# Operator Based Multi-Scale Analysis of Simulation Bundles

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VAVID

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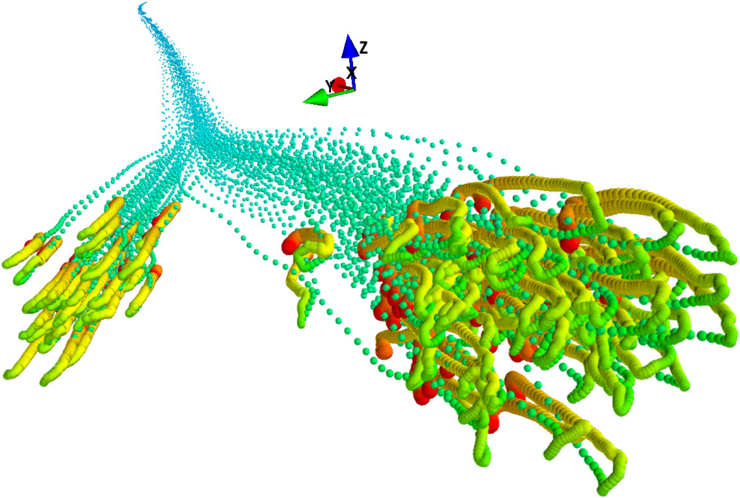
# Visualization of Many Simulations over Time

290 simulations $\times$141 time steps



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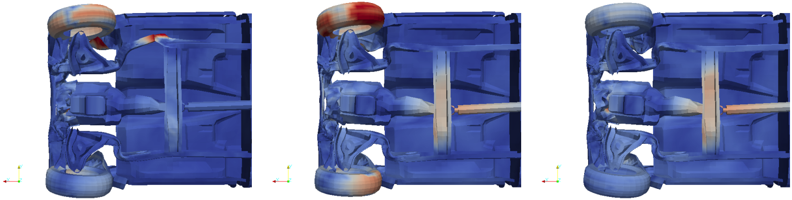
# Numerical Simulation as a Data Source

- numerical simulation used in many industries and sciences
  - automotive engineering – crash simulation applications
  - wind turbine design - behaviour under lots of different winds
  - wind farm design – computational fluid dynamics simulation
  - automotive engineering – Aeroacoustic CFD simulations
  - numerical weather forecasts / climate simulations
  - oil- and gas reservoir simulation
  - ...
- typical goal in engineering: analyse influence of parameters
- each parameter gives a full simulation run as a data point
  - one million grid points (or more)
  - a couple of hundred saved time steps
  - very high dimensional data
- per R&D-step a couple of hundred simulation runs
- data needs to be investigated and analyzed interactively

# Virtual Product Development in Automotive

- for car crash many disciplines, load cases, and requirements
- mostly limited to scalar outputs (e.g. HIC, firewall intrusion)
- no tools for geometric input variations or deformations
- analyzing full 3D simulation is very time consuming



- our aim: automatic organisation of (full) simulation results
- represent $d$-dimensional data in $s$-dimensional space, $d \gg s$
- goal: find intrinsic dimension $s$ of simulation vectors

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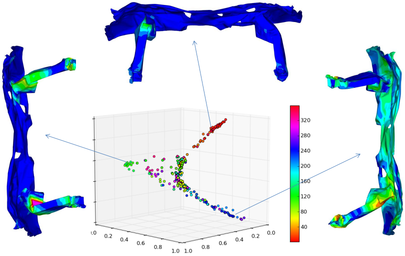
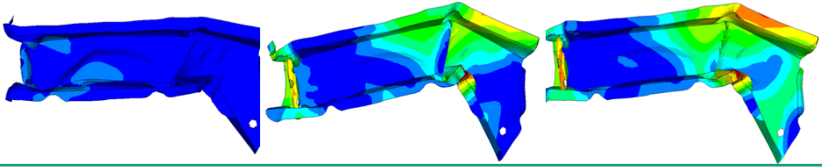
# Dimensionality Reduction / Simulation Space

