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Empirical Interpolation of Nonlinear Parametrized Evolution Operators

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Bernard Haasdonk,

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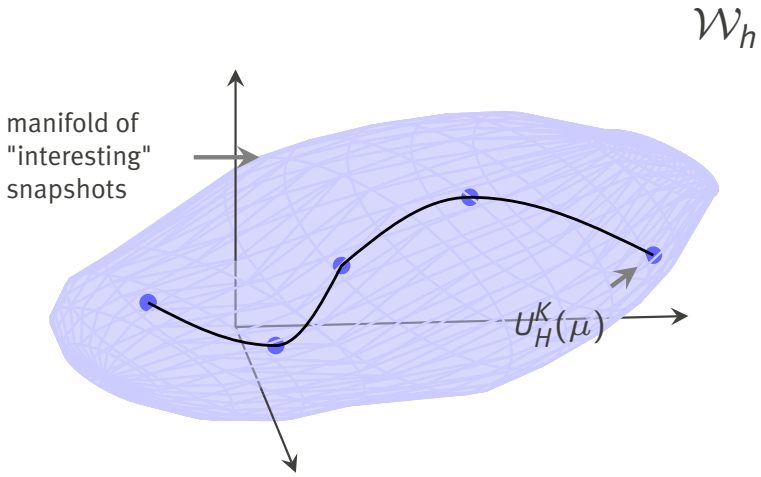
Motivation: Reduced Basis Method

RB Scenario:

- Parametrized partial differential equations for (non-stationary) problems
- Applications relying on time-critical or many repeated simulations

Goals:

- Offline-/Online decomposition
- Efficient reduced simulations
- A posteriori error control



References: [Patera&Rozza, 2006], [Haasdonk et al., 2008]

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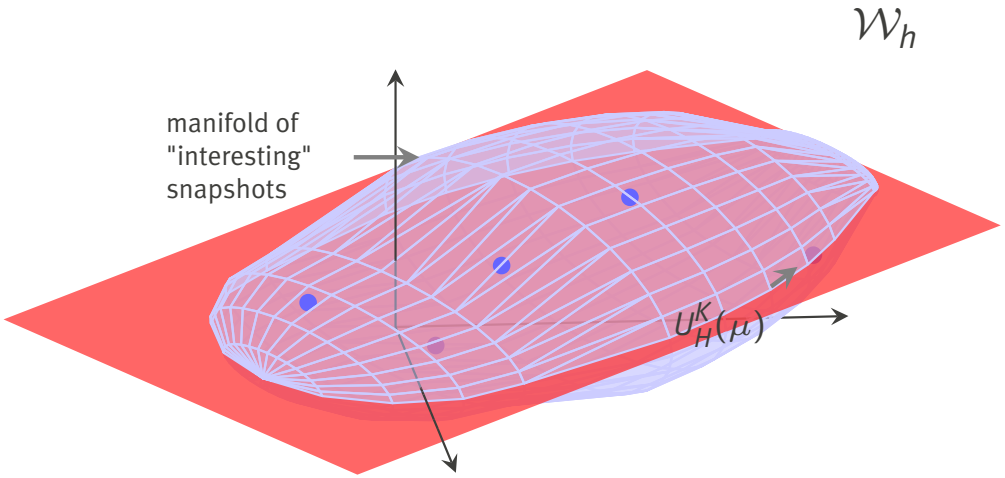

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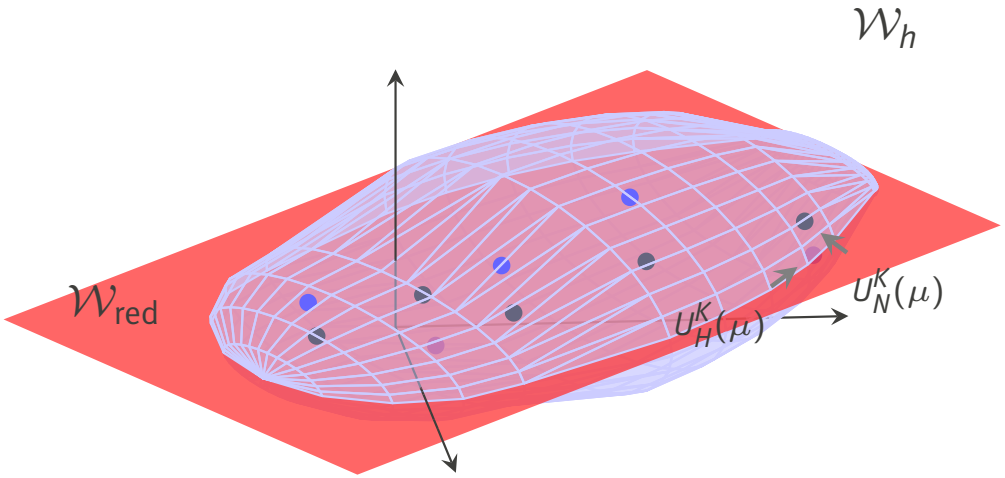

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Motivation: Parametrized Evolution Equation

Analytical Formulation

For $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$, find $u : [0, T_{\max}] \to \mathcal{W}_h \subset L^2(\Omega)$, s.t.

$$u(0) = u_0(\boldsymbol{\mu}), \qquad \partial_t u(t) - \mathcal{L}(\boldsymbol{\mu})\,[u(t)] = 0$$

plus (parameter dependent) boundary conditions.

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plus (parameter dependent) boundary conditions.

