A reduced basis method for evolution equations on parametrized geometries

Martin Drohmann, Bernard Haasdonk, Mario Ohlberger

Institut für Numerische und Angewandte Mathematik
Universität Münster
http://wwwmath.uni-muenster.de/num

March 3, 2012

Westfälische Wilhelms-Universität Münster

Outline

1. Reduced basis method for evolution problems
2. Classification of evolution problems
3. Methodology: parametrised DEIM
4. Reduced basis scheme with linear implicit operator
5. Reduced basis scheme with non-linear implicit operator
6. Numerical results and validation
7. Summary & Outlook

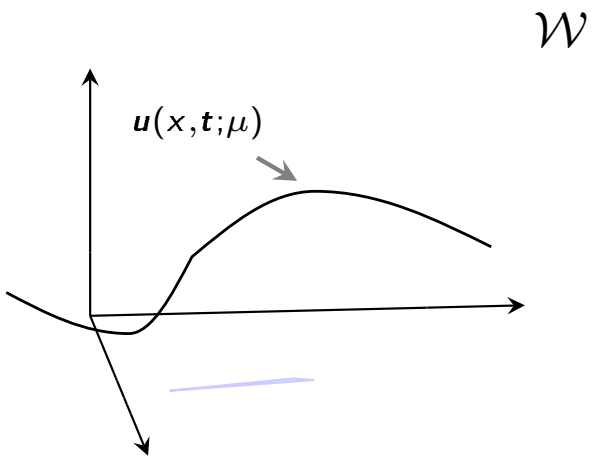
Parametrised evolution equation

$\mathcal{L}$			
$\mathcal{W}$			
$u(x,t;\mu)$			

Solve

$$u(x,0;\mu) := u_0(x;\mu)$$
$$\partial_t u(x,t;\mu) - \mathcal{L}[u(x,t;\mu)] := 0$$

plus boundary conditions. Solutions $u(\cdot,t;\mu)$ live in a (Sobolev) space $\mathcal{W}$ for each $t \in [0, T_{\max}]$.



Discrete simulations (FV, FE, DG, ...)

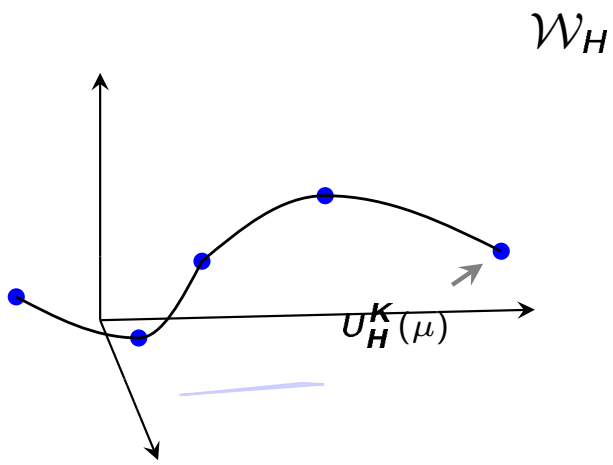
$\mathcal{L}$	L_I, L_E, P		
$\mathcal{W}$	$\mathcal{W}_H$		
$u(x,t;\mu)$	$\{U_H^k(\mu)\}_{k=1}^K$		

Solve

$$U_H^0(\mu) := P[u_0(x;\mu)]$$

$$L_I(\mu, \Delta t^k)[U_H^{k+1}] - L_E(\mu, \Delta t^k)[U_H^k] := 0,$$

with $\Delta t = \frac{T_{\max}}{K}$. Solutions build trajectories in high dimensional discrete function space $\mathcal{W}_H$.



Discrete simulations (FV, FE, DG, ...)

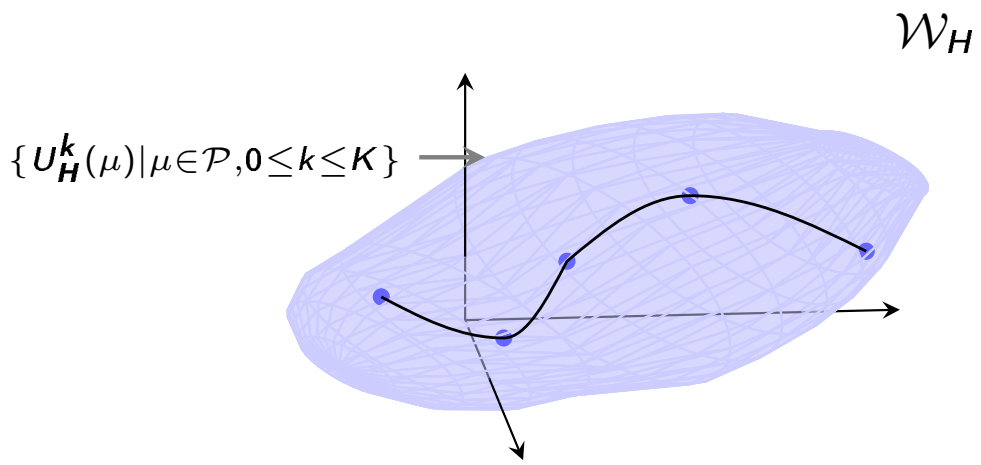
$\mathcal{L}$	L_I, L_E, P		
$\mathcal{W}$	$\mathcal{W}_H$		
$u(x,t;\mu)$	$\{U_H^k(\mu)\}_{k=1}^K$		

Solve

$$U_H^0(\mu) := P[u_0(x;\mu)]$$

$$L_I(\mu, \Delta t^k)[U_H^{k+1}] - L_E(\mu, \Delta t^k)[U_H^k] := 0,$$

with $\Delta t = \frac{T_{\max}}{K}$. Solutions build trajectories in high dimensional discrete function space $\mathcal{W}_H$.



Discrete simulations (FV, FE, DG, ...)

