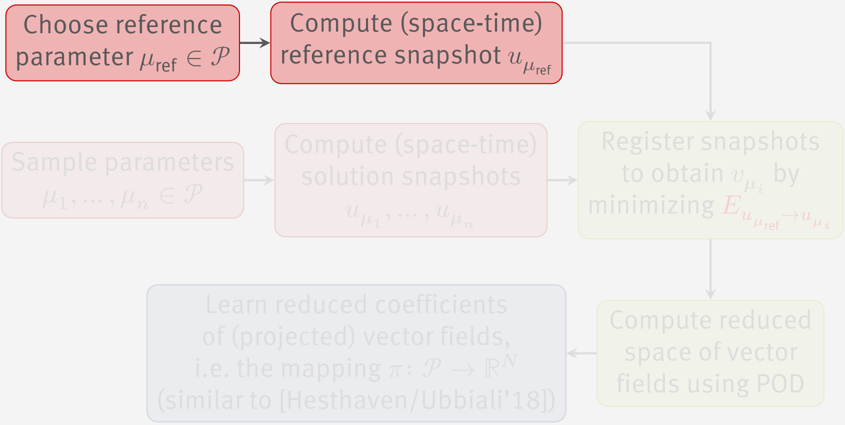

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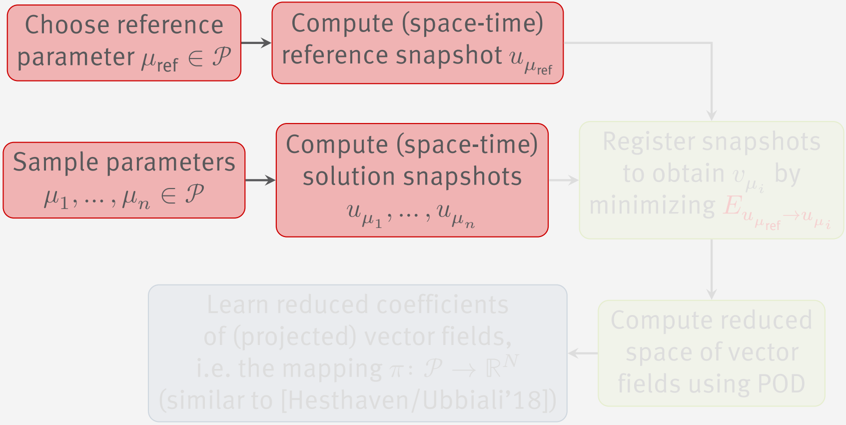

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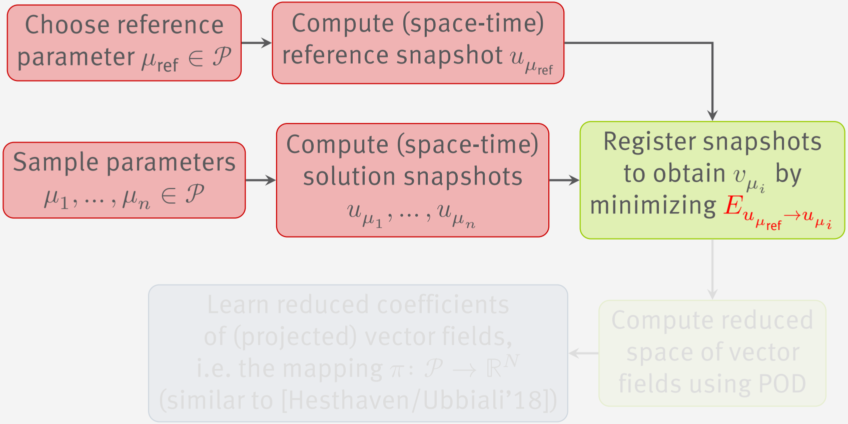

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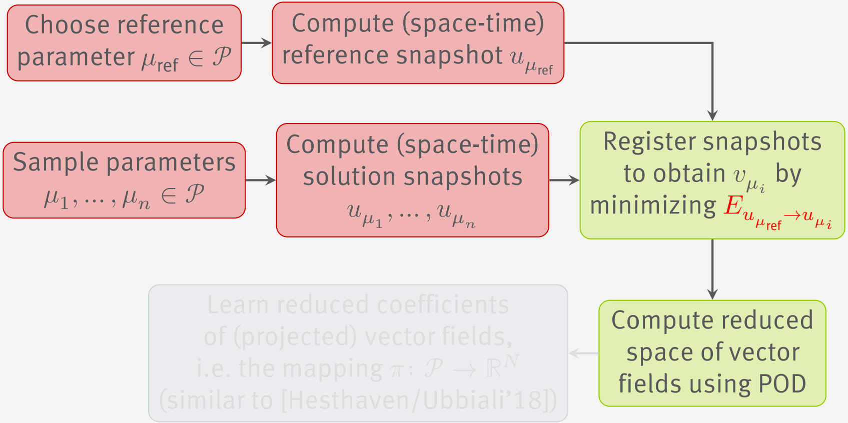

