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MÜNSTER

dune-pyMor

Model Order Reduction with Python and Dune



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- ▶ 0.2 release coming soon!



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- ▶ It's a great language!



Outline

1. The Reduced Basis Method.
2. Design of pyMor and dune-pyMor.
3. dune-pyMor in action.

Reduced Basis Method

in a Nutshell

Discrete Problem

For given parameter $\mu \in \mathcal{P}$, find $u_{\mu,h} \in V_h$ satisfying

$$\sum_{k=1}^K \theta_k(\mu) B_k(u_{\mu,h}, v_h) = F(v_h) \quad \forall v_h \in V_h. \quad (*)$$

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 - ▶ compute snapshots $\mathcal{S} := \{u_{\mu_s,h} \mid s = 1, \dots, S\}$
 - ▶ determine $V_N \subseteq \text{span}(\mathcal{S})$ with $N = \dim V_N \ll \dim V_h$.

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- ▶ Let b_1, \dots, b_N be a basis of V_N and define

$$\underline{B}_k = [B_k(b_j, b_i)]_{i,j=1}^N \quad \underline{F} = [F(b_i)]_{i=1}^N.$$

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- ▶ In coordinates, $(**)$ becomes

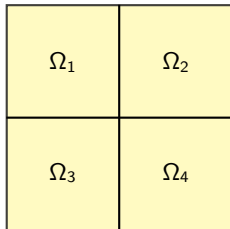
$$\sum_{k=1}^K \theta(\mu) \underline{B}_k \cdot \underline{u}_{\mu,N} = \underline{F}$$

with reconstruction equation

$$u_{\mu,N} = \sum_{i=1}^N b_i \cdot \underline{u}_{\mu,N,i}.$$

Reduced Basis Method

Example



$$\Omega = \bigcup_{k=1}^4 \Omega_k, \mathcal{P} = [\alpha, 1]^4, \alpha > 0$$

$$a_\mu(x) = \sum_{k=1}^4 \mu_k \cdot \chi_{\Omega_k}(x), \quad x \in \Omega, \mu \in \mathcal{P}$$

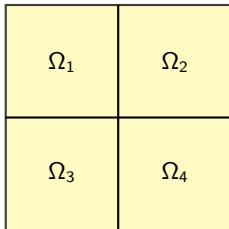
Thermal-Block Problem

For $f \in L^2(\Omega)$ and $\mu \in \mathcal{P}$, find $u_\mu \in H_0^1(\Omega)$ s.t.

$$-\nabla \cdot (a_\mu \nabla u_\mu) = f$$

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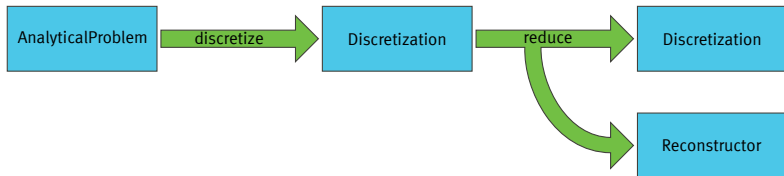
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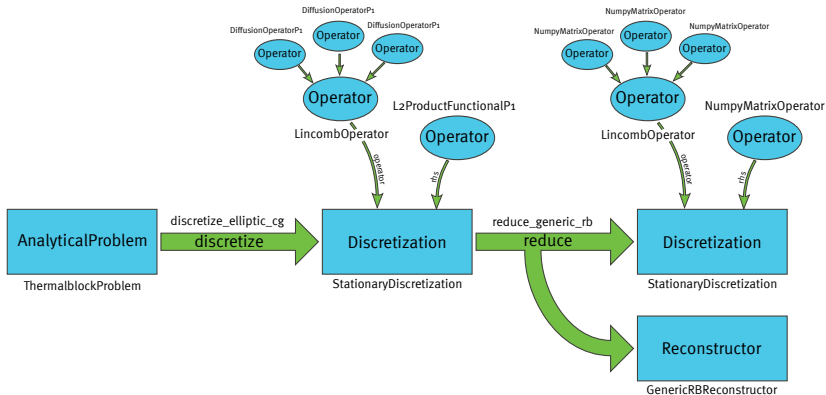
Architecture of pyMor

Workflow



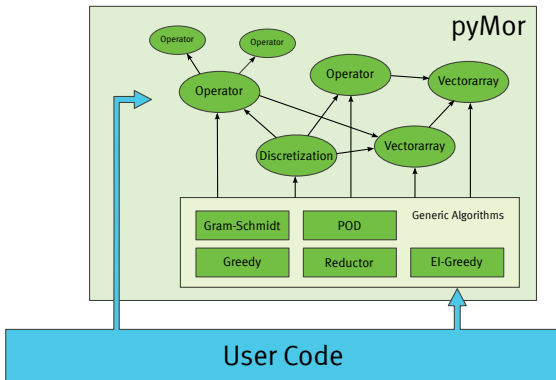
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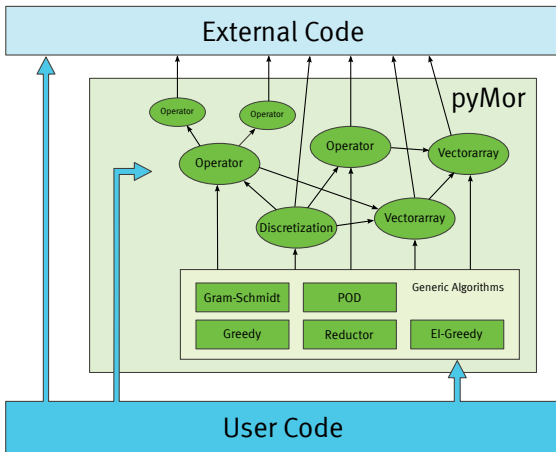
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Interfaces