Discretization (implicit/explicit with Newton scheme)

For $\boldsymbol{\mu} \in \mathcal{P}$ find $\{u_h\}_{k=0}^{K} \subset \mathcal{W}_h \subset L^2(\Omega)$, s.t.

$$u_h^0 := P_h\left[u_0(\boldsymbol{\mu})\right], \qquad u_h^{k+1} := u_h^{k+1,\nu_{\max}(k)}$$

with Newton iteration

$$u_h^{k+1,0} := u_h^k, \qquad u_h^{k+1,\nu+1} := u_h^{k+1,\nu} + \delta_h^{k+1,\nu+1},$$

$$\left(\mathrm{Id} + \Delta t \mathbf{D}\mathcal{L}_h^I\big|_{u_h^{k+1,\nu}}\right)\left[\delta_h^{k+1,\nu+1}\right] = u_h^k - u_h^{k+1,\nu} - \Delta t\left(\mathcal{L}_h^I\left[u_h^{k+1,\nu}\right] + \mathcal{L}_h^E\left[u_h^k\right]\right).$$

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Empirical interpolation: Idea

General operator approximation

Approximate operator evaluations

$$\mathcal{L}_h(\boldsymbol{\mu})\left[u_h^k(\boldsymbol{\mu})\right] \approx \mathcal{I}_M\left[\mathcal{L}_h(\boldsymbol{\mu})\right]\left[u_h^k(\boldsymbol{\mu})\right] = \sum_{m=1}^{M} l_m(\boldsymbol{\mu})\left[u_h^k(\boldsymbol{\mu})\right] \quad \xi_m \ ,$$

where $l_m(\boldsymbol{\mu}) : \mathcal{W}_h \to \mathbb{R}$ are efficiently computable functionals and ξ_m collateral reduced basis functions.

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Empirical interpolation[Barrault et al, 2004]

- collateral reduced basis $\mathcal{W}_M$ made out of operator evaluations: $\left\{\mathcal{L}_h(\boldsymbol{\mu}_m)\left[u_h^{k_m}(\boldsymbol{\mu}_m)\right]\right\}_{m=1}^{M}$ ("Greedy search in parameter space")
- coefficients are exact operator evaluations at interpolation points $\{x_m\}_{m=1}^{M}$: $l_m(\boldsymbol{\mu}) := \mathcal{L}_h(\boldsymbol{\mu})\left[\cdot\right](x_m)$.

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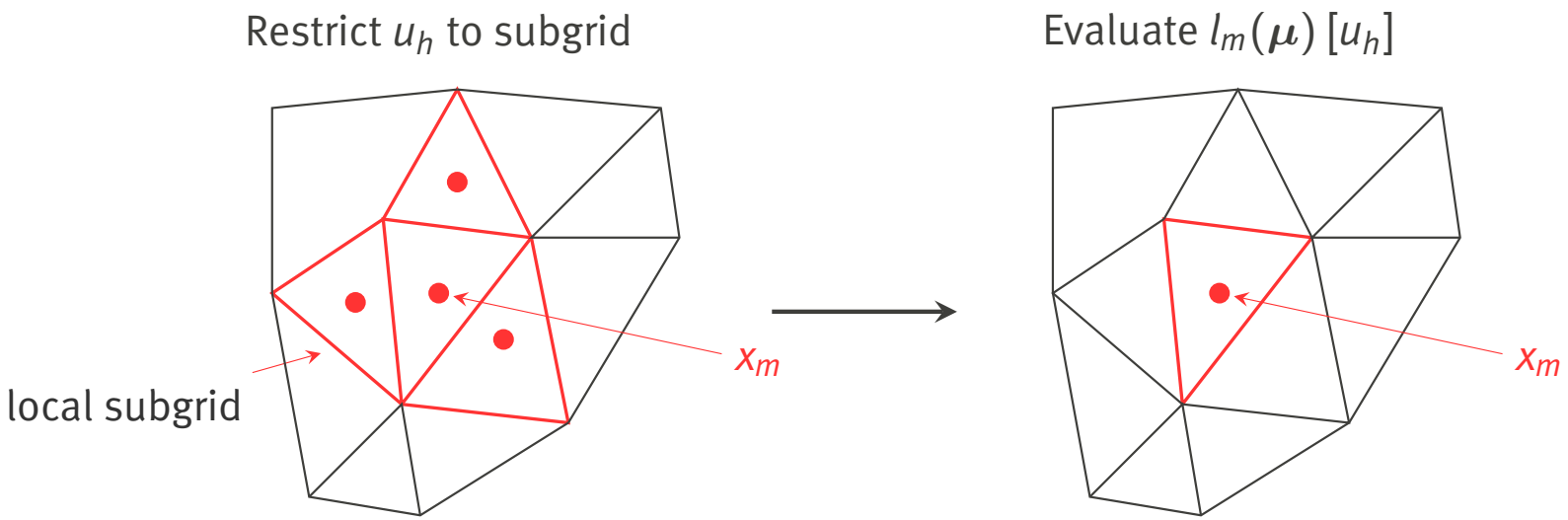
- coefficients are exact operator evaluations at interpolation points $\{x_m\}_{m=1}^{M}$: $l_m(\boldsymbol{\mu}) := \mathcal{L}_h(\boldsymbol{\mu})\left[\cdot\right](x_m)$.
- CRB functions ξ_m are nodal in interpolation points: $\xi_m(x_n) = \delta_{nm}$.

Empirical interpolation: Online evaluations

Efficient evaluations of $l_m(\boldsymbol{\mu})$

The coefficient functionals $l_m(\boldsymbol{\mu}) = \mathcal{L}_h(\boldsymbol{\mu})[\cdot](x_m)$ can be computed efficiently during online phase, if

- operator has localized structure (small stencil) and
- local geometry information is precomputed in offline phase.



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Empirical interpolation: CRB generation

CRB extension algorithm

$m \leftarrow 0, q_0 \leftarrow 0$ ▷ Initialization.

repeat

  for $u_h \in L_{\text{train}}$ **do**

    $u_h^* \leftarrow \arg\inf_{v_h \in \operatorname{span}\{q_i\}_{i=1}^m} \|u_h - v_h\|$. ▷ Find the best approximation.

  end for

  $u_m \leftarrow \arg\sup_{u_h \in L_{\text{train}}} \|u_h - u_h^*\|$. ▷ Find approximation with worst error.

  $r_m \leftarrow u_m - \mathcal{I}_m[u_m]$ ▷ Compute the residual between u_m and its interpolant.

  $x_m \leftarrow \arg\sup_{x \in X_H} |r_m(x_i)|$ ▷ Find new interpolation point.

  $q_m \leftarrow \frac{r_m}{r_m(x_m)}$ ▷ Find new CRB function.

