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Nonlinear Model Order Reduction using Diffeomorphic Transformations of a Space-Time Domain

MATHMOD 2022 – Minisymposium on “Recent Advances in Model Reduction and Surrogate Modeling”

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Parametrized hyperbolic conservation laws

We consider equations of the form

$$\partial_t u_\mu + \nabla_x \cdot f(u_\mu; \mu) = 0.$$

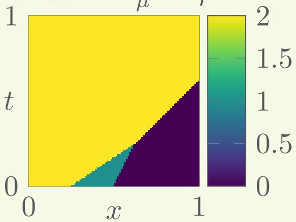
Example – Burgers equation

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

$$u_\mu(0) = u_0, \qquad x \in \Omega,$$

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

Full solution u_μ for $\mu = 1$

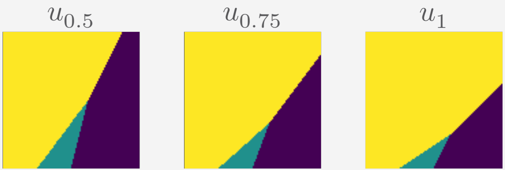


Need for nonlinear methods

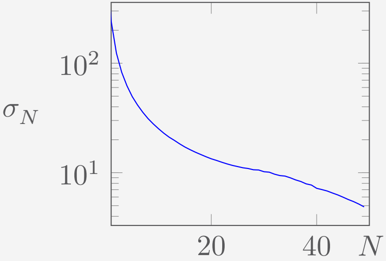
Main issues:

- Slowly decaying Kolmogorov N-width (e.g. $N^{-1/2}$ for linear transport [Ohlberger/Rave'16] or the linear wave equation [Greif/Urban'19])
- Complex shock topologies
- Interaction of shocks

$\longrightarrow$ Nonlinear transformations of space-time domains!



Singular values of space-time snapshots



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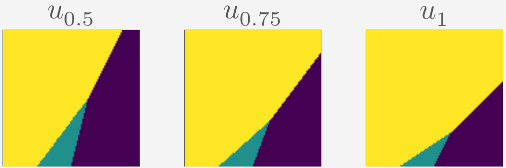

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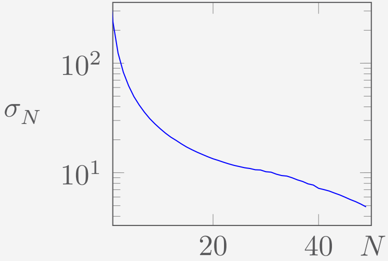

Transformations of space-time domains to align shocks and discontinuities

- 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 image registration.

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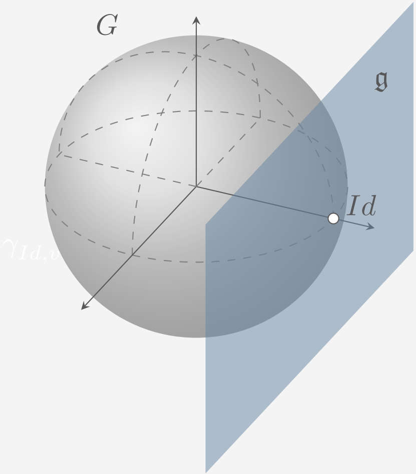
Lie groups and Lie algebras

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 $Id \in G$.



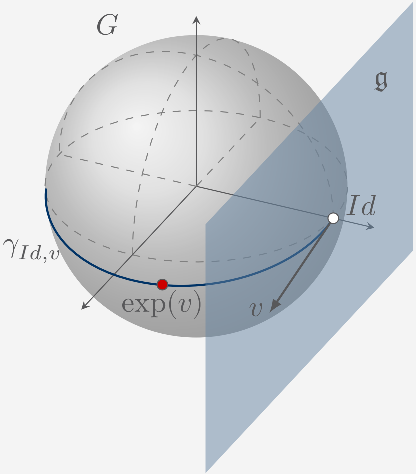
Lie groups and Lie algebras

Geodesic curve

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

Exponential map

Maps the Lie algebra into the Lie group, i.e. $\exp\colon \mathfrak{g} \to G$, by $\exp(v) = \gamma_{Id,v}(1)$.



