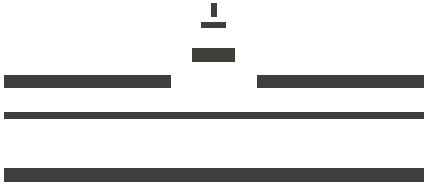

Westfälische
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Model Order Reduction with Python

Linus Balicki, René Fritze, Petar Mlinarić, Stephan Rave, Felix Schindler

Outline

- What is Model Order Reduction?
- The design philosophy behind pyMOR.
- Some things you can do with pyMOR.

pyMOR main developers


Linus Balicki


René Fritze


Petar Mlinarić


Stephan Rave


Felix Schindler

What is Model Order Reduction?

System-Theoretic Model Order Reduction

Linear time invariant system (full order model)

Input $u(t) \in \mathbb{R}^m$ to state $x(t) \in \mathbb{R}^n$ to output $y(t) \in \mathbb{R}^p$ mapping is given by

$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t).$$

System-Theoretic Model Order Reduction

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$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t).$$

Model Reduction Magic

Compute 'good' $W,\ V \in \mathbb{R}^{n \times r},\ r \ll n, \qquad s.t. \qquad W^T V = I$

Linear time invariant system (reduced order model)

Input $u(t) \in \mathbb{R}^m$ to state $x(t) \in \mathbb{R}^r$ to output $y(t) \in \mathbb{R}^p$ mapping is given by

$$\dot{x}(t) = (W^T AV)\, x(t) + (W^T B)\, u(t)$$
$$y(t) = (CV)\, x(t).$$

System-Theoretic MOR – Computing V and W

Balanced Truncation

- Compute reachability Gramian $\mathcal{P}$ and observability Gramian $\mathcal{Q}$ subject to

$$A\mathcal{P} + \mathcal{P}A^T + BB^T = 0$$
$$A^T\mathcal{Q} + \mathcal{Q}A + C^TC = 0.$$

- Simultaneously diagonalize $\mathcal{P}$ and $\mathcal{Q}$.
- Select V, W by truncating states which are both hard to reach and hard to observe.

System-Theoretic MOR – Computing V and W

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- Select V, W by truncating states which are both hard to reach and hard to observe.

Rational interpolation

- Construct V, W, s.t. the transfer function (Laplace transform of impulse response)

$$H(s) = C(sI - A)^{-1}B$$

  is interpolated (including higher moments) at points $s_1, \ldots, s_k$ by a rational function.
- Methods: Moment matching, Padé approximation, IRKA, ...
- Computed using rational Krylov methods.

Reduced Basis Methods

Parametric linear parabolic problem (full order model)

For given parameter $\mu \in \mathcal{P}$, find $u_\mu(t) \in V_h$ s.t.

$$\begin{aligned} u_\mu(0) &= u_0 \\ \langle v, \partial_t u_\mu(t) \rangle + b_\mu(v, u_\mu(t)) &= f(v) \qquad \forall v \in V_h, \\ y_\mu(t) &= g(u_\mu(t)). \end{aligned}$$

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Parametric linear parabolic problem (reduced order model)

For given $V_N \subset V_h$, let $u_{\mu,N}(t) \in V_N$ be given by Galerkin proj. onto V_N, i.e.

$$\begin{aligned} u_{\mu,N}(0) &= P_{V_N}(u_0), \\ \langle v, \partial_t u_{\mu(t),N} \rangle + b_\mu(v, u_{\mu(t),N}) &= f(v) \qquad \forall v \in V_N, \\ y_{\mu,N}(t) &= g(u_{\mu,N}(t)), \end{aligned}$$

where $P_{V_N} : V_h \to V_N$ is orthogonal proj. onto V_N.