  $m \leftarrow m + 1$

until $\|r_m\| \leq \varepsilon_{\text{tol}}$ or $m = M_{\max}$

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- Use $L^\infty - \|\cdot\|$ or $L^2 - \|\cdot\|$

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- Use $L^\infty - \|\cdot\|$ or $L^2 - \|\cdot\|$
- For notation: nodal basis $\boldsymbol{\xi} := \{\xi_m\}_{m=1}^M$ made out of $\{q_m\}_{m=1}^M$

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Emprical interpolation: Fréchet derivative

Observation

$$\mathbf{D}\mathcal{I}_M\left[\mathcal{L}_h(\boldsymbol{\mu})\right]|_{u_h}[v_h] = \boxed{\sum_{m=1}^{M} \mathbf{D}l_m(\boldsymbol{\mu})|_{u_h}[v_h]\ \boxed{\xi_m}}$$

parameter dependent parameter independent

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parameter dependent parameter independent

Coefficient functionals

$\mathcal{W}_h$ is finite dimensional

$$\mathbf{D}l_m(\boldsymbol{\mu})|_{u_h}\left[v_h\right] = \sum_{m=1}^{M}\sum_{i=1}^{H} \frac{\partial}{\partial \psi_i} l_m(\boldsymbol{\mu})\left[u_h\right]\left(\underline{v}_{h,i}\right)$$

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$$= \sum_{m=1}^{M}\sum_{i\in I_{x_m}} \frac{\partial}{\partial \psi_i} l_m(\boldsymbol{\mu})\left[u_h\right](\underline{v}_{h,i}).$$

$\mathcal{L}_h$ has local stencil

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$\mathcal{L}_h$ has local stencil

Note: $\mathrm{card}(I_{x_m}) < C$ for all $m = 1, \ldots, M$. $\Rightarrow$ Complexity still $\mathcal{O}(M)$.

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Reduced basis method for nonlinear schemes

- Generate reduced basis space with POD-Greedy algorithm: $\mathcal{W}_{\text{red}} := \text{span}\,\{\varphi_i\}_{i=1}^{N} \subset \mathcal{W}_h$
- Reduced model order by Galerkin projection: $P_{\text{red}} : \mathcal{W}_h \to \mathcal{W}_{\text{red}}$
- Offline-/online decomposition of operators:

$$\left(P_{\text{red}}[u_{h,\text{o}}(\boldsymbol{\mu})]\right)_n = \underbrace{\boxed{\sum_{q=1}^{Q_{u\text{o}}} \sigma_{u\text{o}}^q(\boldsymbol{\mu}) \; \boxed{\int_\Omega u_\text{o}^q \varphi_n}}}_{\text{online} \qquad \text{offline}} \quad \text{assuming: } u_\text{o}(\boldsymbol{\mu}) = \sum_{q=1}^{Q_{u\text{o}}} \sigma_{u\text{o}}^q(\boldsymbol{\mu}) u_\text{o}^q$$

$$\left(\mathcal{L}_{\text{red}}^l(\boldsymbol{\mu})\left[u_{\text{red}}^k(\boldsymbol{\mu})\right]\right)_n = \underbrace{\boxed{\sum_{m=1}^{M} l_m^l(\boldsymbol{\mu})\,[u_{\text{red}})] \; \boxed{\int_\Omega \xi_m \varphi_n}}}_{\text{online} \qquad \text{offline}}$$

$$\left(\mathbf{D}\mathcal{L}_{\text{red}}^l(\boldsymbol{\mu})|_{u_{\text{red}}}\,[\delta_{\text{red}}]\right)_n = \underbrace{\boxed{\sum_{m=1}^{M} \frac{\partial}{\partial \psi_i} l_m^l(\boldsymbol{\mu})\,[u_{\text{red}}] \; \boxed{\int_\Omega \xi_m \varphi_n}}}_{\text{online} \qquad \text{offline}}$$

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Reduced basis method for nonlinear schemes

Projection of Operators:

- $P_{\text{red}} : \mathcal{W}_h \to \mathcal{W}_{\text{red}}$ Galerkin projection onto $\mathcal{W}_{\text{red}} \subset \mathcal{W}_h$
- $\mathcal{L}^I_{\text{red}} := P_{\text{red}} \circ \mathcal{I}_M \circ \mathcal{L}^I_h$
- $\mathcal{L}^E_{\text{red}} := P_{\text{red}} \circ \mathcal{I}_M \circ \mathcal{L}^E_h$

Reduced simulation

For $\boldsymbol{\mu} \in \mathcal{P}$ find $\{u_{\text{red}}\}_{k=0}^K \subset \mathcal{W}_{\text{red}}$, s.t.

$$u^{k+1}_{\text{red}} := u^{k+1,\nu_{\max}(k)}_{\text{red}}, \qquad u^0_{\text{red}} := P_{\text{red}}\left[u_{h,0}(\boldsymbol{\mu})\right]$$

with Newton iteration

$$u^{k+1,0}_{\text{red}} := u^k_{\text{red}}, \qquad u^{k+1,\nu+1}_{\text{red}} := u^{k+1,\nu}_{\text{red}} + \delta^{k+1,\nu+1}_{\text{red}},$$

$$\left(\mathrm{Id} + \Delta t \mathbf{D}\mathcal{L}^I_{\text{red}}\big|_{u^{k+1,\nu}_{\text{red}}}\right)\left[\delta^{k+1,\nu+1}_{\text{red}}\right] = u^k_{\text{red}} - u^{k+1,\nu}_{\text{red}} - \Delta t\left(\mathcal{L}^I_{\text{red}}\left[u^{k+1,\nu}_{\text{red}}\right] + \mathcal{L}^E_{\text{red}}\left[u^k_{\text{red}}\right]\right).$$

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Reduced basis generation

POD-greedy algorithm

INPUT: $M_{\text{train}} \subset \mathcal{P}, \varepsilon_{\text{tol}}, N_{\max}$
OUTPUT: $\mathcal{W}_{\text{red}}$
Initialize reduced basis space: $\Phi_{N_0} \leftarrow \{\varphi_n\}_{n=1}^{N_0}, \qquad N \leftarrow N_0$
repeat