- simulations are high dimensional objects Manifold Learning




- simulations are transformed from reference Orbit Space



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# Mathematical Motivation: Orbit Space

- assume simulations are obtained by transformation from reference simulation $f_0$
  - $f = \gamma \cdot f_0, \quad \gamma \in G$ with $f, f_0 \in \mathcal{M}$

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- parametrize simulations according to such transformations
  - $\mathcal{M}$ space of all simulations objects
  - $\mathcal{M}/G$ space of simulations modulo a transformation group
  - $G \cdot f := \{(\gamma, f)\ \gamma \in G\}$ is the orbit

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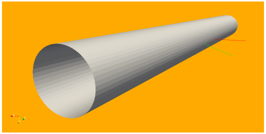

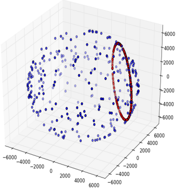


- exploit $G$ to understand the space of simulations objects $\mathcal{M}$
- study objects invariant under group of transformations $G$

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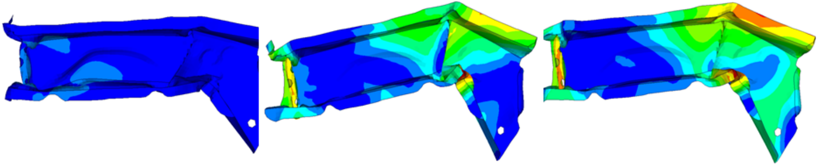
# Symmetry

## Structure Preservation in Transformation of Objects

- isometric invariant $\rightarrow$ distance preserving



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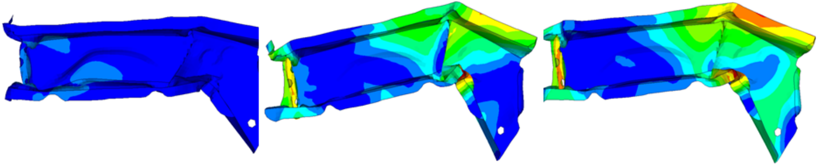
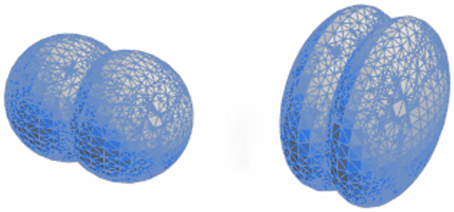


- affine invariant → collinearity preserving



- conformal invariant → angle preserving

# Invariance: Simple ODE Example

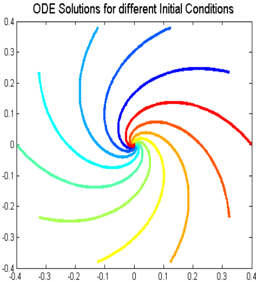
- simulations as solutions of the ODE system in some interval for different initial conditions

$$\begin{aligned} \dot{y} &= y^3 + x^2 y - x - y \\ \dot{x} &= x^3 + xy^2 - x + y \end{aligned}$$

- substitute $x = r \cdot cos(\theta)$, $y = r \cdot sin(\theta)$ to get the invariant,

$$\frac{dr}{d\theta} = r(1 - r^2)$$

- invariant for transformation $(r, \theta) \to (r, \theta + \gamma)$ i.e. a rotation with group parameter $\gamma$
- based on Lie group methods for solving ODE
- for simulations: no closed form available

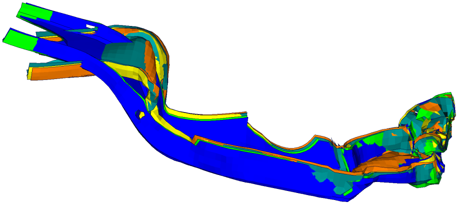


# Invariance for Simulation Bundles

- although no closed form available, principle can be used

  invariance
- variability is in many cases distance preserving

  look for distance preserving operator

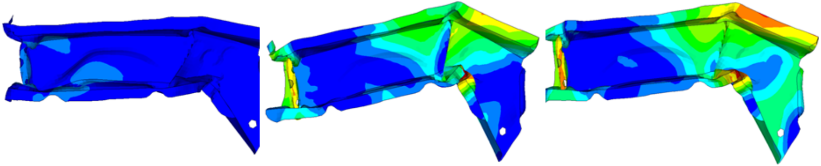


- different simulations have different surface deformations
- Laplace-Beltrami operator is distance preserving on a mesh
- ‘NICA operator’ for nonlinear transformation of point cloud