RB Methods – Computing V_N

Weak greedy basis generation

function WEAK-GREEDY($\mathcal{S}_{train} \subset \mathcal{P}$, ε)
  $V_N \leftarrow \{0\}$
  while $\max_{\mu \in \mathcal{S}_{train}}$ ERR-EST(ROM-SOLVE(μ), μ) $> \varepsilon$ **do**
    $\mu^* \leftarrow$ arg-$\max_{\mu \in \mathcal{S}_{train}}$ ERR-EST(ROM-SOLVE(μ), μ)
    $V_N \leftarrow$ BASIS-EXT(V_N, FOM-SOLVE(μ^*))
  end while
  return V_N
end function

BASIS-EXT

1. Compute $u^{\perp}_{\mu^*}(t) = (I - P_{V_N})u_{\mu^*}(t)$.
2. Add POD($u^{\perp}_{\mu^*}(t)$) to V_N (leading left-singular vectors of snapshot matrix).

ERR-EST

Use residual-based error estimate w.r.t. FOM (finite dimensional $\rightsquigarrow$ can compute dual norms).

RB Methods – Online Efficiency

Parametric linear parabolic problem (reduced order model)

$$
\begin{aligned}
u_{\mu,N}(0) &= P_{V_N}(u_0), \\
\langle v, \partial_t u_{\mu(t),N} \rangle + b_\mu(v, u_{\mu(t),N}) &= f(v) \qquad \forall v \in V_N, \\
y_{\mu,N}(t) &= g(u_{\mu,N}(t)),
\end{aligned}
$$

Parameter separability

Assume that b_μ can be written as

$$
b_\mu(v, u) = \sum_{q=1}^{Q} \theta_q(\mu) b_q(v, u).
$$

RB Methods – Online Efficiency

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$$

Offline/online splitting

By pre-computing

$$
\langle \varphi_i, \varphi_j \rangle, \; b_q(\varphi_i, \varphi_j), \; f(\varphi_i), \; g(\varphi_i)
$$

for a reduced basis $\varphi_1, \ldots, \varphi_N$ of V_N, solving ROM becomes independent of dim V_h.

RB Methods – Nonlinear Problems

Parametric nonlinear parabolic problem (full order model)

$$
\begin{aligned}
u_\mu(0) &= u_0, \\
\langle v, \partial_t u_\mu(t) \rangle + \langle v, \mathcal{A}_\mu(u_\mu(t)) \rangle &= f(v) \qquad \forall v \in V_h, \\
y_\mu(t) &= g(u_\mu(t)),
\end{aligned}
$$

where $\mathcal{A}_\mu : V_h \to V_h^*$ is a nonlinear operator.

RB Methods – Nonlinear Problems

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RB Methods – Nonlinear Problems

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Problem: No offline/online splitting of nonlinear

$$\mathcal{A}_\mu : V_N \longrightarrow V_h^* \longrightarrow {V_N}^*.$$

Same problem for non-affinely decomposed b_μ.

RB Methods – Empirical Interpolation

EI – abstract version

Let normed Space V, functionals $\Psi \subseteq V^*$ and training set $\mathcal{M} \subset V$ be given.
Construct via EI-GREEDY algorithm:

1. Interpolation basis $b_1, \dots b_M \in \operatorname{span} \mathcal{M}$,
2. Interpolation functionals $\psi_1, \dots, \psi_M \in \Psi$.

The empirical interpolant $\mathcal{I}_M(v)$ of an arbitrary $v \in V$ is then determined by

$$\mathcal{I}_M(v) \in \operatorname{span}\{b_1, \dots, b_M\} \quad \text{and} \quad \psi_m(\mathcal{I}_M(v)) = \psi_m(v) \quad 1 \leq m \leq M.$$

EI Cheat Sheet

	V	Ψ	online
function EI	function space	point evaluations	evaluation at 'magic points'
DEIM	range of (discrete) operator	DOFs	local evaluation at selected DOFs
matrix DEIM	matrices of given shape	matrix entries	assembly of selected entries

RB Methods – Hyper-Reduction

Reduced Order Model (with EI)