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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Diffeomorphisms and vector fields

- Diffeomorphism $\phi_t \colon \Omega \to \Omega$, $\Omega \subset \mathbb{R}^d$, given as flow of (time-dependent) velocity field $v_t \colon \Omega \to \mathbb{R}^d$, i.e.

$$\frac{\partial \phi_t}{\partial t} = v_t \circ \phi_t.$$

- Differential operator $L = (Id - \alpha\Delta)^s$, with inverse $K = L^{-1}$.
- Geodesic evolution of v_t is given by EPDiff equation

$$\frac{\partial v_t}{\partial t} = -K\left[(Dv_t)^T \cdot Lv_t + D(Lv_t) \cdot v_t + Lv_t \cdot \operatorname{div} v_t\right].$$

- Knowledge of v_0 sufficient to compute ϕ_1!
  $\longrightarrow$ Main idea of *geodesic shooting* [Miller/Trouvé/Younes'06].

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Ideas and concepts from image registration

How to compute v_0 given a "template image" $u_0\colon \Omega \to \mathbb{R}$ and a "target image" $u_1\colon \Omega \to \mathbb{R}$?

Minimize energy

$$E_{u_0\to u_1}(v_0) := \underbrace{(Lv_0, v_0)_{L^2(\Omega)}}_{\text{Regularization term}} + \frac{1}{\sigma^2}\underbrace{\|u_0 \circ \phi_1^{-1} - u_1\|_{L^2(\Omega)}^2}_{\text{Mismatch measurement}}$$

using descent methods (e.g. L-BFGS).

(Linear) Model order reduction in the Lie algebra

- Lie algebra of smooth vector fields $\mathfrak{g}$ forms 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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Offline procedure

Choose reference parameter $\mu_{\text{ref}} \in \mathcal{P}$

Compute (space-time) reference snapshot $u_{\mu_{\text{ref}}}$

Sample parameters $\mu_1, \dots, \mu_n \in \mathcal{P}$

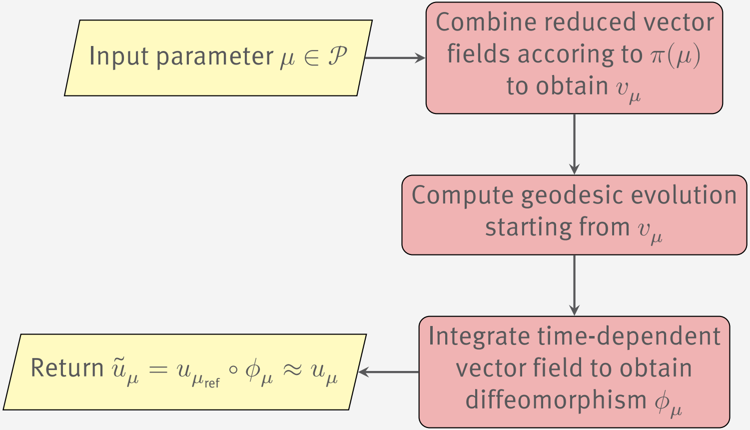
Compute (space-time) solution snapshots $u_{\mu_1}, \dots, u_{\mu_n}$

Register snapshots to obtain v_{μ_i} by minimizing $E_{u_{\mu_{\text{ref}}} \to u_{\mu_i}}$

Compute reduced space of vector fields using POD

Learn reduced coefficients of (projected) vector fields, i.e. the mapping $\pi\colon \mathcal{P} \to \mathbb{R}^N$ (similar to [Hesthaven/Ubbiali'18])

Online procedure



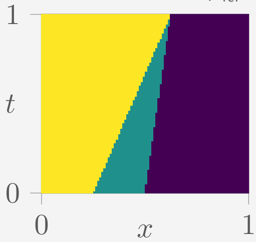
Numerical results – Burgers' equation with two shocks

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

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

Parameter domain	$\mathcal{P} = [0.25, 1.5]$
Discretization	$N_x = N_t = 100$
Training parameters	$n = 50$
Reference parameter	$\mu_{\text{ref}} = 0.25$
Reduced dimension	$N = 10$

