Westfälische
Wilhelms-Universität
Münster

Reduced Basis methods with a DUNE–Matlab–Communication–Interface

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M. Drohmann, B. Haasdonk
S. Kaulmann, M. Ohlberger

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› Outline

Reduced basis method

RBmatlab–Dune-RB-Interface

dune-rb Module

RBMatlab

› Reduced Basis Method Overview

RB Scenario:

- Parametrized partial differential equations for (non-stationary) problems
- Applications relying on time-critical or many repeated simulations, e.g. design, control, optimization applications.

Goals:

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

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

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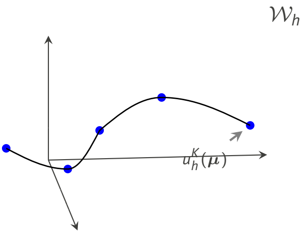

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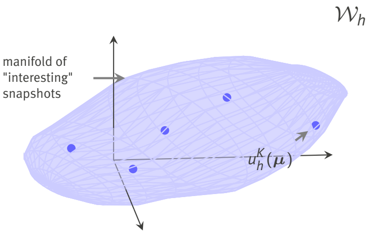

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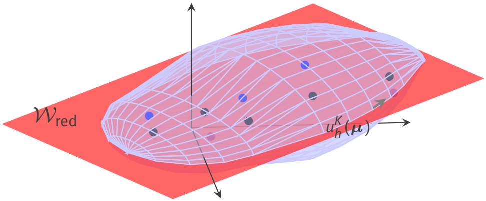

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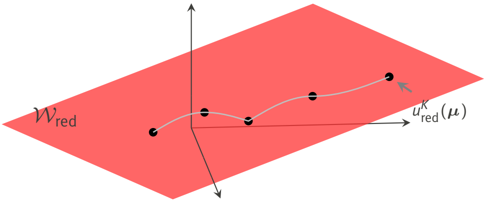

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› Derivation of Reduced Numerical Scheme

1. Analytical formulation

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

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

plus (parameter dependent) boundary conditions.

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plus (parameter dependent) boundary conditions.

2. Discretization (e.g. FV,FE,DG)

For $\boldsymbol{\mu} \in \mathcal{P}$ compute $\left\{u_h^k(\boldsymbol{\mu})\right\}_{k=0}^{K} \subset \mathcal{W}_h \subset L^2(\Omega)$ by

$$u_h^0(\boldsymbol{\mu}) := P_h[u_0(\boldsymbol{\mu})]$$
$$u_h^k(\boldsymbol{\mu}) := u_h^{k-1}(\boldsymbol{\mu}) + \Delta t \mathcal{L}_h(\boldsymbol{\mu})[u_h^{k-1}(\boldsymbol{\mu})].$$

› Derivation of Reduced Numerical Scheme (cont.)

- Generate reduced basis space $\mathcal{W}_{\text{red}} := \text{span}\,\{\varphi_i\}_{i=1}^{N} \subset \mathcal{W}_h$ with POD-Greedy algorithm.
- Assume separable initial data and operator

$$u_0 = \sum_{q=1}^{Q_{u0}} \boxed{\sigma_{u0}^{q}(\boldsymbol{\mu})}\,\boxed{u_0^{q}} \qquad \mathcal{L} = \sum_{q=1}^{Q_L} \boxed{\sigma_L^{q}(\boldsymbol{\mu})}\,\boxed{\mathcal{L}^{q}}$$

  with parameter dependent and independent parts.
- Compute offline–vectors and –matrices from parameter independent contributions for numerical scheme

$$\left(\mathbf{P}^{0,q}\right)_n = \int_\Omega u_0^q \varphi_n, \qquad q = 1,\ldots,Q_{u0},\, n = 1,\ldots,N$$

$$\left(\mathbf{L}^{q}\right)_{n,m} = \int_\Omega \mathcal{L}^q\left[\varphi_m\right]\varphi_n, \qquad q = 1,\ldots,Q_L,\, m,n = 1,\ldots,N$$

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and a posteriori error estimation (not discussed here).