Find $u_{\mu,N} \in V_N$ s.t.

$$\langle v, \partial_t u_{\mu,N}(t) \rangle + \langle v, \{ I_M \circ \mathcal{A}_{M,\mu} \circ R_{M'} \}(u_{\mu,N}(t)) \rangle = f(v) \quad \forall v \in V_N,$$

where

$R_{M'}\colon V_h \to \mathbb{R}^{M'}$	restriction to M' DOFs needed for local evaluation
$\mathcal{A}_{M,\mu}\colon \mathbb{R}^{M'} \to \mathbb{R}^{M}$	local evaluation of $\mathcal{A}_\mu$ at M interpolation DOFs
$I_M\colon \mathbb{R}^{M} \to V_h^*$	linear interpolation operator

Offline/Online splitting

- Pre-compute the linear operators $\langle \cdot, I_M(\cdot) \rangle$ and $R_{M'}$ w.r.t. basis of V_N.
- Effort to evaluate $\langle \cdot, I_M \circ \mathcal{A}_{M,\mu} \circ R_{M'}(\cdot) \rangle$ w.r.t. this basis:

$$\mathcal{O}(MN) + \mathcal{O}(M) + \mathcal{O}(MN).$$

MULTIBAT: RB Approximation of Li-Ion Battery Models

ulm university universität ulm

DLR Institute of Technical Thermodynamics

MULTIBAT

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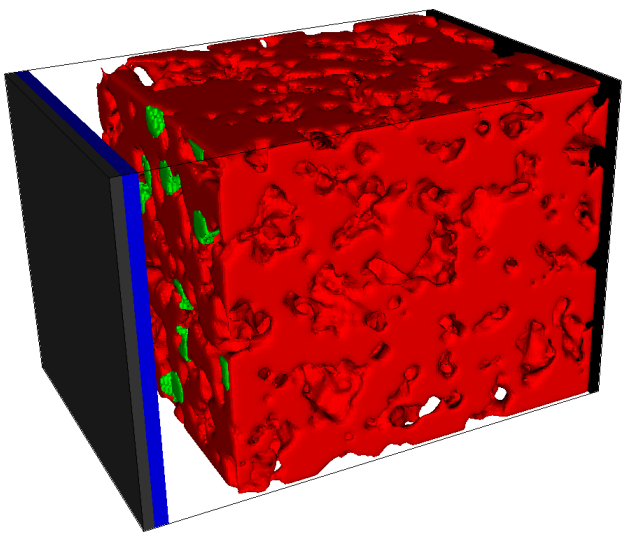
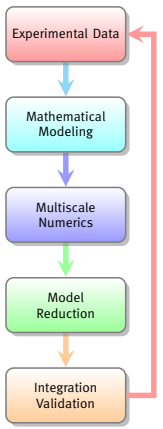




MULTIBAT: Gain understanding of degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.

- Focus: Li-Plating.
- Li-plating initiated at interface between active particles and electrolyte.
- Need microscale models which resolve active particle geometry.
- Very large nonlinear discrete models.

MULTIBAT: Numerical Results

Model:

- Half-cell with plated Li
- $\mu =$ discharge current
- 2.920.000 DOFs

Reduction:

- Snapshots: 3
- $N = 178 + 67$
- $M = 924 + 997$
- Rel. err.: $< 4.5 \cdot 10^{-3}$

Timings:

- Full model: $\approx$ 15.5h
- Projection: $\approx$ 14h
- Red. model: $\approx$ 8m
- Speedup: **120**