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Accessing External Code from pyMor

as a Python Extension Module



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Accessing External Code from pyMor

as a Python Extension Module

- ▶ Implement Operators, VectorArrays, Discretizations.
- ▶ Create Python module (e.g. using PyBindGen).
- ▶ Write Python wrapper classes implementing the full pyMor interfaces.



DUNE-Bindings with dune-pyMor



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 - ▶ `Dune::DynamicMatrix` and `Eigen` based operators already provided.
 - ▶ Bindings for LA backend of PDELab in development.

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- ▶ Utilize provided helper methods (`inject_operator, ...`) and build system to semi-automatically create Python module.

DUNE-Bindings with dune-pyMor

- ▶ Implement Operators, Vectors, Discretizations by deriving from the corresponding `dune-pyMor` interface classes.
 - ▶ `Dune::DynamicMatrix` and `Eigen` based operators already provided.
 - ▶ Bindings for LA backend of PDELab in development.
- ▶ Utilize provided helper methods (`inject_operator, ...`) and build system to semi-automatically create Python module.
- ▶ In `pyMor`, simply call `dune.pyMor.core.wrap_module` to obtain wrappers for all implemented DUNE classes.



Live Demo



Thank you for your attention!

pyMor – Model Order Reduction with Python

<https://github.com/pyMor>

dune-pyMor demo application

<https://github.com/pyMor/dune-hdd-demos>

Interfaces

VectorArrays

```
1 class VectorArrayInterface(BasicInterface):
2     # array creation
3     @classmethod
4     def empty(cls, dim, reserve=0): pass
5     @classmethod
6     def zeros(cls, dim, count=1): pass
7
8     # comparing arrays
9     def __len__(self): pass
10    @property
11    def dim(self): pass
12    def almost_equal(self, other, ind, o_ind, rtol, atol): pass
13
14    # array manipulation
15    def copy(self, ind): pass
16    def append(self, other, o_ind, remove_from_other=False): pass
17    def remove(self, ind): pass
18    def replace(self, other, ind, o_ind, remove_from_other=False): pass
19    # ...
```



Interfaces

VectorArrays

```
1  #class VectorArrayInterface (continued)
2      # linear algebra
3      def scal(self, alpha, ind): pass
4      def axpy(self, alpha, x, ind, x_ind): pass
5      def dot(self, other, pairwise, ind, o_ind): pass
6      def lincomb(self, coefficients, ind): pass
7      def l2_norm(self, ind): pass
8
9      # empirical interpolation
10     def components(self, component_indices, ind): pass
11     def amax(self, ind): pass
```

Interfaces

Operators

```
1 class OperatorInterface(ImmutableInterface, Parametric, Named):
2     dim_source = None
3     dim_range = None
4     type_source = None
5     type_range = None
6     linear = False
7     invert_options = None
8
9     def apply(self, U, ind, mu): pass
10    def apply2(self, V, U, U_ind, V_ind, mu, product, pairwise): pass
11    def apply_inverse(self, U, ind, mu, options): pass
12
13    @staticmethod
14    def lincomb(operators, coefficients, ...): pass
```

Interfaces

RB-Projection in pyMor (more or less)

$$\sum_{k=1}^K \theta_k(\mu) B_k(u_{\mu,N}, v_N) = F(v_N) \quad \forall v_N \in V_N.$$

```
1 def reduce_generic_rb(discretization, RB):
2     projected_ops = {k: rb_project_operator(op, RB)
3                       for k, op in discretization.operators.items()}
4     rd = discretization.with_(operators=projected_operators)
5     rc = GenericRBReconstructor(RB)
6     return rd, rc
7
8 def rb_project_operator(op, RB):
9     source_basis = RB
10    range_basis = RB if op.dim_range == op.dim_source else None
11    return op.projected(source_basis, range_basis)
12
13 class LincombOperatorBase(OperatorBase, LincombOperatorInterface):
14     def projected(self, source_basis, range_basis):
15         proj_ops = [op.projected(source_basis, range_basis)
16                     for op in self.operators]
17         return proj_ops[0].lincomb(proj_operators, self.coefficients)
```

Interfaces

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$$\sum_{k=1}^K \theta_k(\mu) B_k(u_{\mu,N}, v_N) = F(v_N) \quad \forall v_N \in V_N.$$

```
1 class OperatorBase(OperatorInterface):
2     def projected(self, source_basis, range_basis):
3         assert self.linear and not self.parametric
4         mat = self.apply2(source_basis, range_basis, pairwise=False)
5         return NumpyMatrixOperator(mat)
6
7 class GenericRBReconstructor(ImmutableInterface):
8     def __init__(self, RB):
9         self.RB = RB
10
11     def reconstruct(self, U):
12         assert isinstance(U, NumpyVectorArray)
13         return self.RB.lincomb(U.data)
```