Reference solution $u_{\mu_{\text{ref}}} = u_{0.25}$



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

Numerical results – Burgers' equation with two shocks

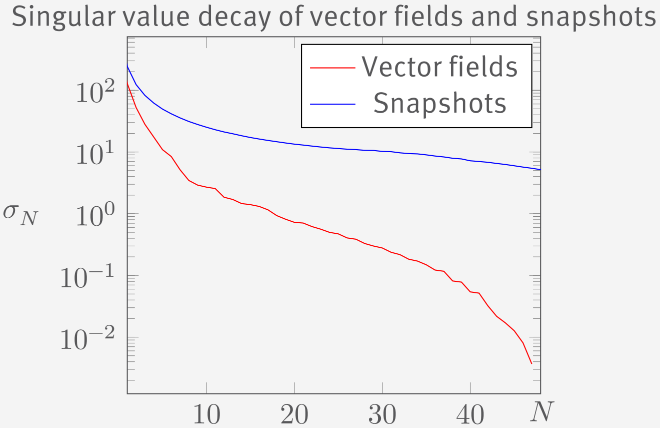
Offline phase

Average relative L^2-error on the n training snapshots: 5.1%.

Online phase

Average relative L^2-error for parameter $\mu \in \{0.5, 0.75, 1, 1.25\}$: 5.5%.

Numerical results – Burgers' equation with two shocks



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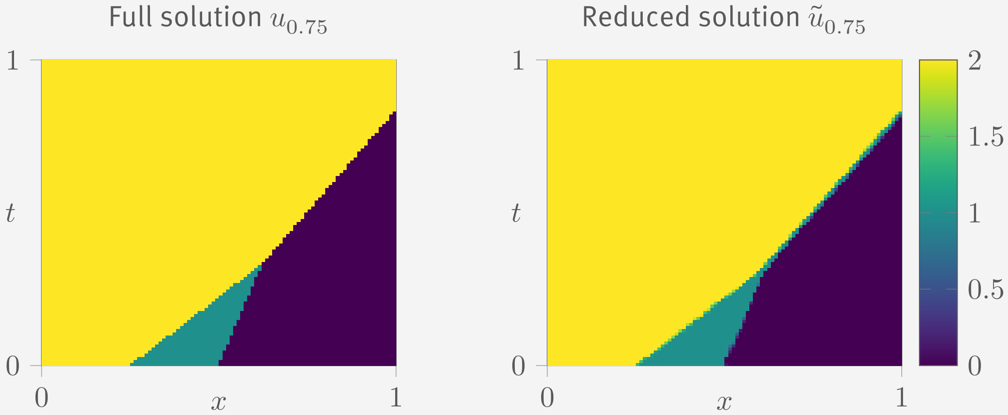
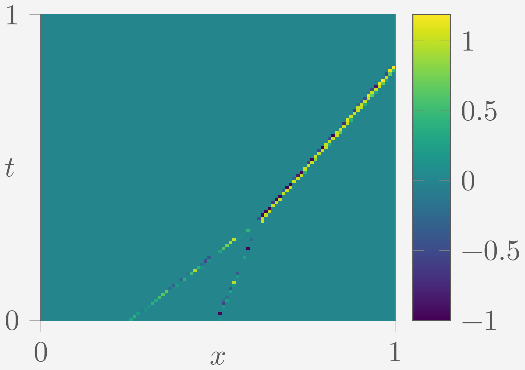
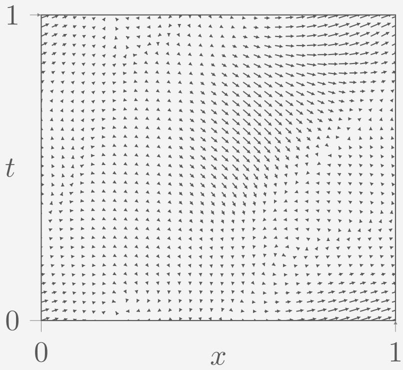


Numerical results – Burgers' equation with two shocks

Difference $\tilde{u}_{0.75} - u_{0.75}$



Initial vector field for $\mu = 0.75$



Thank you for your attention!

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