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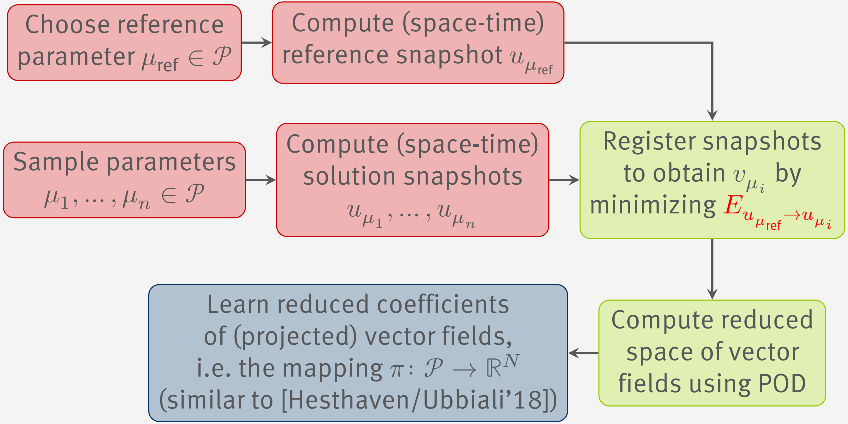

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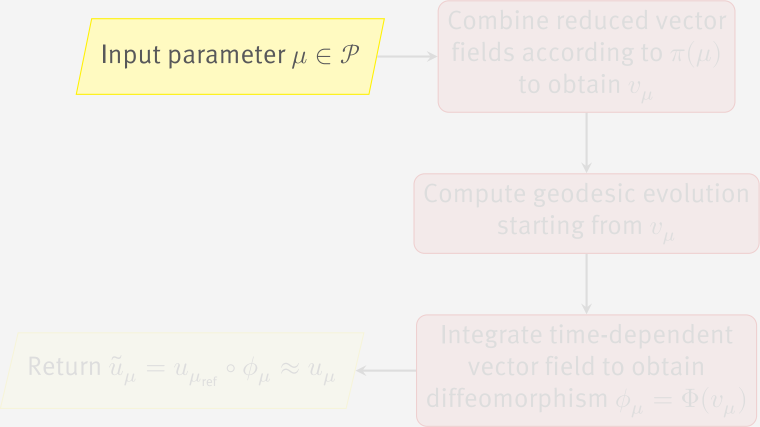

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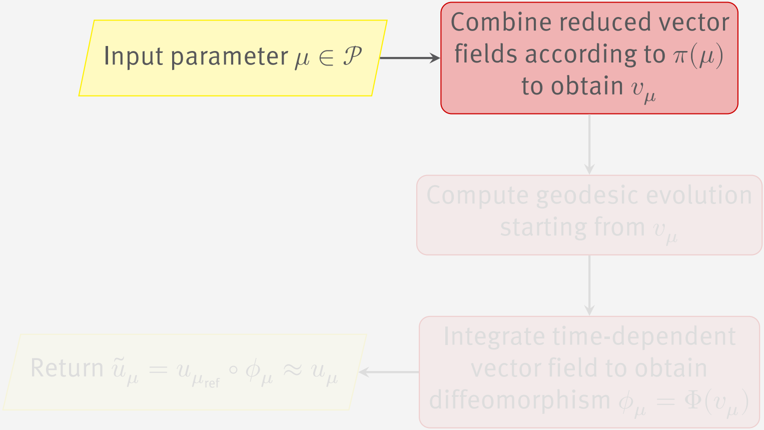