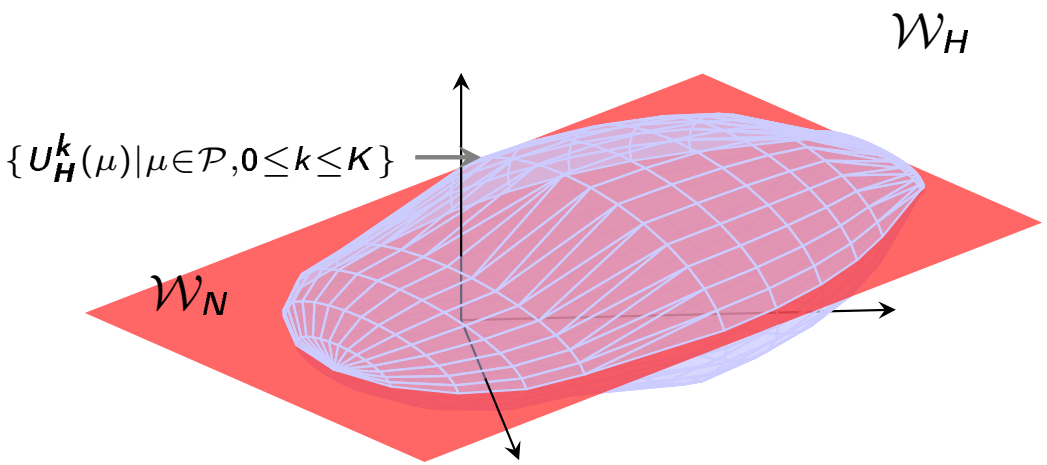
$\mathcal{L}$	L_I, L_E, P		
$\mathcal{W}$	$\mathcal{W}_H$		
$u(x,t;\mu)$	$\{U_H^k(\mu)\}_{k=1}^K$		

Solve

$$U_H^0(\mu) := P[u_0(x;\mu)]$$

$$L_I(\mu, \Delta t^k)[U_H^{k+1}] - L_E(\mu, \Delta t^k)[U_H^k] := 0,$$

with $\Delta t = \frac{T_{\max}}{K}$. Solutions build trajectories in high dimensional discrete function space $\mathcal{W}_H$.



Reduced simulations (Projection on RB space)

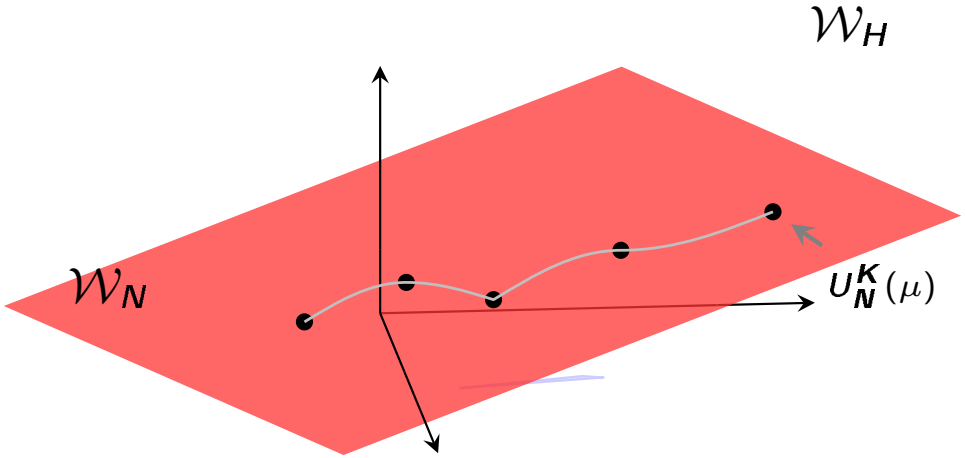
$\mathcal{L}$	L_I, L_E, P	$\mathbf{L}_I, \mathbf{L}_E, \mathbf{P}$	
$\mathcal{W}$	$\mathcal{W}_H$	$\mathcal{W}_N := \text{span}\,\{\varphi_n\}_{n=1}^N$	
$u(x,t;\mu)$	$\{U_H^k(\mu)\}_{k=1}^K$	$\{\mathbf{a}^k(\mu)\}_{k=1}^K$	

Solve

$$\mathbf{a}^0(\mu) := \mathbf{P}[u_0(\mu)]$$

$$\mathbf{L}_I(\mu, \Delta t^k)[\mathbf{a}^{k+1}] - \mathbf{L}_E(\mu, \Delta t^k)[\mathbf{a}^k] := 0.$$

Solutions build trajectories in low dimensional discrete function space $\mathcal{W}_N$.



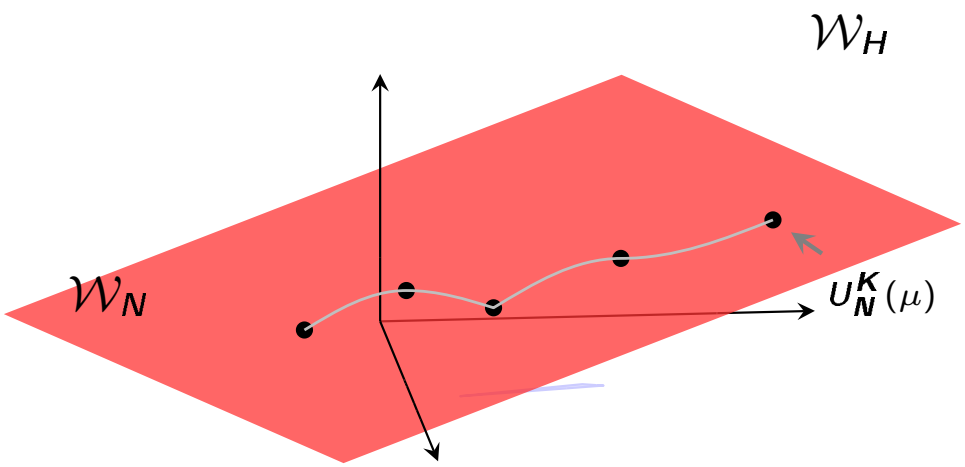
Reduced simulations (Projection on RB space)