› Derivation of Reduced Numerical Scheme (cont.)

3. Reduced numerical scheme

For $\boldsymbol{\mu} \in \mathcal{P}$ compute $\left\{u_{\text{red}}^{k}(\boldsymbol{\mu})\right\}_{k=0}^{K} \subset \mathcal{W}_{\text{red}} \subset \mathcal{W}_{h}$ by

$$\begin{aligned} \left(u_{\text{red}}^{0}(\boldsymbol{\mu}) - P_h[u_0(\boldsymbol{\mu})], \varphi\right) &= 0 \quad \forall \varphi \in \mathcal{W}_{\text{red}}, \\ \left(u_{\text{red}}^{k}(\boldsymbol{\mu}) - u_{\text{red}}^{k-1}(\boldsymbol{\mu}) + \Delta t \mathcal{L}_h(\boldsymbol{\mu})\left[u_h^{k-1}(\boldsymbol{\mu})\right], \varphi\right) &= 0 \quad \forall \varphi \in \mathcal{W}_{\text{red}}, \end{aligned}$$

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or equivalently compute vectors $\mathbf{a}^k(\boldsymbol{\mu}) \subset \mathbb{R}^N$ for $k = 0, \ldots, K$ such that $u^k_{\text{red}}(\boldsymbol{\mu}) = \sum_{n=1}^N a^k_n \varphi_n$ by

$$\mathbf{a}^0(\boldsymbol{\mu}) := \sum_{q=1}^{Q_{u0}} \sigma^q_{u0}(\boldsymbol{\mu}) \mathbf{P}^{0,q},$$

$$\mathbf{a}^k(\boldsymbol{\mu}) := \mathbf{a}^{k-1}(\boldsymbol{\mu}) + \Delta t \sum_{q=1}^{Q_L} \sigma^q_L(\boldsymbol{\mu}) \mathbf{L}^q \mathbf{a}^{k-1}.$$

› Reduced basis generation

Use error estimator $\eta(\boldsymbol{\mu})$, s.t. $\max_{k=0,\dots,K} \left\| u_h^k(\boldsymbol{\mu}) - u_{\text{red}}^k(\boldsymbol{\mu}) \right\|_{\mathcal{W}_h} \leq \eta(\boldsymbol{\mu})$.

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POD-greedy algorithm

INPUT: $M_{\text{train}} \subset \mathcal{P}, \varepsilon_{\text{tol}}, N_{\max}$
OUTPUT: $\mathcal{W}_{\text{red}}$

Initialize reduced basis:

$$\Phi_{N_0} \leftarrow \{\varphi_n\}_{n=1}^{N_0}$$
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1. *Find worst approximated trajectory:* $\boldsymbol{\mu}_{\text{max}} \leftarrow \arg\max_{\boldsymbol{\mu} \in M_{\text{train}}} \eta(\boldsymbol{\mu})$
2. *Compute trajectory* $\left\{ u_h^k(\boldsymbol{\mu}_{\text{max}}) \right\}_{k=0}^{K}$.
3. *Compute new basis function:*

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

until $\eta(\boldsymbol{\mu}_{\text{max}})$ falls beneath given tolerance ε_{tol} **or** $N = N_{\text{max}}$.

$$\mathcal{W}_{\text{red}} \leftarrow \text{span}\,\{\varphi_n\}_{n=1}^{N}$$

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- Reduced basis methods also work for nonlinear schemes and non-separable operators. ($\Rightarrow$ empirical interpolation)
- A posteriori error estimators with offline/-online decomposition
- More sophisticated reduced basis generation algorithms

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But you got the idea:

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2. Low-dimensional and efficient online computations

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But you got the idea:

1. Usage of existing numerical schemes for basis generation
2. Low-dimensional and efficient online computations

For 1, we want to use DUNE, for 2, we don't.