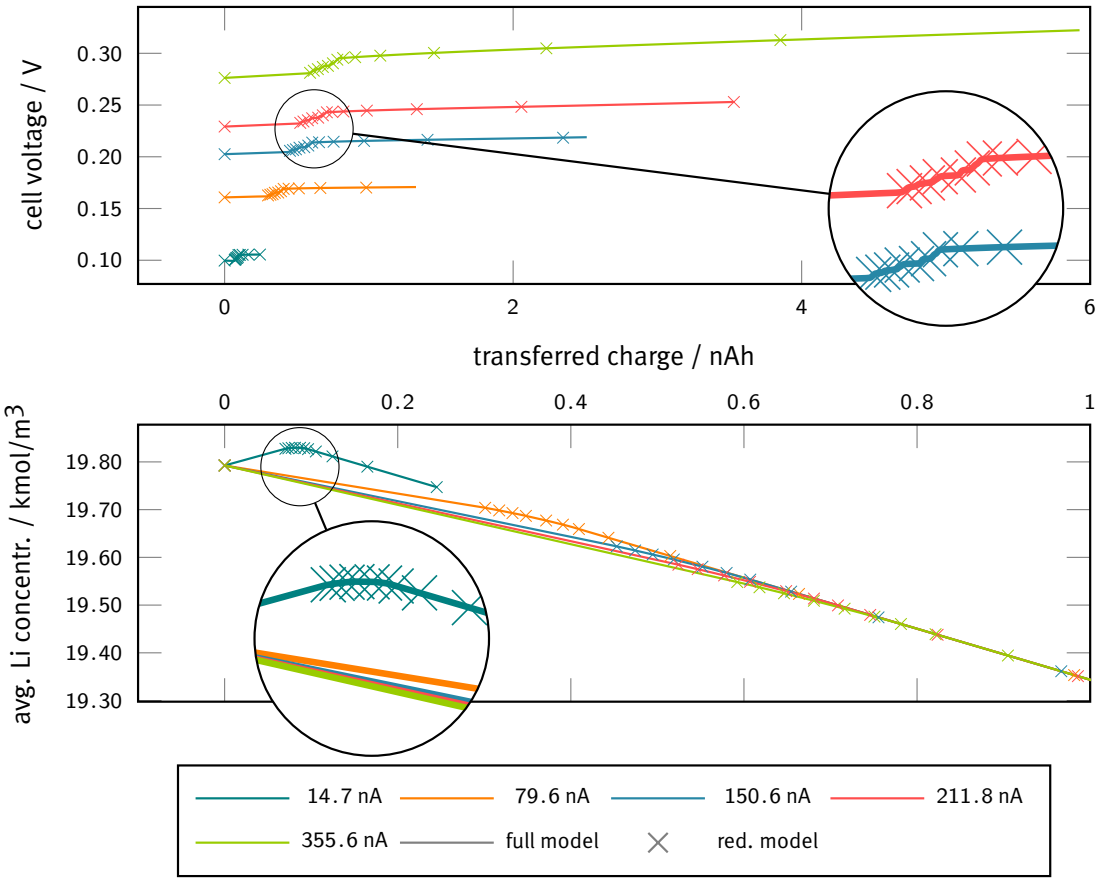


Figure: Validation of reduced order model output for random discharge currents; solid lines: full order model, markers: reduced order model.

The design philosophy behind pyMOR

RB Software Designs

Design 1: write data needed for reduction to disk (e.g. `rbMIT`)

Handle reduction and reduced solving by dedicated MOR code. Read all needed data from disk after run of PDE solver in special MOR output mode.

Design 2: add MOR mode to PDE solver (e.g. `libMesh`)

Add all MOR code needed directly to the PDE solver. Optionally, implement specialized MOR version of solver to run on small devices.