1. *Find worst approximated reduced solution:* $\boldsymbol{\mu}_{\max} \leftarrow \arg\max_{\boldsymbol{\mu} \in M_{\text{train}}} \eta(\boldsymbol{\mu})$
2. *Compute trajectory:* $\left\{u_h^k(\boldsymbol{\mu}_{\max})\right\}_{k=0}^{K}$.
3. *Compute new reduced basis function:*

$$\varphi_{N+1} \leftarrow \text{POD}\left(\left\{u_h^k(\boldsymbol{\mu}_{\max}) - P_{\text{red}}\left[u_h^k(\boldsymbol{\mu}_{\max})\right]\right\}_{k=0}^{K}\right)$$
$$N \leftarrow N + 1$$

until error indicator $\eta(\boldsymbol{\mu}_{\max})$ falls beneath tolerance ε_{tol} **or** $N_{\max}$ is reached.
$\mathcal{W}_{\text{red}} \leftarrow \text{span}\left\{\varphi_n\right\}_{n=1}^{N}$

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A posteriori error estimator

Theorem (A posteriori error estimator)

Assumptions:

- *Operators and* $\mathbf{D}\mathcal{L}_h^l$ *are Lipschitz-continuous.*
- $\mathbf{D}\mathcal{L}_h^l$ *has bounded inverse*
- *Empirical interpolations exact for larger CRB space* $\mathcal{W}_{M+M'}$ *and* $P_h\left[u_0(\boldsymbol{\mu})\right] \in \mathcal{W}_{\text{red}}$

Then:

$$\left\| u_{\text{red}}^k(\boldsymbol{\mu}) - u_h^k(\boldsymbol{\mu}) \right\| \leq \Delta_{N,M}^k(\boldsymbol{\mu}) \qquad \text{with } \Delta_{N,M}(\boldsymbol{\mu}) := \sum_{i=0}^{k-1} \sum_{j=1}^{\nu_{\max}(i)} \bar{\Delta}^{i,j}$$

recursively defined through the Newton step error estimator

$$\bar{\Delta}^{k+1,j+1} := \Delta t \left(C_1 \bar{\Delta}^{k_1,\nu} + C_2 \bar{\Delta}^{k+1,\nu} + \left\| \delta_{\text{red}}^{k+1,\nu+1} \right\| + \left\| R_{D,M}^{k+1,\nu+1} \right\| + \left\| R_{I,M}^{k+1,\nu} \right\| + \left\| R_{E,M}^{k+1,0} \right\| + \left\| R^{k+1,\nu} \right\| \right).$$

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A posteriori error estimator

Theorem (A posteriori error estimator cont.)

Then:

$$\left\| u_{\text{red}}^k(\boldsymbol{\mu}) - u_h^k(\boldsymbol{\mu}) \right\| \leq \Delta_{N,M}^k(\boldsymbol{\mu}) \qquad \textit{with } \Delta_{N,M}(\boldsymbol{\mu}) := \sum_{i=0}^{k-1} \sum_{j=1}^{\nu_{\max}(i)} \bar{\Delta}^{i,j}$$

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The residuals $R_{*,M}$ measure the empirical interpolation error, e.g.

$$R_{I,M}^{k+1,\nu} := \sum_{m=M}^{M+M'} l_m' \left[u_{\text{red}}^{k+1,\nu} \right] \xi_m$$

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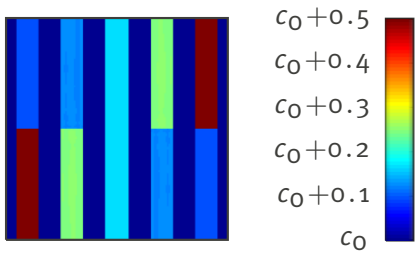
Numerical results: Porous Medium Equation

Problem definition:

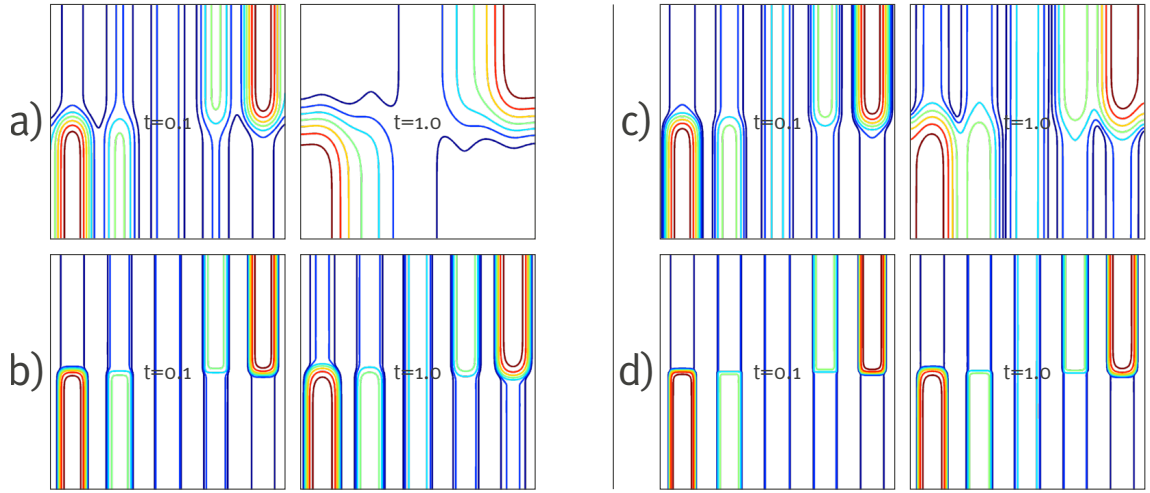
$$\partial_t u - m\Delta u^p = 0 \quad \text{in } \Omega \times [0,1], \qquad u(\cdot,0) = c_0 + u_0 \quad \text{on } \Omega \times \{0\}$$

with homogeneous boundary conditions, $\boldsymbol{\mu} = (p, m, c_0) \in [1,5] \times [0, 0.01] \times [0, 0.2]$

Initial data:



Sample trajectories:



a) $\boldsymbol{\mu} = (1, 0.01, 0.2)$, b) $\boldsymbol{\mu} = (4, 0.01, 0.2)$,
c) $\boldsymbol{\mu} = (1, 0.01, 0.0)$, d) $\boldsymbol{\mu} = (4, 0.01, 0.0)$