$\mathcal{L}$	L_I, L_E, P	$\mathbf{L}_I, \mathbf{L}_E, \mathbf{P}$	
$\mathcal{W}$	$\mathcal{W}_H$	$\mathcal{W}_N := \text{span}\,\{\varphi_n\}_{n=1}^N$	$\mathcal{W}_H, \mathcal{W}_O$
$u(x,t;\mu)$	$\{U_H^k(\mu)\}_{k=1}^K$	$\{\mathbf{a}^k(\mu)\}_{k=1}^K$	$U_N^k(\mu), s(\mu)$

Reconstruct the solution

$$U_N^k(\mu) := \sum_{n=1}^N a_n^k(\mu)\varphi_n \in \mathcal{W}_H$$

or: Evaluate an output functional $s(\mu)$.
The latter is preferable in the RB context because it is independent of any high dimensional computations.



Classification of evolution problems

Operator constraints

	L_I	L_E
1	linear in space, affinely μ-dependent	
2	$=$ Id	localized
3	coercive, non-coercive, linear, non-linear	$=$ Id
4	linear in space	localized **or:** linear in space, affinely μ-dependent
5	localized, nonlinear	

Revision: Affine parameter dependence(*)

An operator is called affinely decomposed if it can be written as a sum of products of parameter dependent and parameter independent parts.

Classification of evolution problems

Operator constraints

	L_I	L_E
1	linear in space, affinely μ-dependent	
2	$=$ Id	localized
3	coercive, non-coercive, linear, non-linear	$=$ Id
4	linear in space	localized **or:** linear in space, affinely μ-dependent
5	localized, nonlinear	

- Case 1 is discussed in [Haasdonk&Ohlberger, 2008].
- Case 2 is discussed in [Haasdonk et al., 2008] and [Drohmann et al.,2009]
- Case 3 is discussed in [Grepl, 2005], [Grepl et al., 2008] and [Knezevic et al., 2009]
- Our focus: nonlinear and non-affinely decomposed implicit operators.

Revision: Affine parameter dependence(*)

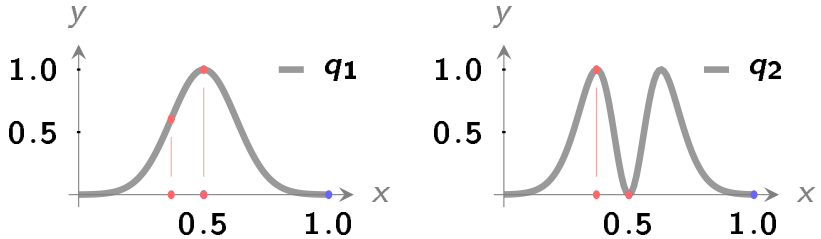
An operator is called affinely decomposed if it can be written as a sum of products of parameter dependent and parameter independent parts.

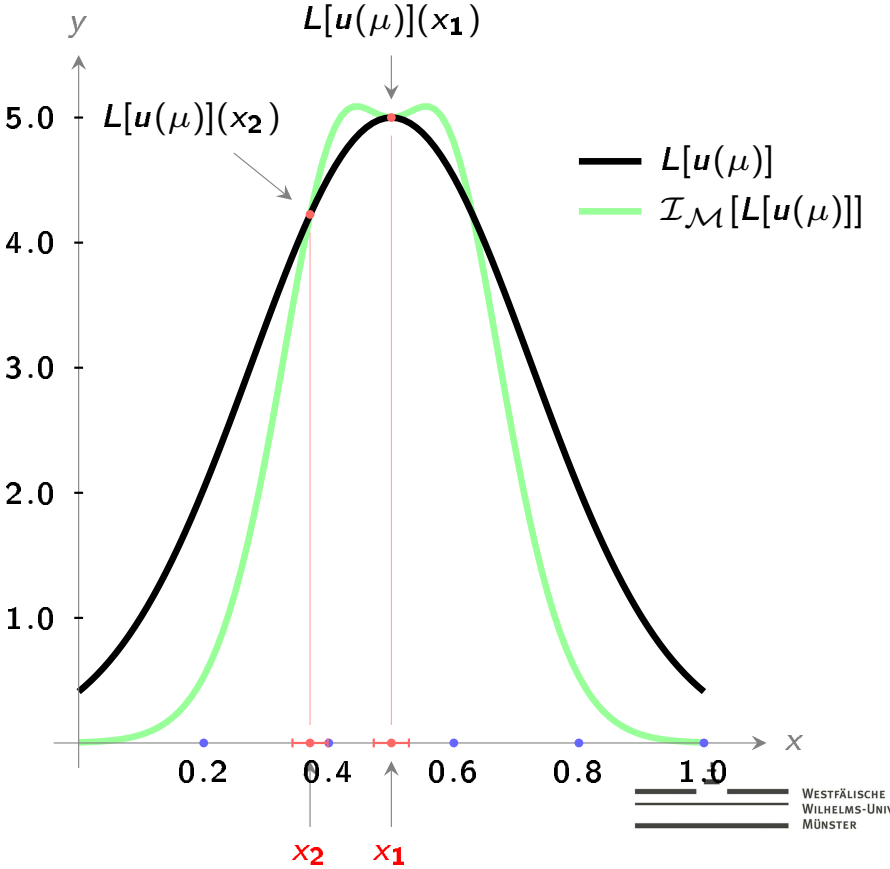
Non-affinely decomposed operators

Idea

Approximate an operator $L(\mu)[U^k(\mu)]$ with few point evaluations.

Base functions:





Non-affinely decomposed operators ⇒ parametrised DEIM

Idea

Approximate an operator $L(\mu)[U^k(\mu)]$ with few point evaluations.