# Invariant Operators: Isometric Invariance

**Proposition (*Iza-Teran, G., 2016*)**

*The discrete approximation $L_K^h$ of the Laplace-Beltrami operator, constructed using graph distances from one mesh $K^{i=\kappa}$, is (approximately) the same for all meshes $i = 1, \ldots, m$ in the set of meshes undergoing isometric transformations.*



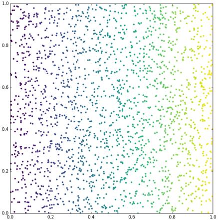
# Spectral Decomposition of an Operator

- on a manifold $(\mathcal{S}, g)$ define eigenvalue problem $-\Delta_{\mathcal{S}}\phi = \lambda\phi$
- the operator is positive semidefinite, all eigenvalues $\lambda_k$, $k \geq 0$ are real positive and isolated with finite multiplicity
- use corresponding discrete operator and its discrete eigenfunctions $\{\phi_i\}_i^N$
- spectral decomposition for function $f$ on mesh gives

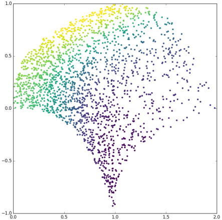
$$f = \sum_{i=1}^{N} \alpha^i \phi_i,\ \alpha^i = < f, \phi_i >$$

- distance of coefficients $\alpha_1^i, \alpha_2^i$ gives good distance measure for the corresponding simulations $f^1, f^2$

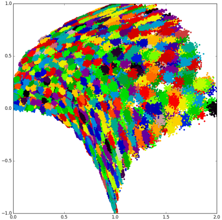
# NICA weighted Graph Laplacian on Point Cloud



non-observable data



observed data



simulation burst

- estimate local covariance matrices per mesh point, this allows approximation of distances in non-observable space
- use these distances (from observed data) as weights in graph, resulting in NICA-weighted graph Laplacian
- constructed NICA-weighted graph Laplacian is invariant to the nonlinear transformation (Singer & Coifman, 2008)

# Operator Basis

## Approximation Properties

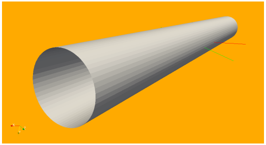
**Proposition** (*Iza-Teran, G., 2016*)

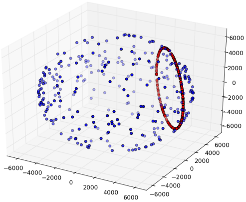
*Using the eigenvectors $\phi$ of the NICA operator as an orthogonal basis, thresholding the orthogonal expansion given by $f = \sum_{i=0}^{\infty} \alpha^i \phi_i$, $\alpha^i =< f, \phi_i >$ using only $N_t-$ terms, the first few coefficients decay very fast, depending on the degree of smoothness of the function $f$.*

- proof uses connection of operator to Sturm-Liouville problem
- approximation properties depend (unsurprisingly) on smoothness of $f$

# Summary: Orbit Space / Simulation Space

- assumption: transformation group $G$ sends simul. to simul.
- project simulation bundle into basis obtained from operator
- $G$ is reflected in the spectral coefficients
- estimate dimensionality based on decay of the coefficients
- exploit $G$ to understand the space of simulations objects $M$
- use projection coefficients of orbits to characterize $M/G$
- or: orbit can be approximated by projection coefficients