› Motivation: Comparison of Matlab and Dune

Matlab

+ Easy to learn and use
+ Huge library of mathematical functions (statistical data, postprocessing, plots,...)
- Slow for interpreted code parts
- Memory constraints

Dune

+ Flexible and efficient
+ Provides complex numerical schemes
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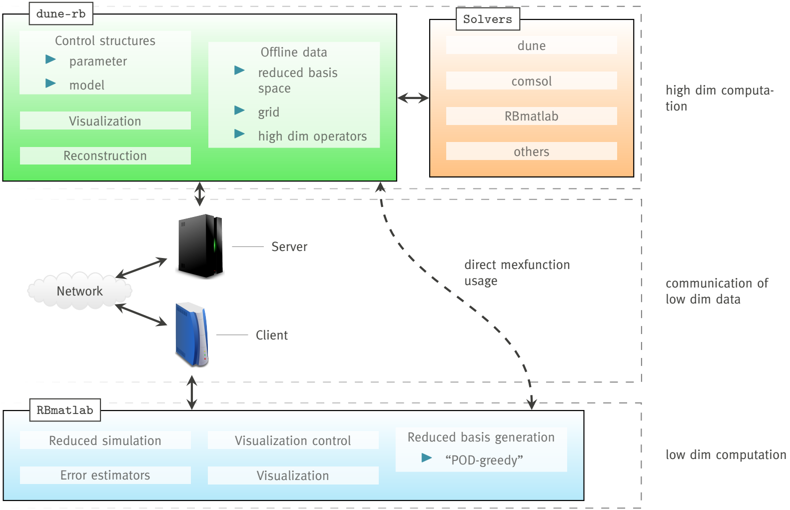
$\Rightarrow$ Separate implementation of offline-/online-phases in RBmatlab and dune-rb, respectively.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Control structures
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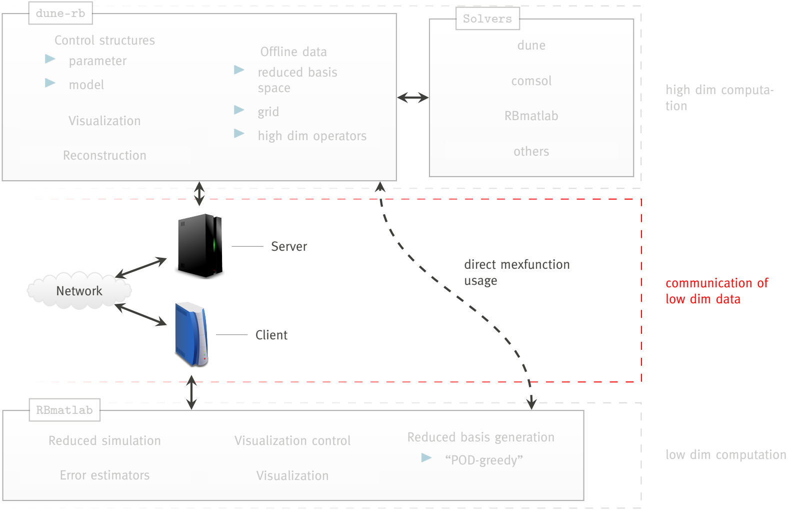
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› Data Structures

Matlab provides a C data structure `mxArray*` that can be used as

- Matrix
- String
- Container-Type (Struct, Cell-Array)

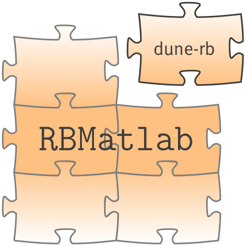
dune-rb provides C++ wrappers

- MXArray (internal data stored as `mxArray*`)
- RBArray (internal data stored as `double*`, `std::string`)

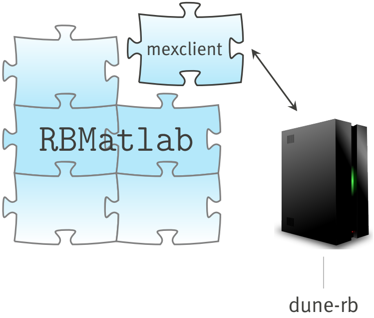
derived from a common interface `SerializedArray`.