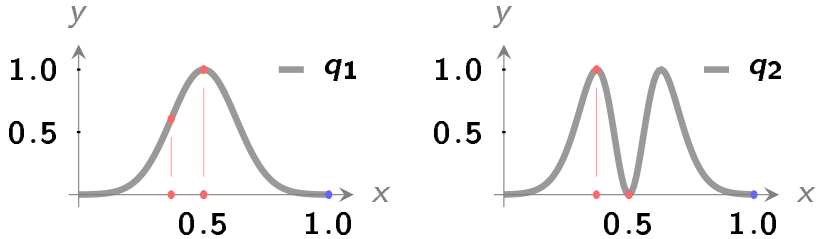
Empirical interpolation [Barrault et al, 2004]

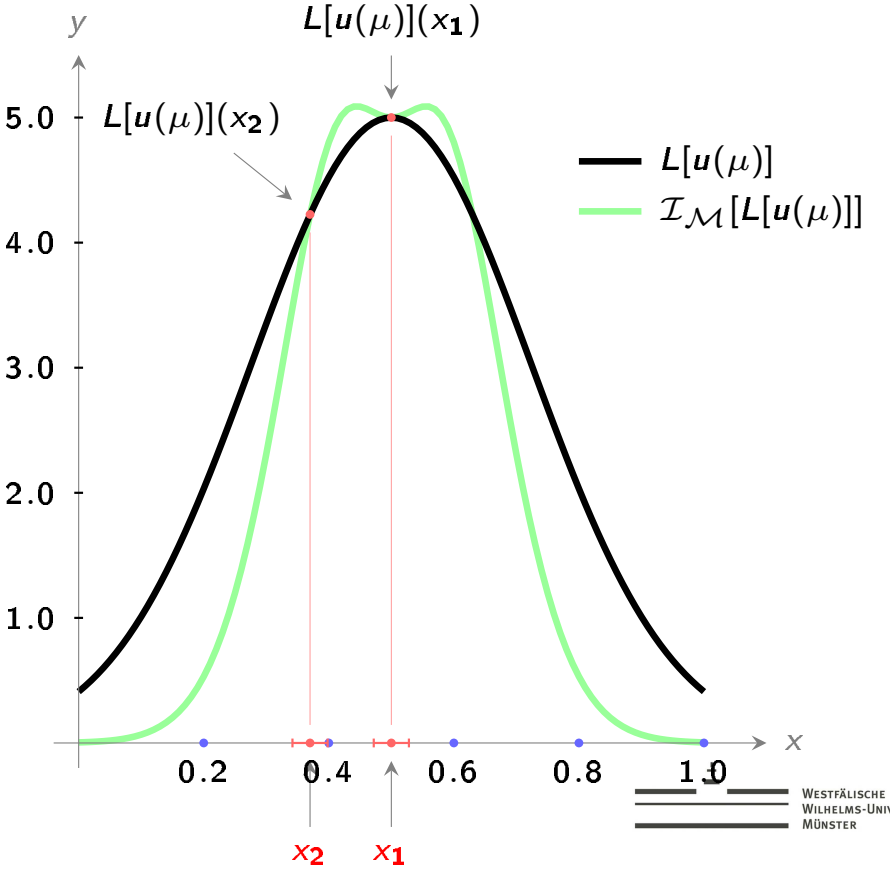
- Collateral reduced basis space of operator evaluations

$$\mathcal{W}_M := \text{span}\{L(\mu_i)[U_H^{k_i}(\mu_i)]\}_{i=1}^M$$

- Collateral reduced basis $\Xi_M := \{\xi_i\}_{i=1}^M$ of nodal base functions
- Interpolation points $x_1, \ldots, x_M$.

Base functions:





Non-affinely decomposed operators ⇒ parametrised DEIM

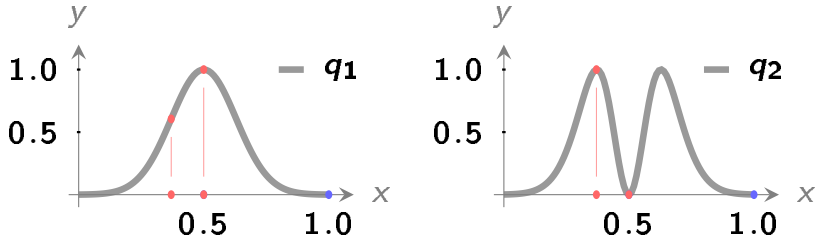
Operator evaluations

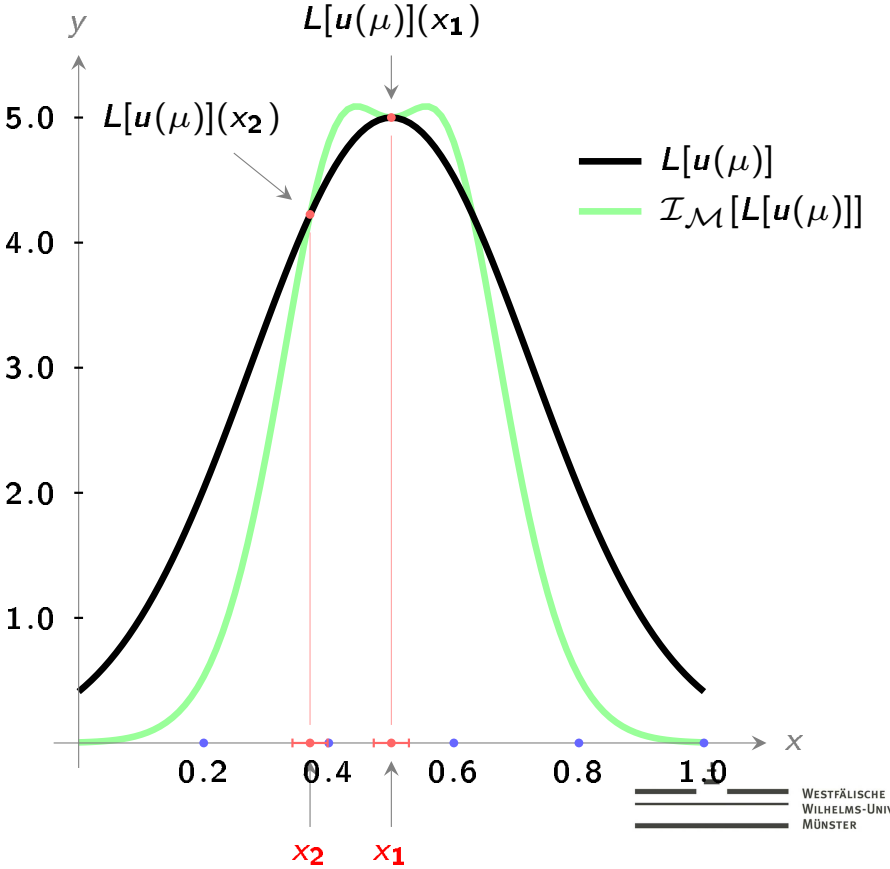
Interpolation is gained through exact operator evaluations at the interpolation points such that