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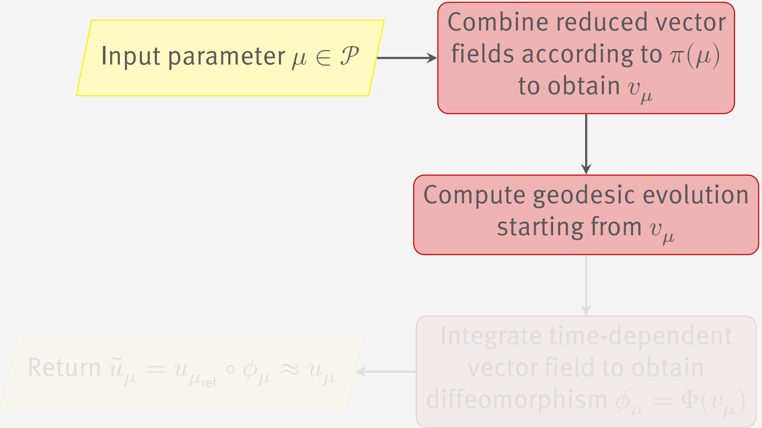

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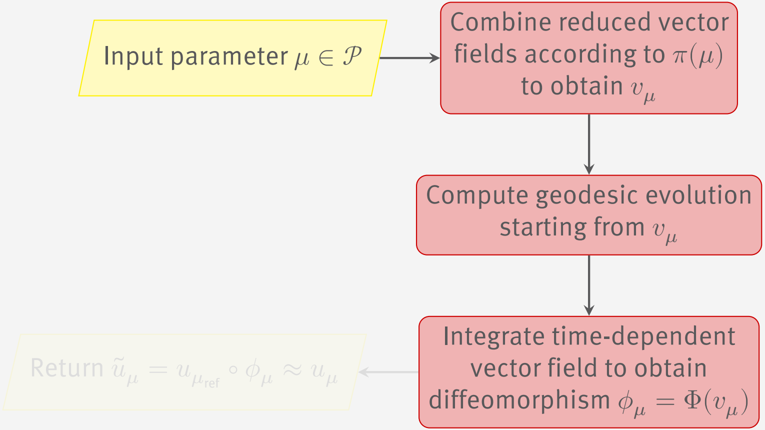

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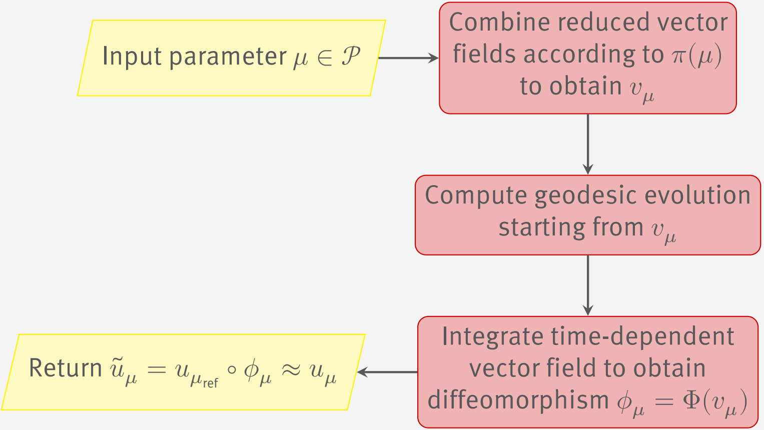


Outline

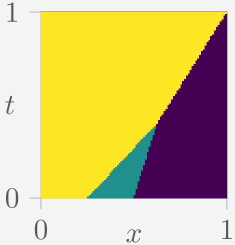
Numerical results – Burgers' equation with two shocks

$$\begin{aligned} \partial_t u_\mu + \mu \partial_x u_\mu^2 &= 0, && (t,x) \in [0,T] \times \Omega, \\ u_\mu(0) &= u_0, && x \in \Omega, \end{aligned}$$

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

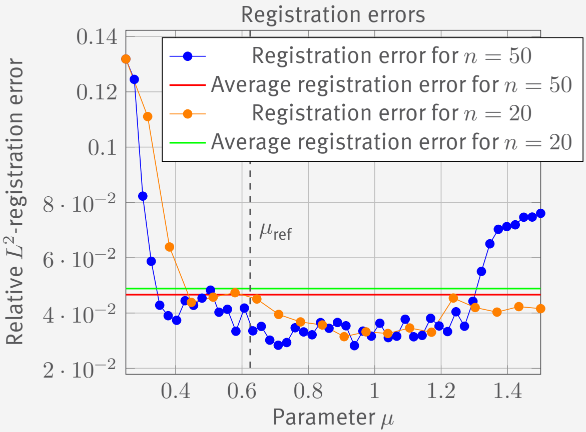
Parameter domain	$\mathcal{P} = [0.25, 1.5]$
Discretization	$N_x = N_t = 100$
Reference parameter	$\mu_{\text{ref}} = 0.625$
Test parameters	$\mu \in \{0.5, 0.75, 1.0, 1.25\}$