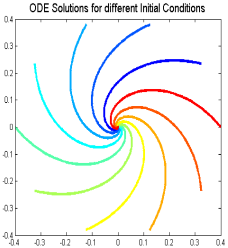


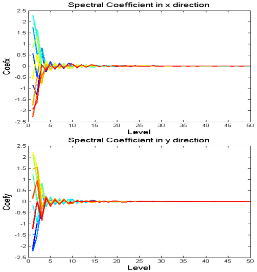
# Analysis of ODE Example with Invariant Operator

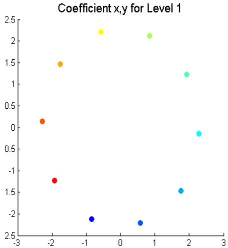
- simulations as solutions of the ODE system in some interval for different initial conditions

$$\begin{aligned}\dot{y} &= y^3 + x^2 y - x - y \\ \dot{x} &= x^3 + x y^2 - x + y\end{aligned}$$

- take a solution and calculate a rotation invariant operator

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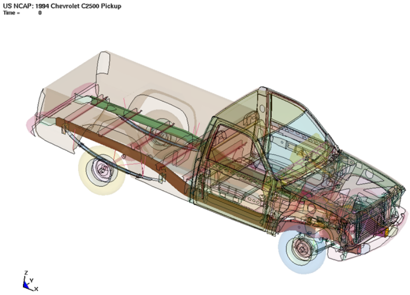
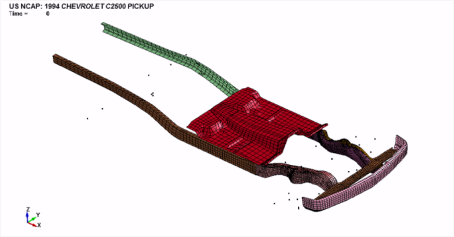
# Analysis of Numerical Simulations of a Car Crash

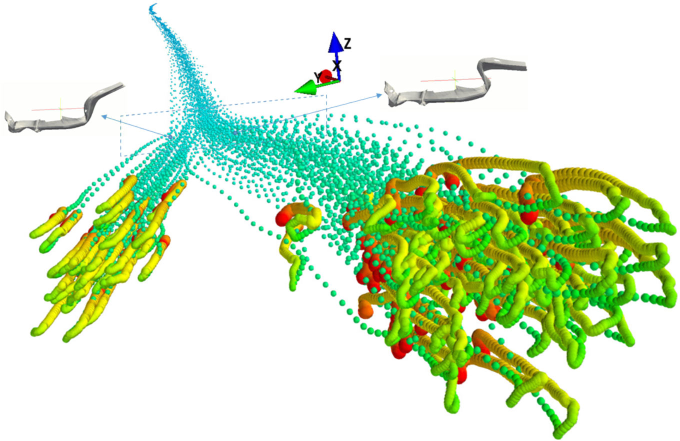



- simulations results are 3D deformations
- thickness values of 9 parts of the car structure are varied randomly up to 30% to obtain 116 numerical simulations
- chose relevant structural part and time step for analysis

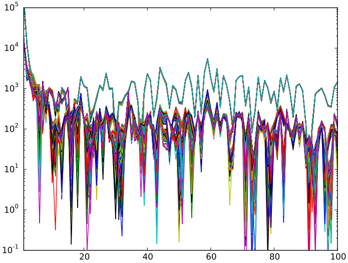
# Visualization of All Time Steps in LB-decomposition



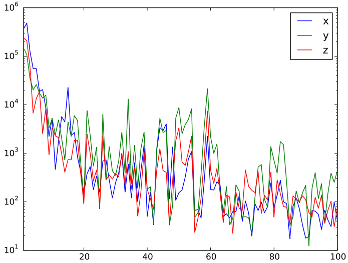

- for each mesh point resulting $x$, $y$, and $z$ coordinates of simulation $i$ gives function values for $\phi_x^i$, $\phi_y^i$, and $\phi_z^i$