$$\mathcal{I}_M[L(\mu)[U]](x) := \sum_{m=1}^{M} y_m(\mu)\xi_m(x)$$

$$y_m(\mu) := L(\mu)[U](x_m)$$

Base functions:





Non-affinely decomposed operators ⇒ parametrised DEIM

Operator evaluations

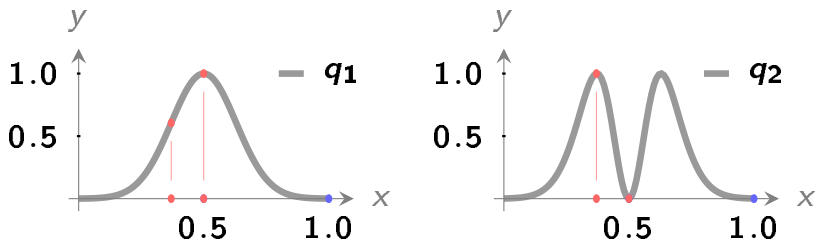
Interpolation is gained through exact operator evaluations at the interpolation points such that

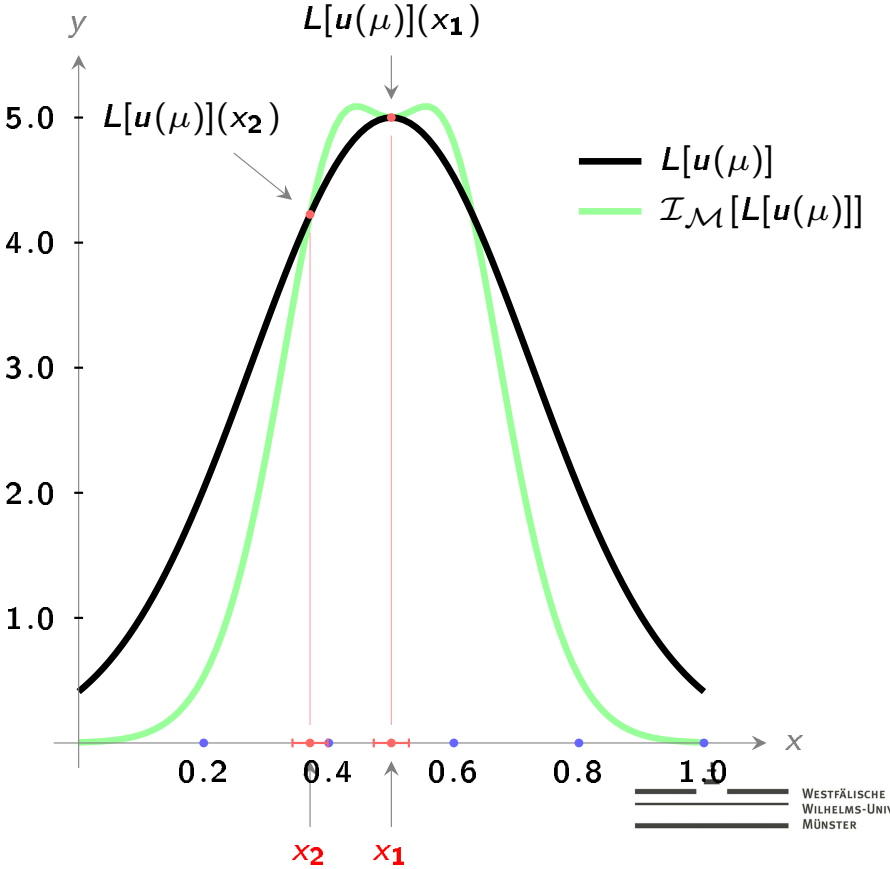
$$\mathcal{I}_M[L(\mu)[U]](x) := \sum_{m=1}^{M} y_m(\mu)\xi_m(x)$$

$$y_m(\mu) := L(\mu)[U](x_m)$$

- The coefficients can be computed efficiently, if the operator is localised.
- A local version of the grid and evaluations of the RB functions at interpolation points need to be precomputed in offline phase.

Base functions:





Linear implicit operator

Projection of empirical interpolated $L_I(\mu)$

Let $U = \sum_{n=1}^{N} a_n \varphi_n$ be a discrete function in the reduced basis space $\mathcal{W}_N := \text{span}\{\varphi_n\}_{n=1}^{N}$. Then

$$\int_\Omega L_I(\mu)[U]\varphi_n \approx$$

$$\int_\Omega \mathcal{I}_M \left[L_I(\mu) \left[\sum_{n=1}^{N} a_n \varphi_n \right] \right] (x)\varphi_{n'}(x) = \sum_{m=1}^{M} \sum_{n=1}^{N} a_n \; y_m(\varphi_n; \mu) \int_\Omega \xi_m(x)\varphi_{n'}(x)$$

with quickly computable online parts and precomputed offline parts.