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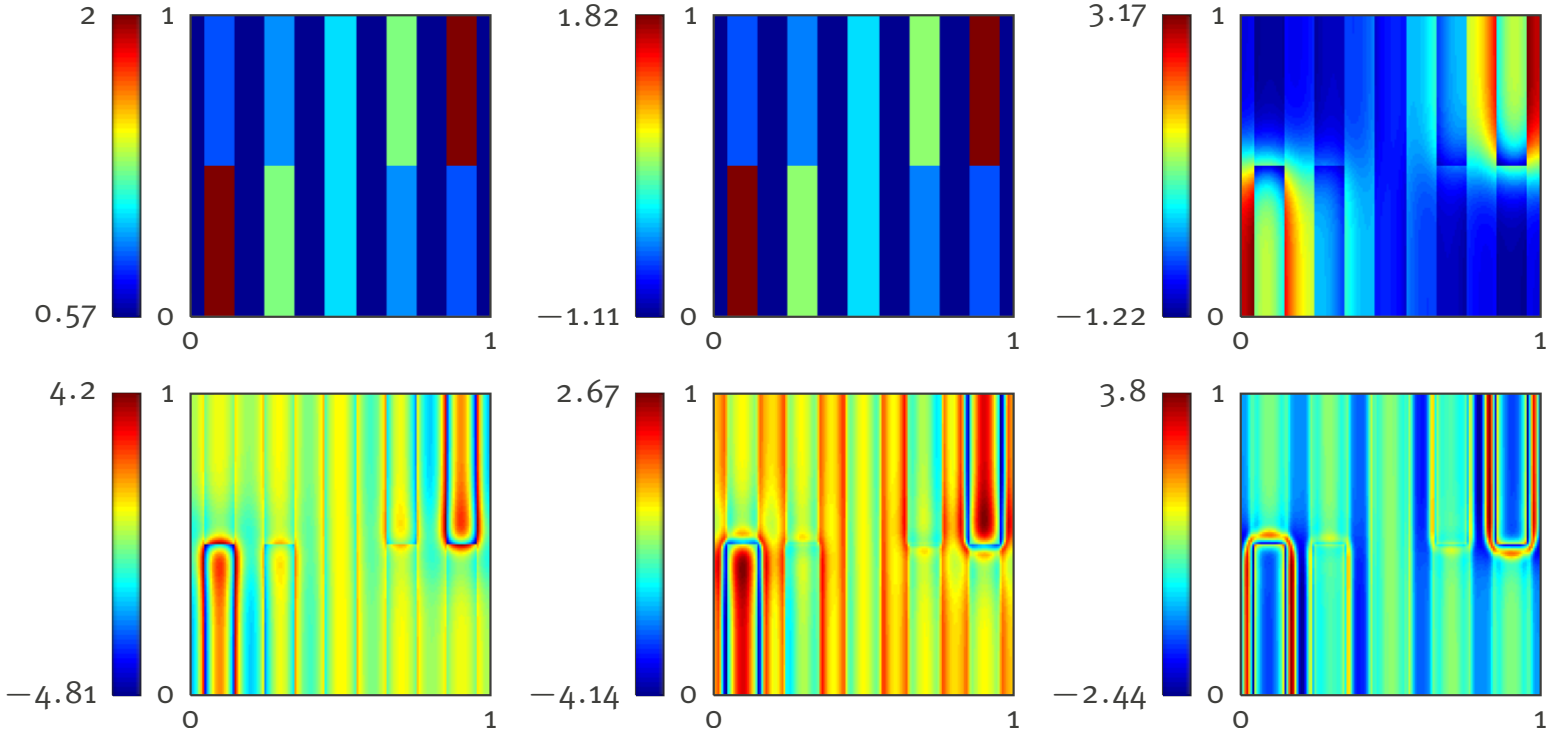
Numerical results: Porous Medium Equation

First 6 reduced basis functions



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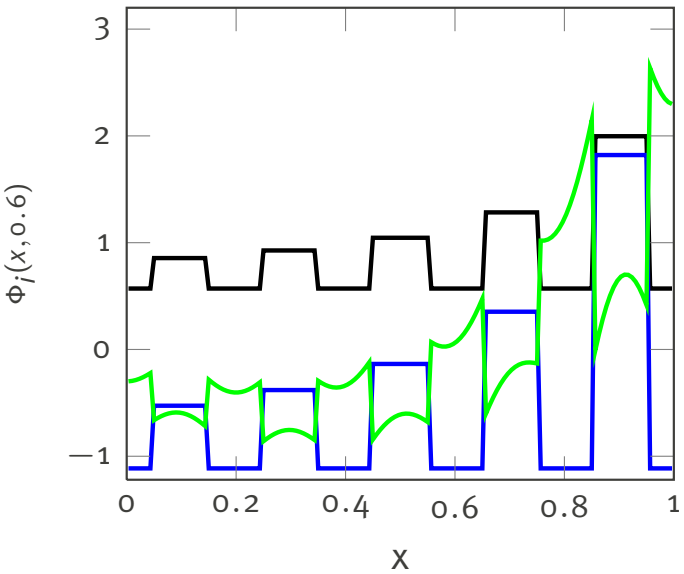
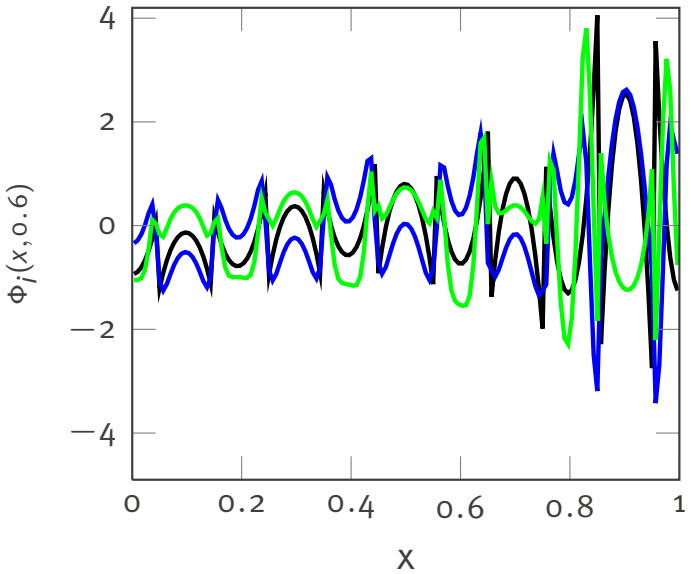
Numerical results: Porous Medium Equation