# NICA-weighted Graph Laplacian

- for each mesh point resulting $x$, $y$, and $z$ coordinates of simulation $i$ gives function values for $\phi_x^i$, $\phi_y^i$, and $\phi_z^i$
- spectral decomposition computed for a selected time step
- consider first 100 spectral coefficients




(a) magnitude of coefficients




(b) variance of coefficients

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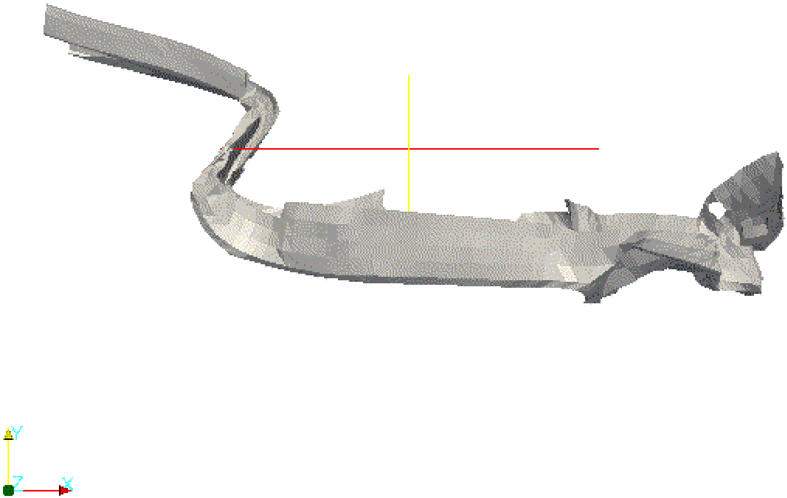
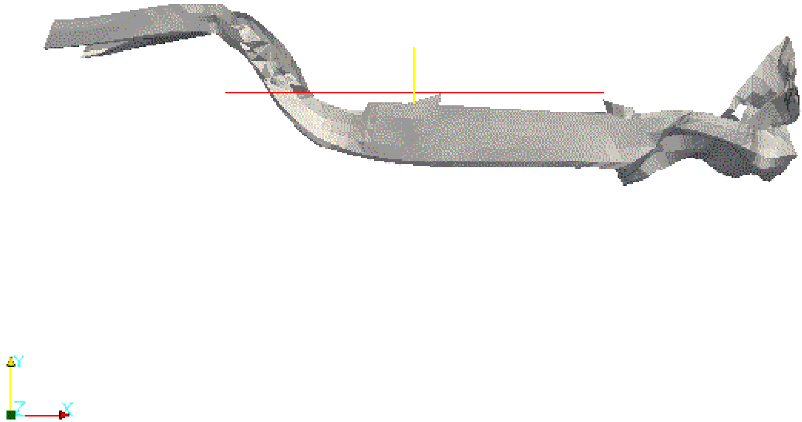
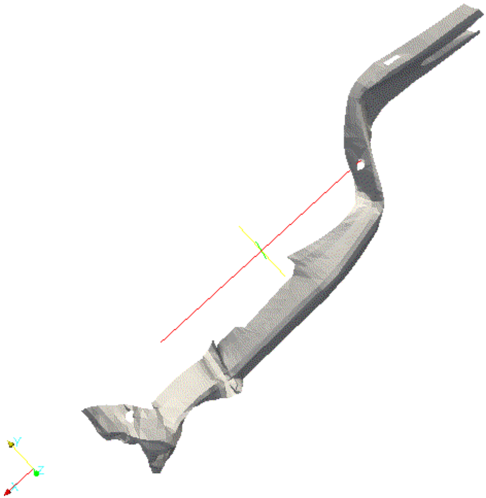
# Mode 1 - Translation