Note: y_m is linear, because the operator $L_I(\mu)$ is linear in space.

$$\Downarrow$$

Linear implicit operator II

Reduced basis scheme

With degrees of freedom $\mathbf{a}^k := (a_1^k, \dots, a_N^k)$ for $k = 1, \dots, K$ and affinely decomposed operators P, $L_E(\mu)$ we get the scheme

$$\mathbf{a}^0 - \sum_{q=1}^{Q_P} \mathbf{P}^q \sigma_P^q(\mu) = 0, \qquad \mathbf{L}_I(\mu)\mathbf{a}^k + \sum_{q=1}^{Q_E} \mathbf{L}_E^q \mathbf{a}^{k-1} \sigma_E^q(\mu) = 0,$$

with

$$(\mathbf{L}_I(\mu))_{n',n} := \sum_{m=1}^{M} y_m(\varphi_n; \mu) \int_\Omega \xi_m \varphi_{n'} \tag{1}$$

Note: $P[u_0(\mu)]$ and $L_E(\mu)$ are linear and affinely decomposed in this scheme, but could be substituted easily by an empirical interpolation.

Non-linear implicit operator

Newton method

Define the defect

$$V^{k+1,\nu+1} := U^{k+1,\nu+1} - U^{k+1,\nu}$$

and solve

$$F_I(U^{k+1,\nu})[V^{k+1,\nu+1}] = -L_I[U^{k+1,\nu}] - L_E[U^k],$$

for each $k = 0, \ldots, K-1$ and each Newton step $\nu = 0, \ldots, S(k)$ with $U^{k+1} := U^{k+1,0} := U^{k,S(k)}$ and F_I being the Fréchet derivative of $L_I(\mu)$.

Non-linear implicit operator

Newton method

Define the defect

$$V^{k+1,\nu+1} := U^{k+1,\nu+1} - U^{k+1,\nu}$$

and solve

$$F_I(U^{k+1,\nu})[V^{k+1,\nu+1}] = -L_I[U^{k+1,\nu}] - L_E[U^k],$$

for each $k = 0, \ldots, K-1$ and each Newton step $\nu = 0, \ldots, S(k)$ with $U^{k+1} := U^{k+1,0} := U^{k,S(k)}$ and F_I being the Fréchet derivative of $L_I(\mu)$.

How to reduce F_I?

Non-linear implicit operator

Newton method

$$F_I(U^{k+1,\nu})[V^{k+1,\nu+1}] = -L_I[U^{k+1,\nu}] - L_E[U^k],$$

Empirical interpolation of F_I

- empirical interpolation of L_I

$$\mathcal{I}_M[L_I] = \sum_{m=1}^{M} y_m(U)\xi_m$$

- leads to an empirical interpolation of $F_I(U)[V]$

$$\mathcal{I}_M[F_I(U)[V]] = \sum_{i=1}^{H}\sum_{m=1}^{M} \partial_i y_m(U) v_i \xi_m = \sum_{i\in\tau}\sum_{m=1}^{M} \partial_i y_m(U) v_i \xi_m$$

- where $\tau \subset \{1,\dots,H\}$ is the smallest possible subset for which the above equation is fulfilled. Note, that $\mathrm{card}(\tau) \in \mathcal{O}(M)$, because L_I is localised.
- $\{v_i\}_{i\in\tau}$ can be evaluated efficiently in case of nodal basis of $\mathcal{W}_H$.

Non-linear implicit operator II

Reduced basis scheme

$$GA(U_N^{k+1,\nu})(\mathbf{a}^{k+1,\nu+1} - \mathbf{a}^{k+1,\nu}) = RHS(\mathbf{a}^{k+1,\nu}, \mathbf{a}^k),$$

with $A(U_N)$ and G defined by

$$(A(U_N))_{m,n} := \sum_{i=1}^{M} \partial_i y_m(U_N)\varphi_n(x_i) \qquad \text{and} \qquad (G)_{n,m} = \int_\Omega \xi_m \varphi_n.$$

The assembling of $A(U_N)$ costs $\mathcal{O}(MN \cdot MN)$ and multiplication with G has costs of $\mathcal{O}(NMN)$. In addition this is still independent of H.

Convection-diffusion equation with parametrized geometry

As a test case we choose a general (maybe nonlinear) convection-diffusion-reaction equation on parametrized geometries.

$$\partial_t u(x,t;\mu) - \nabla \cdot (K \nabla u(x,t;\mu)) - b \cdot \nabla u(x,t;\mu) - r u(x,t;\mu) = 0 \quad \text{in } \Omega(\mu) \times [0, T_{\max}].$$

Convection-diffusion equation with parametrized geometry

The reduced basis space must not depend on the parameter.

Therefore, we introduce a reference geometry $\hat{\Omega}$ and a diffeomorphic mapping $\Phi(\mu) : \hat{\Omega} \to \Omega(\mu)$ for every parameter.