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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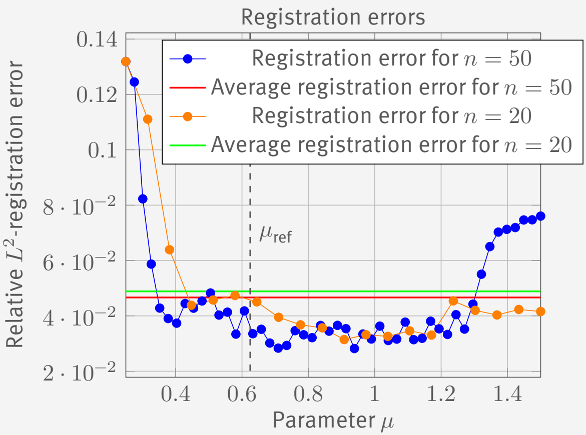
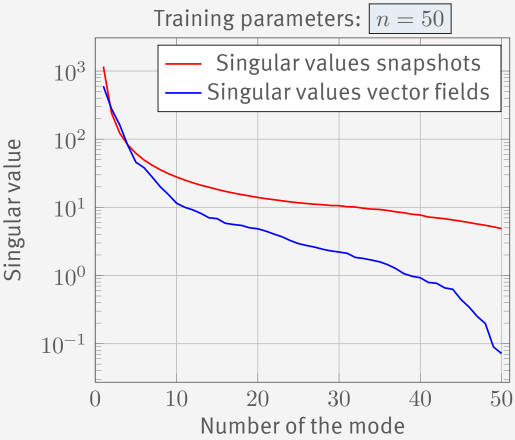
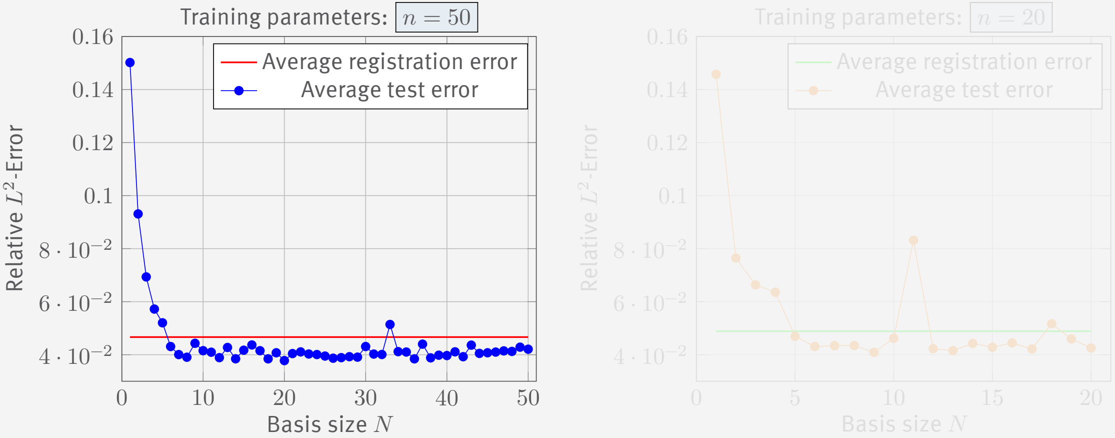