› Transmission of Data

Use dune-rb as
Matlab (mex) library



Use dune-rb as
standalone server



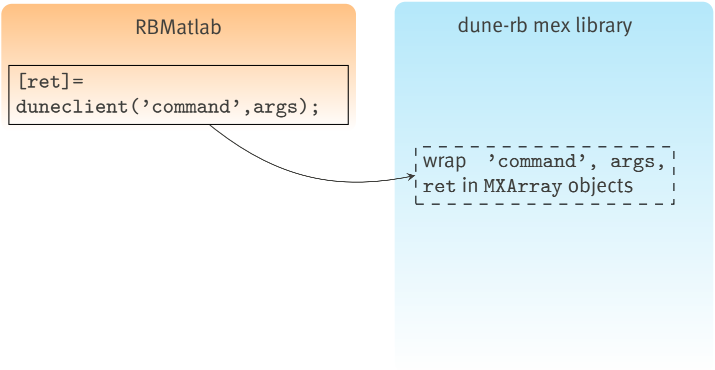
› Communication with mex Library

RBMatlab

```
[ret]=
duneclient('command',args);
```

dune-rb mex library

› Communication with mex Library



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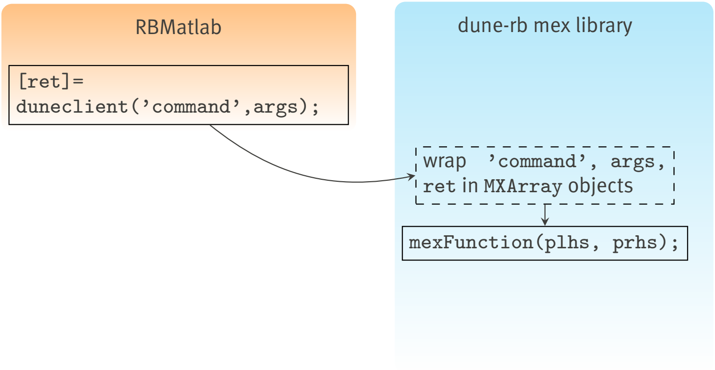

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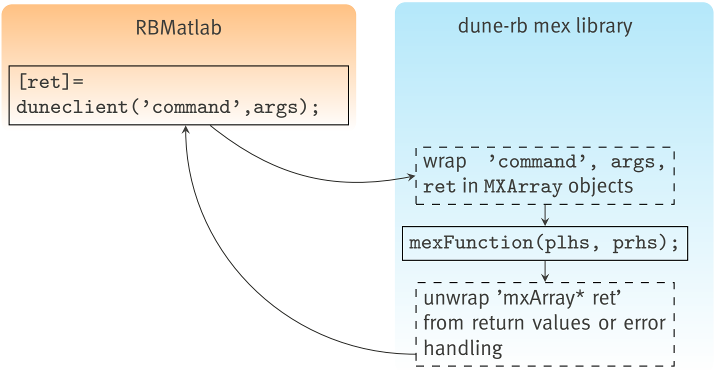

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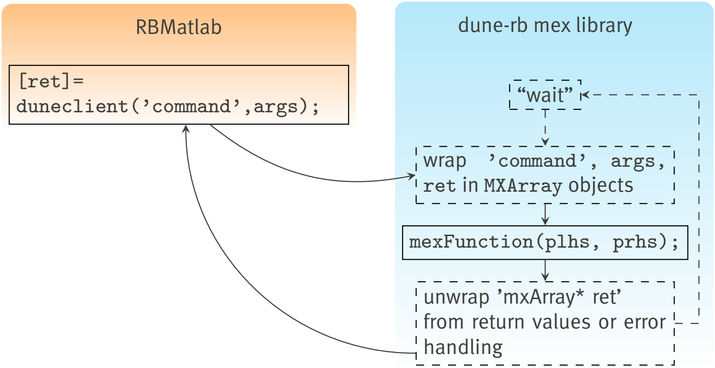