Slices of first 6 reduced basis functions at $y = 0.6$





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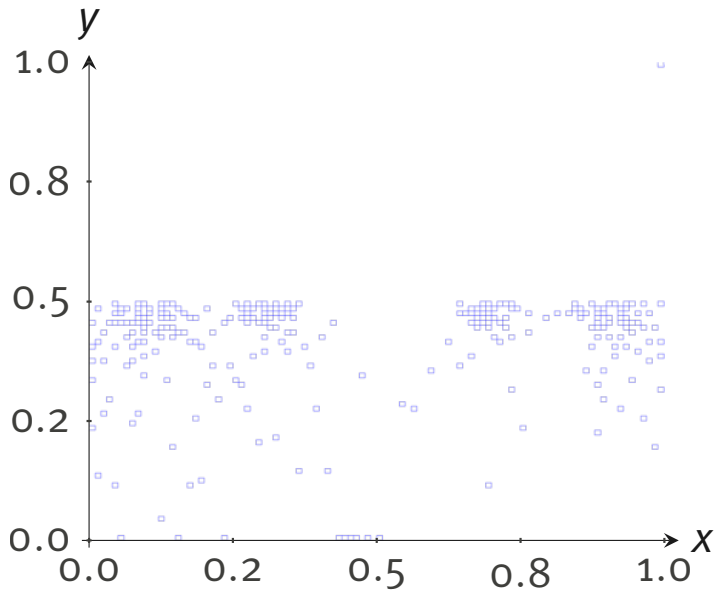
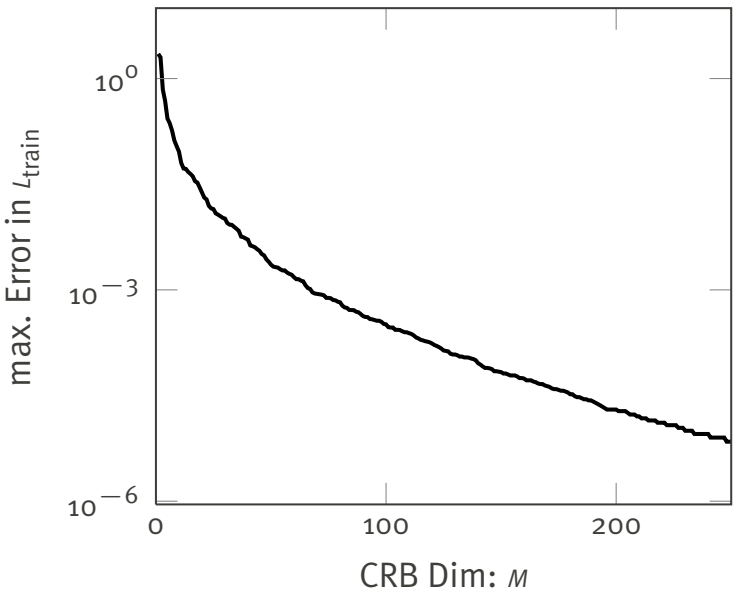
Numerical results: Empirical interpolation of $\mathcal{L}_h^l$

Subgrid at interpolation points



Error decrease during EI-Offline algorithm



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Numerical results: Reduced basis scheme

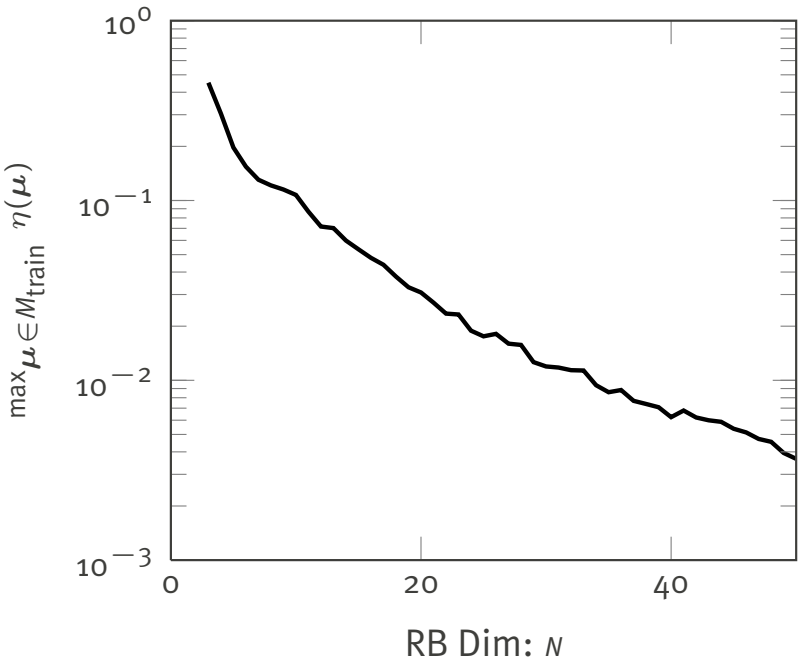

Figure: RB error convergence on 100 test samples

Dimension	Runtime[s]	Error
H=22500	605.66	–
N=15, M=75	5.01	$4.93 \cdot 10^{-3}$
N=30, M=150	7.14	$1.73 \cdot 10^{-3}$
N=40, M=200	8.27	$8.53 \cdot 10^{-4}$
N=50, M=250	9.78	$7.59 \cdot 10^{-4}$

Table: average time measurements on 100 test samples

Number of base functions in $\mathcal{W}_h$:	22500
Number of Newton steps $\nu_{\max}$:	$\approx 1 - 20$
Time gain factor for online phase:	$\approx 25 - 110$