Numerical results – Errors on the test set



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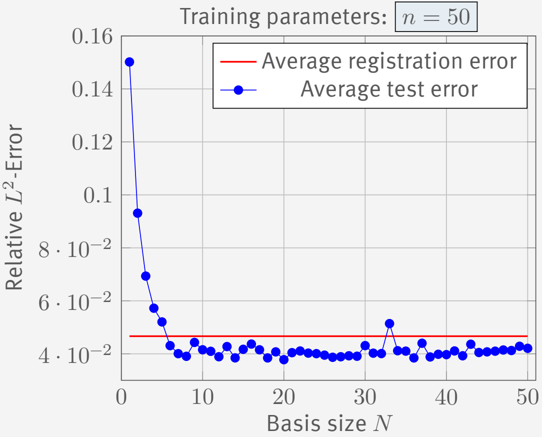
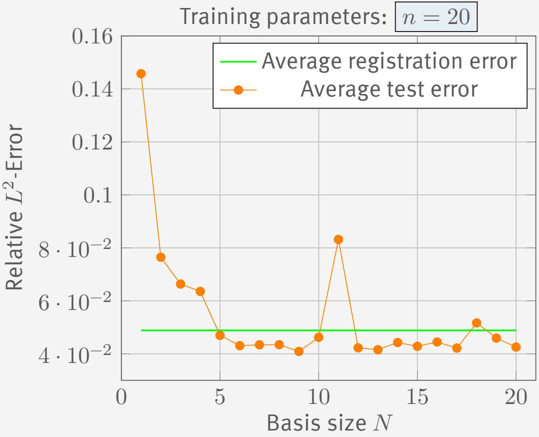
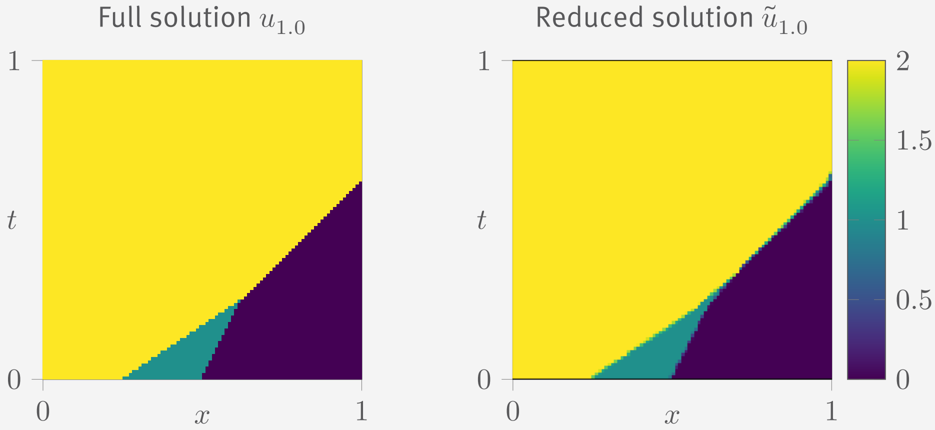


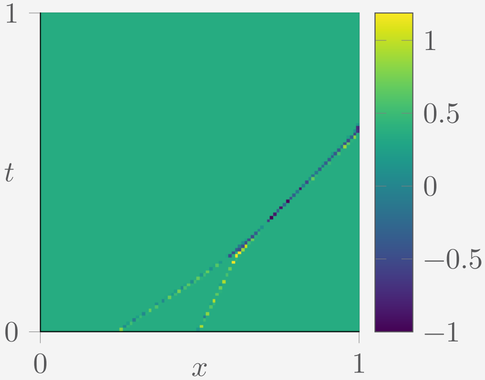


Numerical results – Reduced basis of size $N = 10$

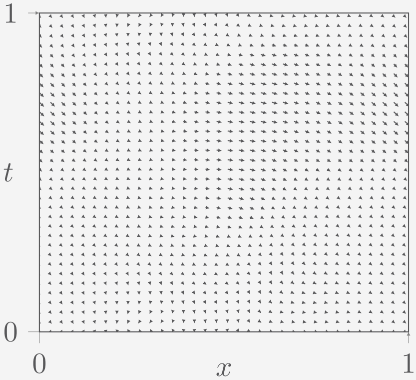


Numerical results – Reduced basis of size $N = 10$

Difference $\tilde{u}_{1.0} - u_{1.0}$



Initial vector field for $\mu = 1.0$



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Outlook and further research perspectives

- Theoretical investigation of reduced subspace of the Lie algebra.
- 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!

References I

- Constantin Greif and Karsten Urban, *Decay of the kolmogorov n-width for wave problems*, Applied Mathematics Letters **96** (2019), 216–222.
- J.S. Hesthaven and S. Ubbiali, *Non-intrusive reduced order modeling of nonlinear problems using neural networks*, Journal of Computational Physics **363** (2018), 55–78.
- Michael Miller, Alain Trouvé, and Laurent Younes, *Geodesic shooting for computational anatomy*, Journal of mathematical imaging and vision **24** (2006), 209–228.
- Mario Ohlberger and Stephan Rave, *Nonlinear reduced basis approximation of parameterized evolution equations via the method of freezing*, Comptes Rendus Mathematique **351** (2013), no. 23, 901 – 906.

References II

- ________, *Reduced basis methods: Success, limitations and future challenges*, Proceedings of the Conference Algoritmy (2016), 1–12.
- Jian Wang, Wei Xing, Robert M. Kirby, and Miaomiao Zhang, *Data-driven model order reduction for diffeomorphic image registration*, Information Processing in Medical Imaging (Cham) (Albert C. S. Chung, James C. Gee, Paul A. Yushkevich, and Siqi Bao, eds.), Springer International Publishing, 2019, pp. 694–705.