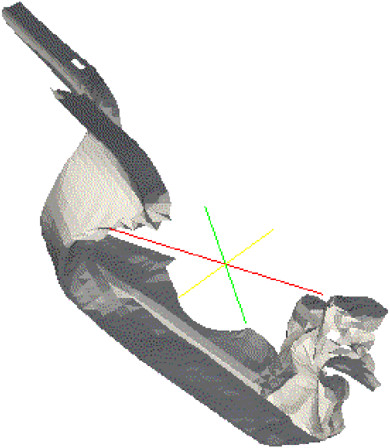
# Mode 2 - Rotation



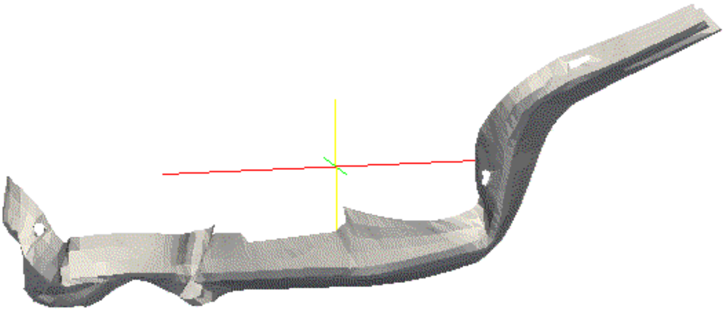
# Mode 3 - Global Deformation



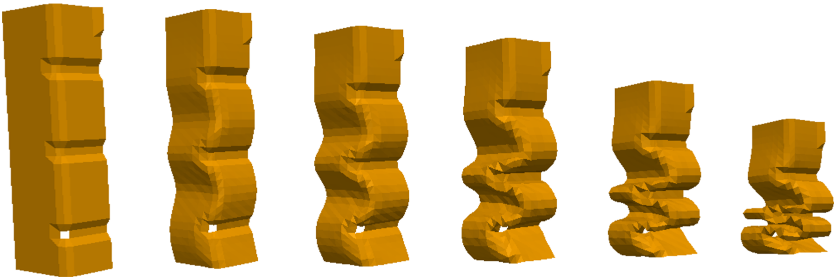
# Mode 4 - Local Deformation



# Combined Modes

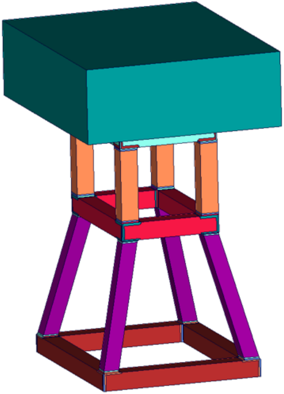


# Geodesic Paths and Orbits

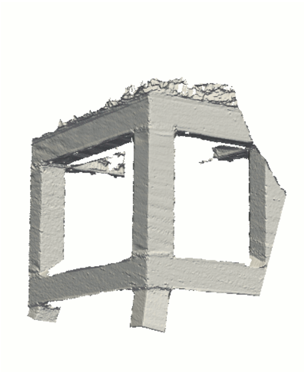


# High Speed 3D-Point Cloud Measurements

results from joint project with Fraunhofer IOF and EMI



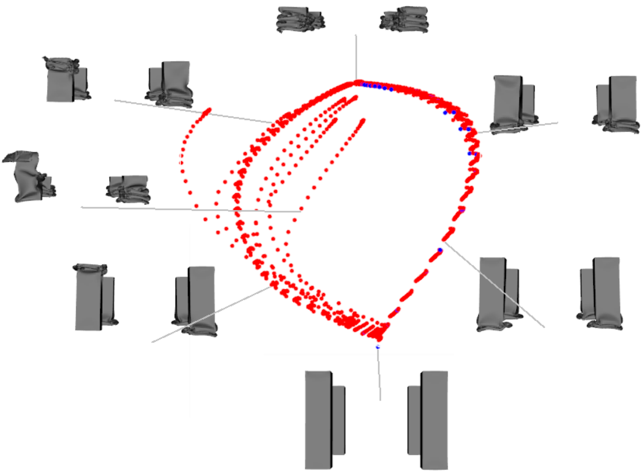
"Hand"-Build Test Structure



3D-Video of Crash

# Matching of 3D-Point Data and Simulation

# Path of Experiment Data in Simulation Space



# Conclusion

- integration of domain knowledge and assumptions into overall data analysis for complex engineering data essential
- introduced orbit space ansatz for analysis of simulation
- allows “virtual” simulations by interpolation in lower dimensional representation of simulation space
- have start of theory and are further extending theory
- approach can be applied to other numerical data, e.g. time series from wind energy plants
- preliminary results using an invariant basis in RBM-context