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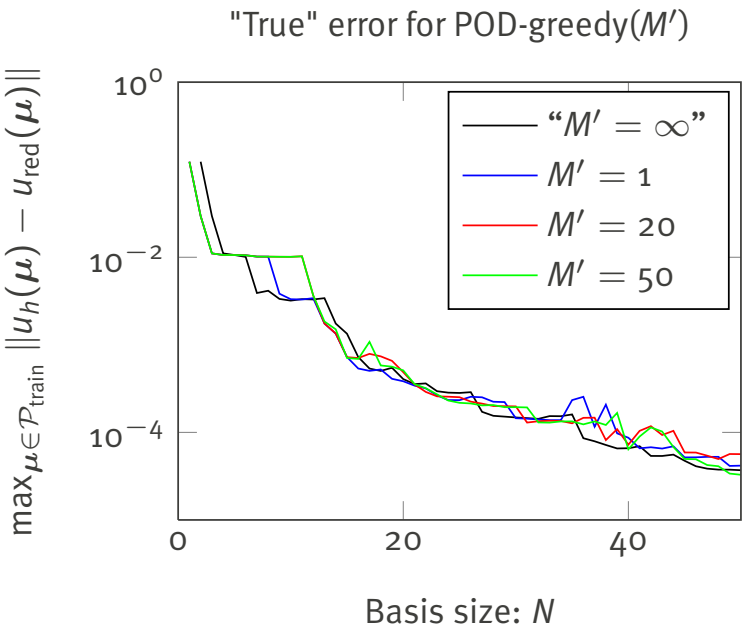
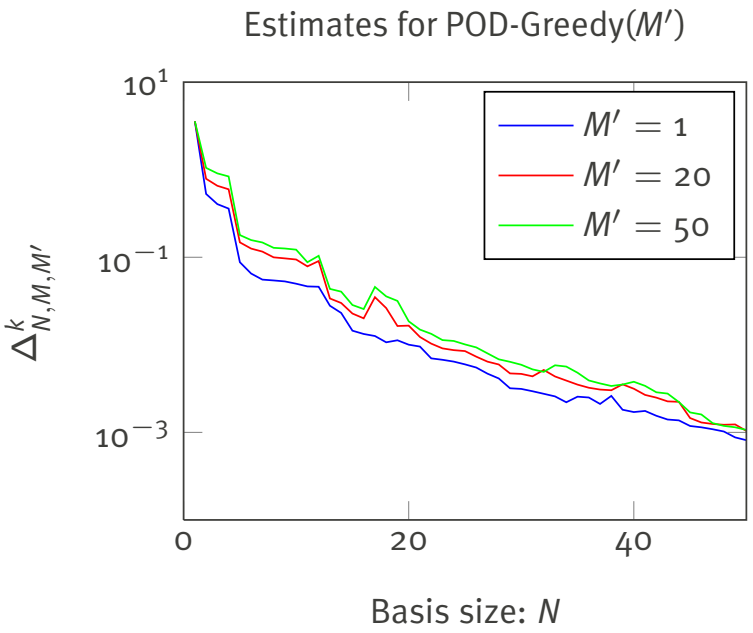
Numerical results: A posteriori error estimator

POD-Greedy with efficient error control (explicit Burgers problem)





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Numerical results: A posteriori error estimator

Efficiency of error estimator η: $\lambda(\boldsymbol{\mu}) := \frac{\eta(\boldsymbol{\mu})}{\|u_h(\boldsymbol{\mu}) - u_{\text{red}}(\boldsymbol{\mu})\|}$

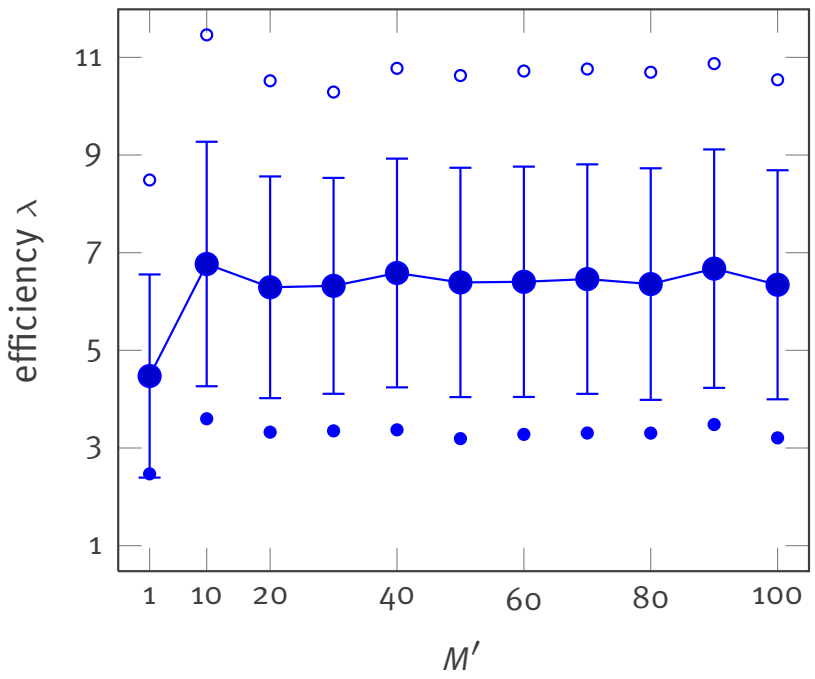

Figure: Error bar plot showing mean and standard deviation of error estimator efficiency over a sample of 20 random parameters for different values of M'. The dots indicate the minimum (●) and maximum (○) efficiency.

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Outlook

Conclusion

- Model order reduction of general (scalar) parametrized evolution schemes
- Main ingredient is the empirical interpolation for discrete operators
- Rigorous error control via a posteriori error estimator is possible

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Some Problems

- Control and measurement of complexity of parametrized solution manifold (“Kolmogorov n-width”)
- Big reduced basis space are inefficient and instable through cancellation
- Variable time step width

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Some solutions/Ideas

- Do intensive tests with “real-world” discretizations (including systems)
- Improve reduced basis generation
  - generate many small reduced bases spaces for parameter and time ranges
  - improve RB approximation by adaptive search algorithms
  - change reduced basis spaces over the time
- Stability analysis of reduced matrices for time-stepping

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Software concepts (DUNE-RB/RBMATLAB interface)

Goals:

- Use C++ software DUNE-RB for high-dimensional computations and RBMATLAB for reduced basis algorithms
- Access to open source implementations of “real world” problems. (Several available in DUNE)
- Testing the reduced basis methods on these implementations.