› Communication over TCP/IP

RBMatlab

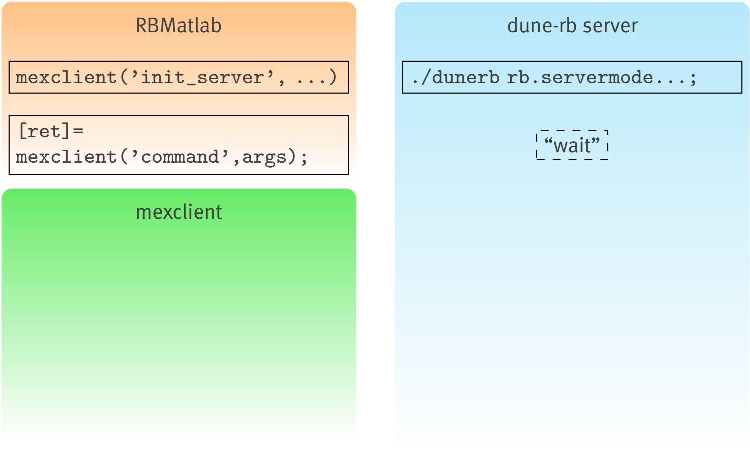
```
mexclient('init_server',
struct('serverhost',
'localhost', 'port', 1234))
```

mexclient

dune-rb server

```
./dunerb rb.servermode:true
rb.port:1234;
```

› Communication over TCP/IP



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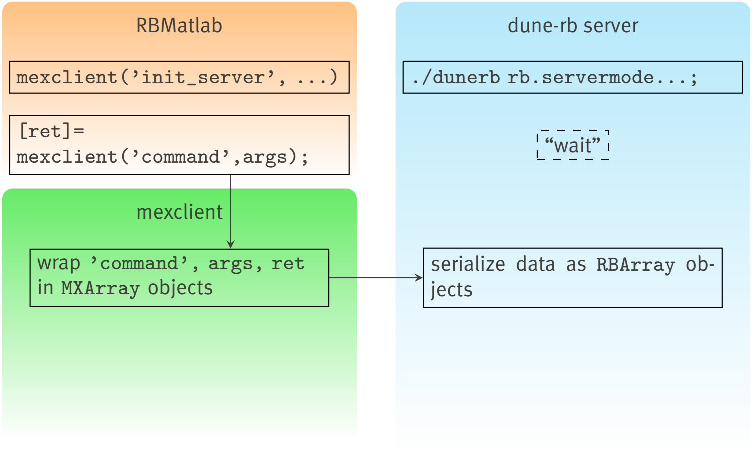

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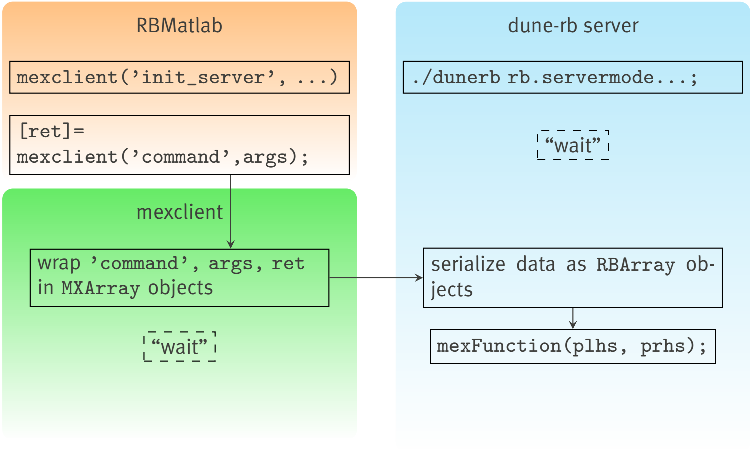