**5th Workshop on Sparse Grids and its Applications**

save the date: 23 – 27 July 2018 @TU München
prelimary webpage: https://www5.in.tum.de/SGA2018/

# The Laplace-Beltrami Operator on a Mesh

Let $\mathcal{S}$ be a manifold surface isometrically embedded in $R^3$, $\Delta_{\mathcal{S}}$ be the Laplace-Beltrami operator on $\mathcal{S}$, and $K$ be an $(\epsilon, \eta)$ approx. of $\mathcal{S}$. For any vertex $w$, the mesh Laplace operator is

$$L_K^h f(w) = \frac{1}{4\pi h^2} \sum_{t \in K} \frac{Area(t)}{\#t} \sum_{p \in V(t)} e^{-\frac{d(p,w)^2}{4h}} (f(p) - f(w)),$$

where $d(p, w)$ denotes the graph distance.

**Theorem (Laplace-Beltrami Approx. (Belkin et.al.2008))**

*Put $h(\epsilon, \eta) = \epsilon^{\frac{1}{2.5+\alpha}} + \eta^{\frac{1}{1+\alpha}}$ for an $\alpha > 0$. Then for any function $f \in C^3(\mathcal{S})$ it holds*

$$\lim_{\epsilon,\eta \to 0} \sup_K \left|\left| L_K^{h(\epsilon,\eta)} f - \Delta_{\mathcal{S}} f|_K \right|\right|_\infty = 0,$$

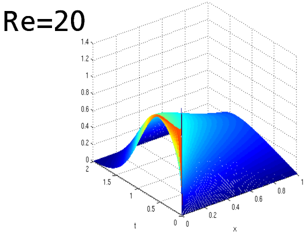
*where $\sup_K$ is taken over all $(\epsilon, \eta)$-approximations $K$ of $\mathcal{S}$.*

# Reduced Basis Method with Invariant Basis

- preliminary tests with Burgers' equation

$$\frac{\partial}{\partial t}u(t,x) + u(x,t)\frac{\partial}{\partial x}u(t,x) - q\frac{\partial^2}{\partial x^2}u(x,t) = 0$$

- generate a snapshot for POD with $Re := 1/q = 20$




- compute invariant basis from operator invariant to changes which preserve path length along the curve (for $t = 0$)
- replace the POD basis by an invariant basis

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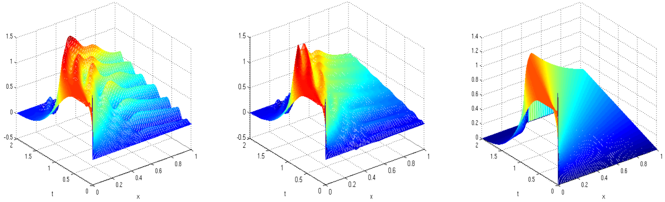
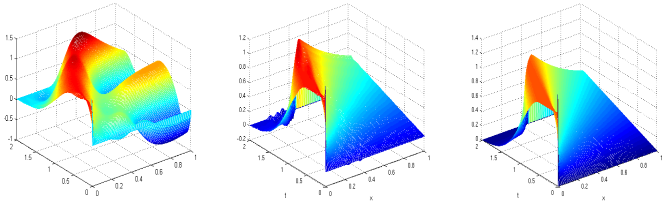
# POD vs. Invariant Basis

- solve problem for $Re = 400$ with both basis from $Re = 20$



(a) POD (b) Inv. Basis (c) solution

- project solution for $Re = 400$ into both basis from $Re = 20$



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# Potential of Invariant Approach for RBMs