As a test case we choose a general (maybe nonlinear) convection-diffusion-reaction equation on parametrized geometries.

$$\partial_t u(x,t;\mu) - \nabla \cdot (K \nabla u(x,t;\mu)) - b \cdot \nabla u(x,t;\mu) - r u(x,t;\mu) = 0 \quad \text{in } \Omega(\cancel{\mu}) \times [0, T_{\max}].$$

Geometry transformation

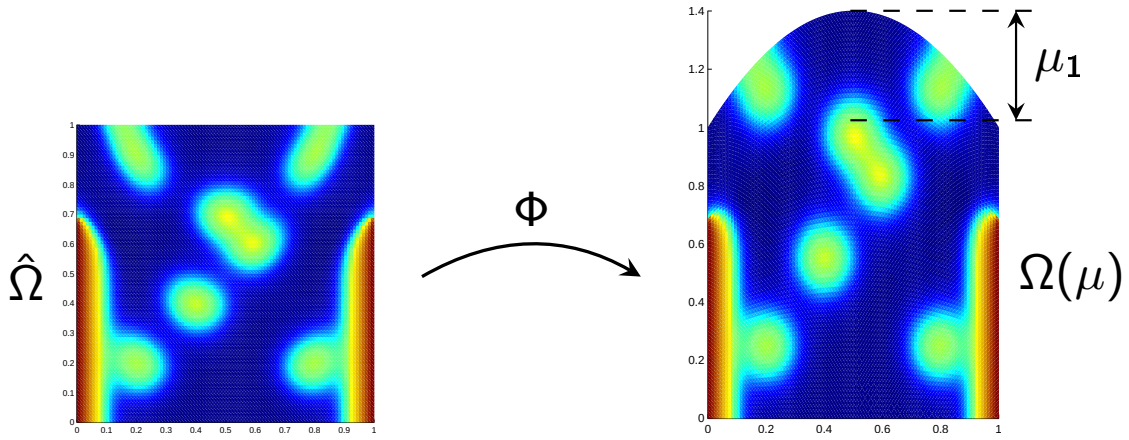
Transformed heat equation

The special case of a transformed linear heat equation with a scalar diffusion factor $k(\mu)$ results in a PDE with (anisotropic) diffusion, convection and a reaction term:

$$\partial_t \hat{u} - k(\mu)\nabla \cdot (GG^t \nabla \hat{u}) + k(\mu)\nabla \cdot (v\hat{u}) - k(\mu)(\nabla \cdot v)\hat{u} = 0 \qquad \text{in } \hat{\Omega} \times [0, T_{\max}],$$

with notations

$$\hat{x} := \Phi^{-1}(x), \qquad \hat{u}(\hat{x}, t) := u(\Phi(\hat{x}), t),$$
$$G(\hat{x}) := D\Phi^{-1}|_{\Phi(\hat{x})}, \qquad v(\hat{x}) := G(\hat{x})\left(\nabla_{\hat{x}} \cdot G(\hat{x})\right).$$



Finite volume scheme

Challenges

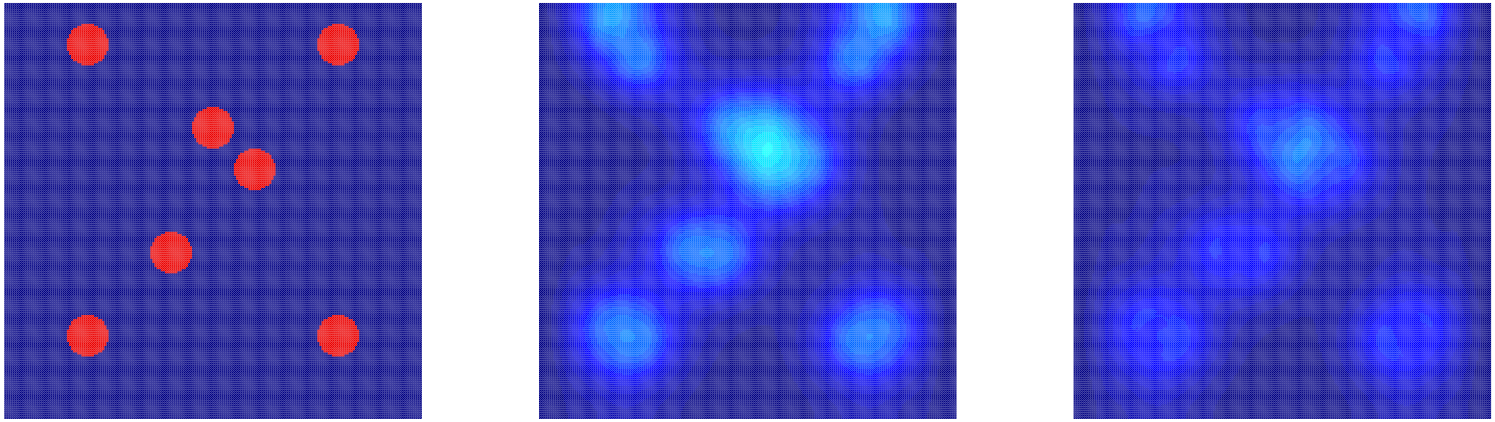
- The geometry transformation introduces a diffusion tensor.
- For non-affine geometry transformations the discrete operators do not depend affinely on the parameter. $\Rightarrow$ Empirical interpolation of the purely explicit discretization operator (case 2) or the implicit and explicit operators (case 4).

Numerical scheme for transformed heat equation

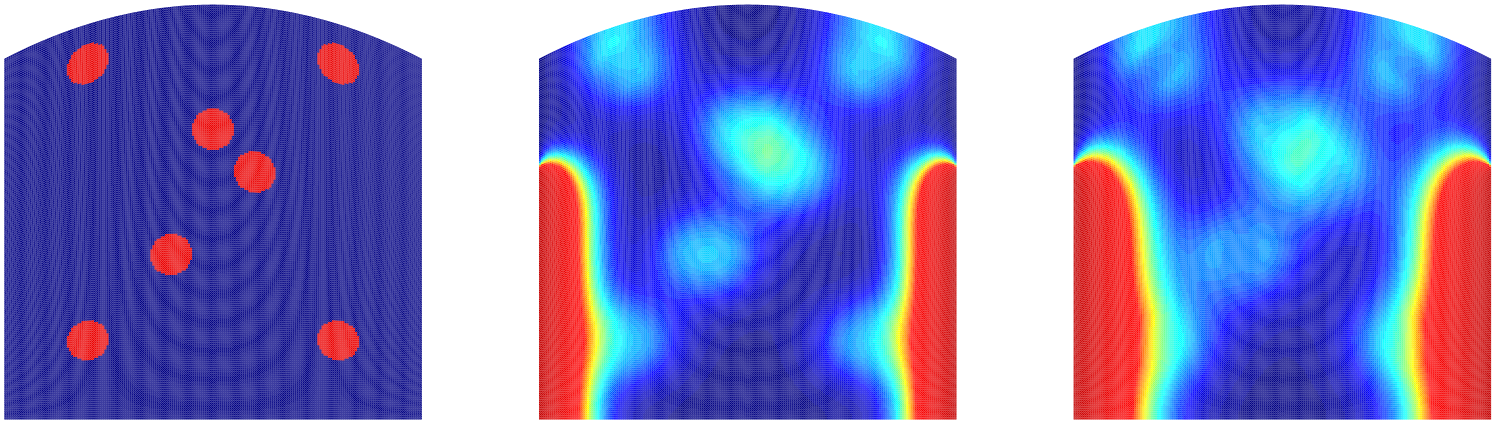
- Discretization with a semi-implicit finite volume scheme on a structured grid with gradient reconstruction. [Drblíková&Mikula, 2007]
- Implicit discretization of diffusion term.