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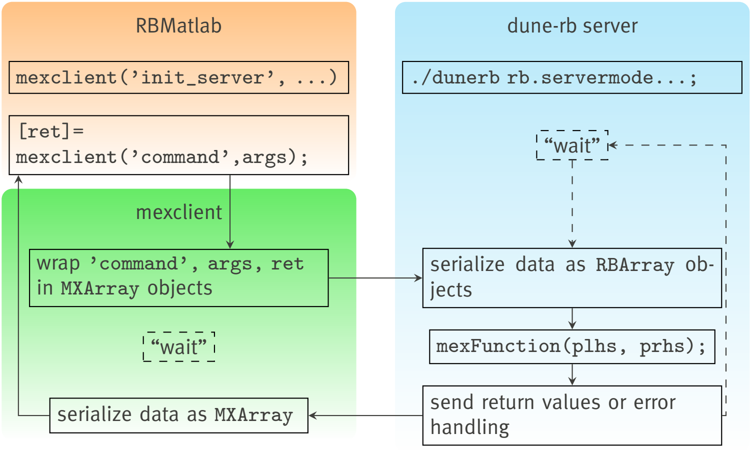

› dune-rb Module

Goals

- Enhance dune-fem operators with parametrization
  - Affine parametrized operators
  - Library of finite volume operators and problems
- Storage and management of reduced bases
  - discrete function lists
  - reduced basis space
- High-dimensional matrix computations
  - PCA
  - Gramian matrix computation
- Reconstruction and visualization of reduced basis solutions.

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Goals

- Enhance dune-fem operators with parametrization
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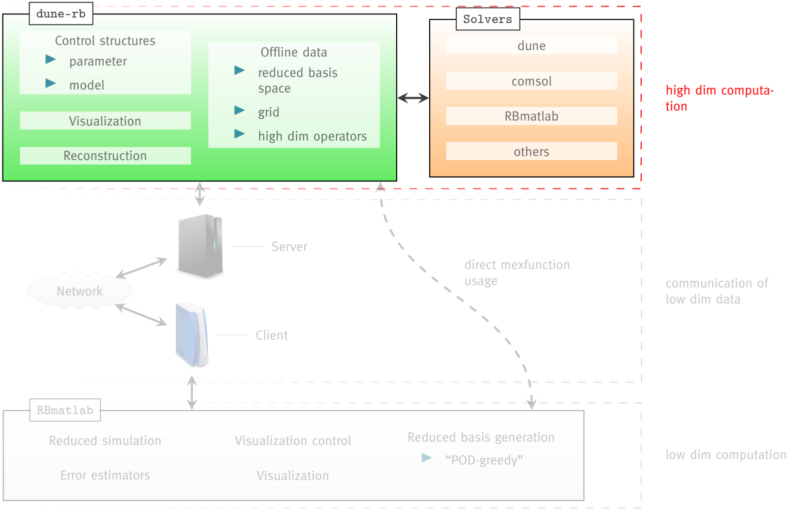
Dependencies

- dune-common, dune-grid
- dune-fem
- LAPACK (for PCA)
- Matlab (for mexclient)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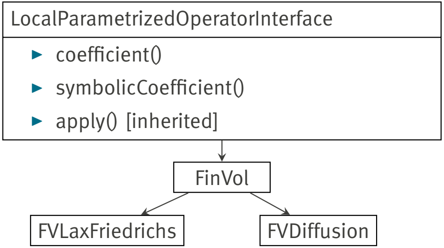
› Separable Discrete Operators

$$\mathcal{L} \quad := \sum_{q=1}^{Q} \sigma_L^q \mathcal{L}^q$$

Implement a class for each summand as instance of `LocalParametrizedOperatorInterface`.