For further information see: http://morepas.org

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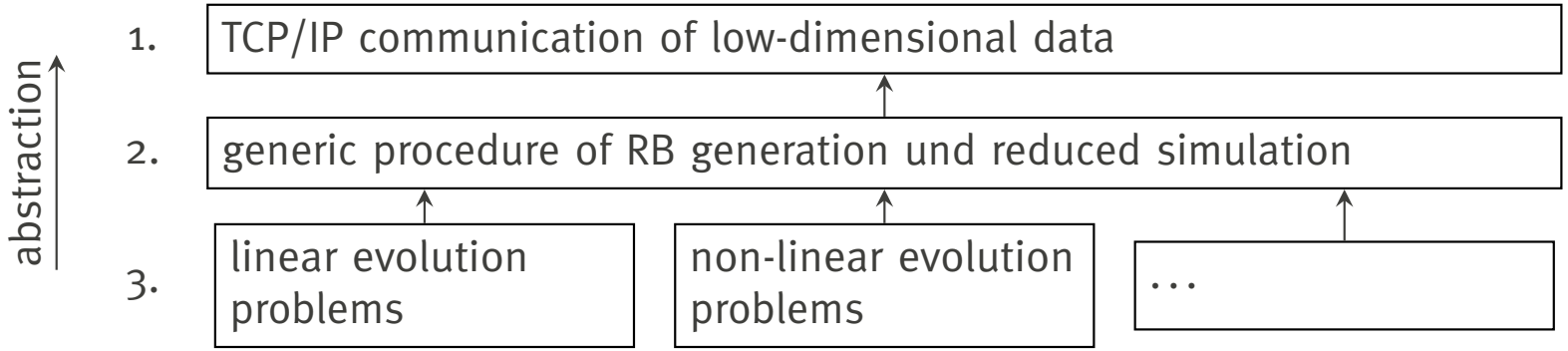
Illustration of interface concept:



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Status:

- Communication interface between RBMATLAB and DUNE-RB exists
- Example implementation: linear heat equation in Dune affinely parameter dependent structure. (No empirical interpolation necessary)
- Empirical interpolation of simple operators.

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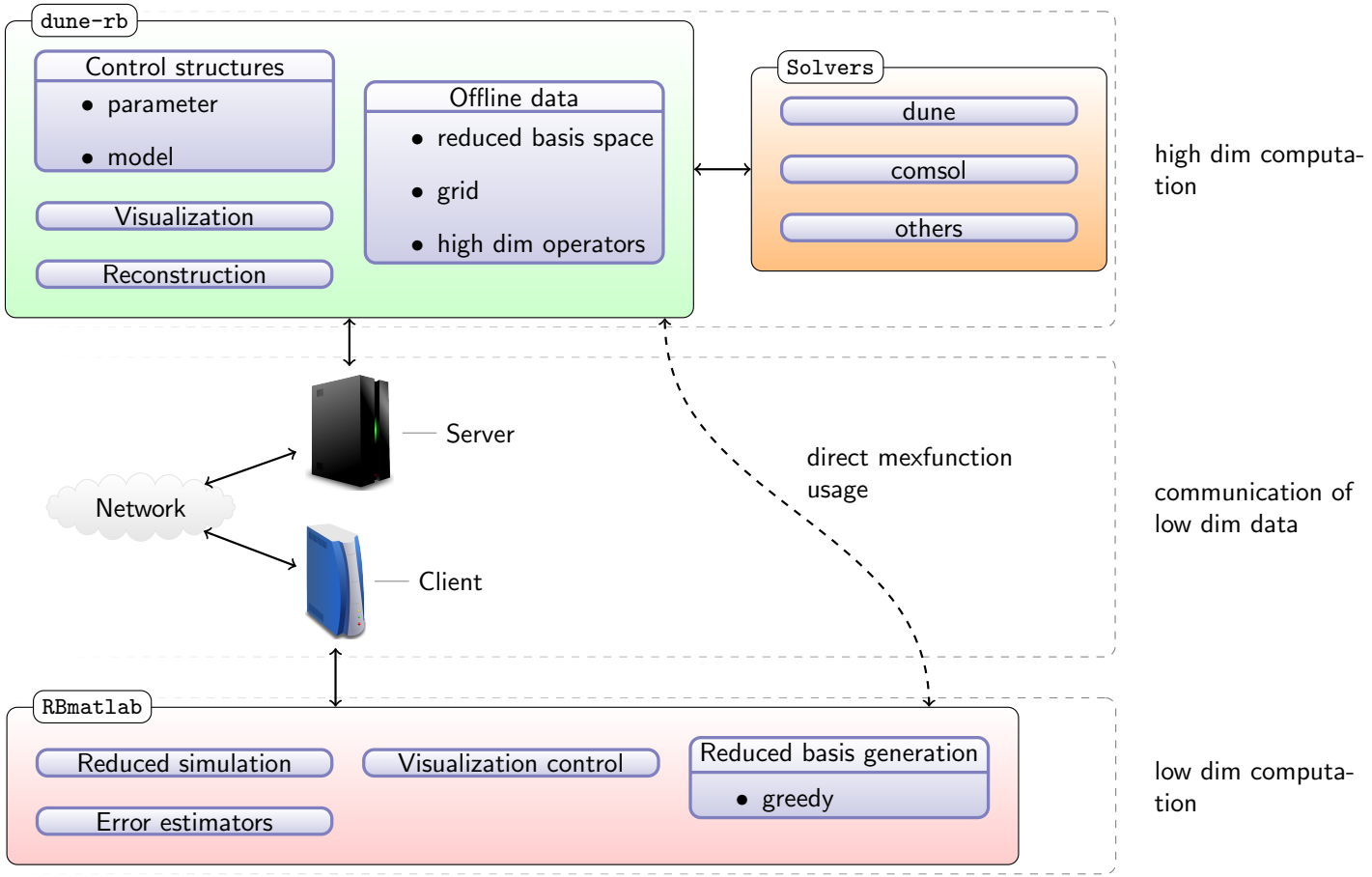
Software concepts (DUNE-RB/RBMATLAB interface)



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