Westfälische Wilhelms-Universität Münster

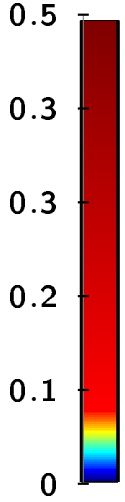
Results



Solutions for $\mu = (0, 0)$ at timesteps $t = 0.0$, $t = 0.75$, $t = 1.5$.



Solutions for $\mu = (0.2, 0.2)$ at timesteps $t = 0.0$, $t = 0.75$, $t = 1.5$.



Results II

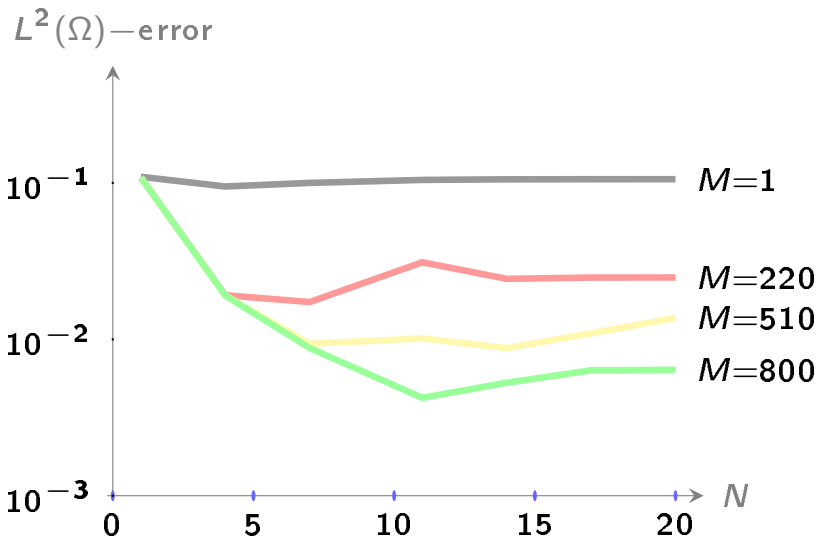


Figure: RB error convergence on 100 test samples

dimension	time [s]
$H = 40000$	24.3675
$N = 7, M = 267$	1.2224
$N = 7, M = 800$	2.0501
$N = 14, M = 267$	1.246
$N = 14, M = 800$	2.104
$N = 20, M = 267$	1.2707
$N = 20, M = 800$	2.1127

Table: average time measurements on 100 test samples

Number of base functions in $\mathcal{W}_H$: 40000
Time gain factor for online phase: ≈ 10

Summary and Outlook

Summary

- Reduced bases allow model reduction for parametrized evolution problems
- RB framework can be applied to implicit and explicit schemes. (tested for implicit linear operators)
- Geometry parametrization is possible for diffeomorphic reference mappings
- Reliability through a posteriori estimators in some cases

Outlook

- Improvement of methodical parts (error estimators, RB/EI generation, stability)
- Test case for schemes with non-linear implicit operators (nonlinear diffusion term)
- Application to PDE systems
- Implementation of a framework that works with efficient numerical software packages like Dune. (c.f. poster)

Westfälische Wilhelms-Universität Münster

References

[Patera, 2006] A. Patera and G. Rozza.
Reduced Basis Approximation and A Posteriori Error Estimation for Parametrized Partial Differential Equations.
Version 1.0, Copyright MIT 2006, to appear in (tentative rubric) MIT Pappalardo Graduate Monographs in Mechanical Engineering

[Drblíková, 2007] O. Drblíková and K. Mikula,
Convergence Analysis of Finite Volume Scheme for Nonlinear Tensor Anisotropic Diffusion in Image Processing.
SIAM J. Numer. Anal., 46, 27–60, 2007

[Haasdonk&Ohlberger, 2008] B. Haasdonk und M. Ohlberger
Reduced Basis Method for Finite Volume Approximations of Parametrized Linear Evolution Equations
M2AN, Math. Model. Numer. Anal. 42, 277–302, 2008

[Haasdonk et al., 2008] B. Haasdonk, M. Ohlberger und G. Rozza.
A Reduced Basis Method for Evolution Schemes with Parameter-Dependent Explicit Operators
ETNA, Electronic Transactions on Numerical Analysis, vol. 32, 2008

[Barrault et al., 2004] M. Barrault, M., Y. Maday, N. Nguyen and A. Patera,
An 'empirical interpolation' method: application to efficient reduced-basis discretization of partial differential equations
C. R. Math. Acad. Sci. Paris Series I, 2004, 339, 667-672

[Drohmann et al., 2009] M. Drohmann, B. Haasdonk and M. Ohlberger,
Reduced Basis Method for Finite Volume Approximation of Evolution Equations on Parametrized Geometries
Proceedings of ALGORITMY 2009, 111–120

Westfälische Wilhelms-Universität Münster