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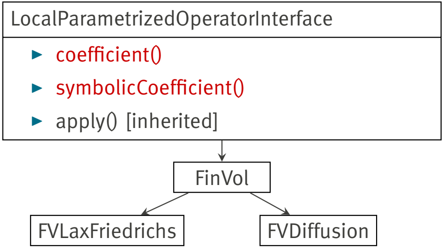

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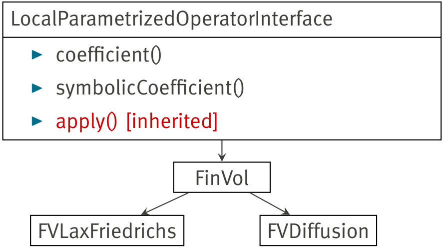

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```
typedef Tuple<LocalParametrizedOperatorImp,...> LPOTuple;
LPOTuple lpoTuple(lpo1,...);
DiscreteDecomposedOperator<LPOTuple,
                           DiscreteFunction, // type of domain
                           DiscreteFunction> // type of range
  ddo(discreteFunctionSpace, lpoTuple);

ddo.coefficients();
ddo.complete();
ddo.component(i);
```

› Reduced Basis Space (by M. Nolte)

- Derived from `DiscreteFunctionSpaceDefault`

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- `baseFunctionSet(const Entity& en)` provides restriction of the base functions to the entity `en`
- Allows manipulation of base functions:
  - `addBaseFunction()`
  - `setBaseFunction()`
- Saves base functions in *discrete function list*

› Discrete Function Lists

- Save/ load list of discrete functions

```
typedef DiscreteFunctionList_xdr<DFType> ListType;
ListType list(discreteFunctionSpace, name);
list.push_back(function); // calls AttributeType()
list.push_back(function, attribute);
list.getFunc(i, destination);
list.getFuncByAttribute(attribute, destination);
```

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- Save/ load list of discrete functions
  - in memory

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- Save attribute (of arbitrary serializable type) for each function

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```

› Discrete Function Lists

- Save/ load list of discrete functions
  - in memory
  - on hard disk
- Save attribute (of arbitrary serializable type) for each function
- Access function by index or attribute

```
typedef DiscreteFunctionList_xdr<DFType> ListType;
ListType list(discreteFunctionSpace, name);
list.push_back(function); // calls AttributeType()
list.push_back(function, attribute);
list.getFunc(i, destination);
list.getFuncByAttribute(attribute, destination);
```

› Gramian Pipeline

- Efficient computation of Gramian-matrices with entries like $G_{ij} = \left(\mathcal{L}\left[\varphi_i\right], \varphi_j\right)$
- few grid iterations
- efficient memory management (optimization of hard disk access)

```
GramianPipeline pipe(DFList&)
OpHandle hId = pipe.getIdentityHandle();
OpHandle hL = pipe.registerDiscreteOperator(ℒ);
pipe.addGramMatrixComputation(hL,hId, G);
... // further computations added
pipe.run();
```

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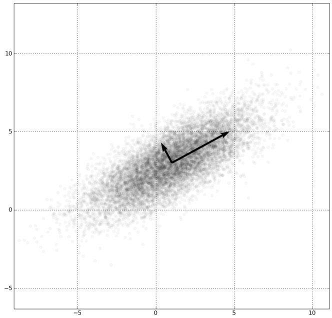
› Principal Component Analysis

- Principal Component Analysis (PCA) of discrete function lists
- Uses `LAPACK::dsyev`
- Usage: `pca(U, pcomps, ratio)`



PCA of a Gaussian Scatter plot, Source: Wikipedia

› Prospects: Empirical Interpolation

The Empirical Interpolation puts arbitrary discrete operators into “separable” form.

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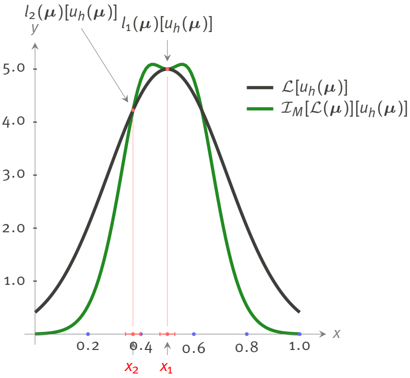
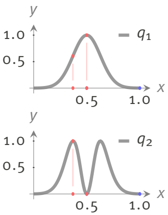


Base functions:



› Prospects: Empirical Interpolation

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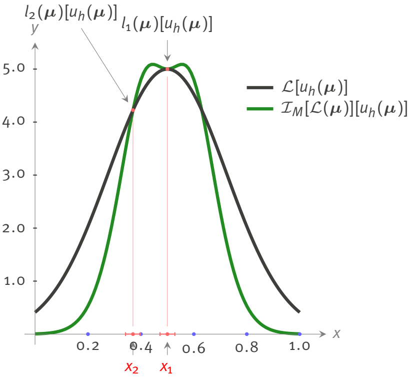
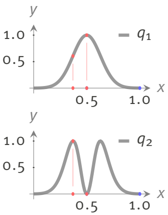
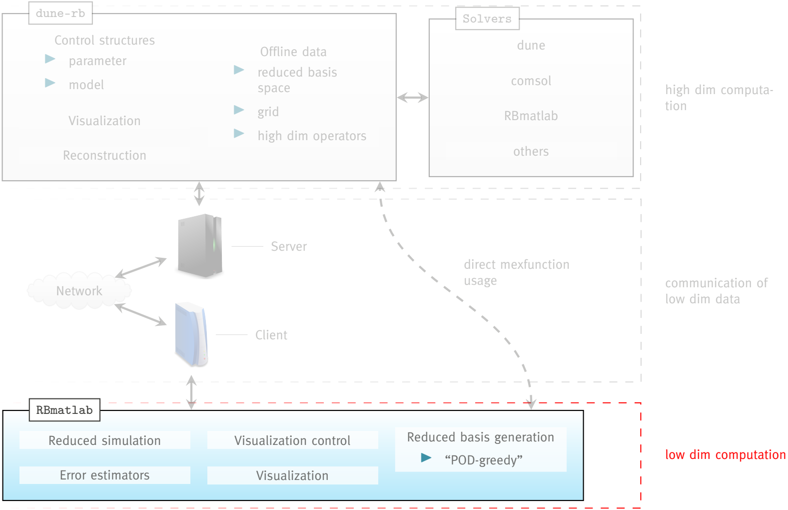




References: [Barrault et al., 2004], [Haasdonk et al., 2008]


dune-rb
Control structures
parameter
model
Visualization
Reconstruction
Offline data
reduced basis space
grid
high dim operators
Solvers
dune
comsol
RBmatlab
others
high dim computation
Server
Network
Client
direct mexfunction usage
communication of low dim data
RBmatlab
Reduced simulation
Visualization control
Reduced basis generation
“POD-greedy”
Error estimators
Visualization
low dim computation

› RBMatlab

```
model_data    = gen_model_data(model)
```
- generate grid

```
detailed_data = gen_detailed_data(model, model_data)
```
- compute high dim simulations
- generate reduced basis space

```
reduced_data  = gen_reduced_data(model, detailed_data)
```
- generate reduced matrices and vectors for reduced simulation and error estimation

Offline

```
sim_data      = rb_simulation(model, reduced_data)
```
- perfom reduced simulation
- evaluate error estimators

Online

› Further Capabilities of RBMatlab

- Different basis generation algorithms

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- Different basis generation algorithms
  - adaptive/fixed training set search in parameter space

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  - adaptive/fixed training set search in parameter space
  - multiple basis generation

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- Visualization

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- Empirical interpolation

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- Different basis generation algorithms
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- Visualization
- Post processing
- Empirical interpolation
- Finite volume discretization of parametrized PDEs

Thank you for your attention!