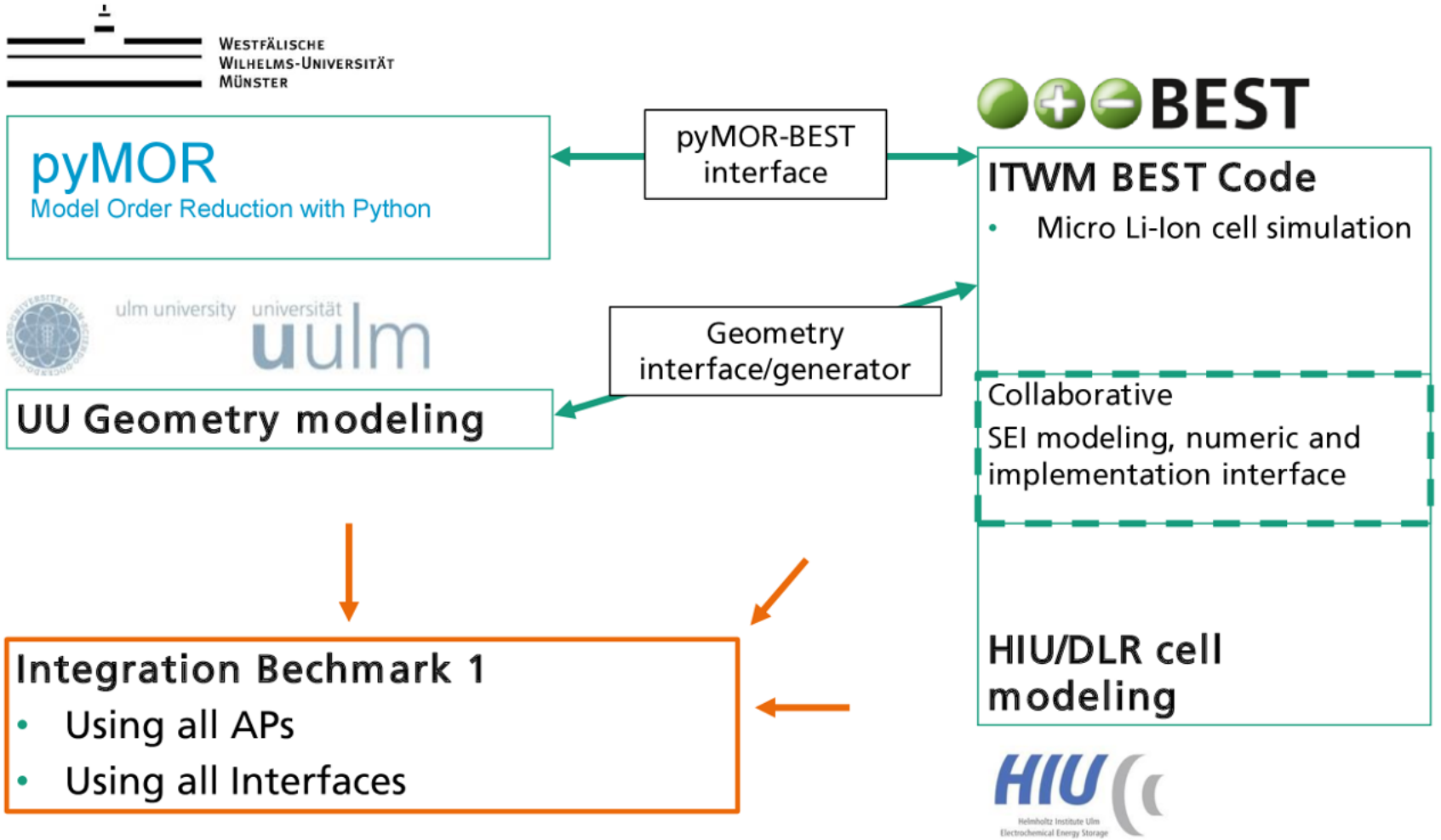
Design 3: communicate only reduced data (e.g. `RBmatlab + dune-rb`)

Write MOR code which communicates with running PDE solver. MOR code can, e.g., instruct solver to enrich basis with snapshot for certain μ and to compute data for reduced model.

RB Software Design Comparison

	via disk	in solver	low-dim
large (e.g. matrix-free) problems			
empirical interpolation			
reusability w. new solver			
reusability w. new MOR alg.			
MOR alg. easy to implement			
easy to maintain			
MOR and solver dev. decoupled			

Software Interfaces in MULTIBAT



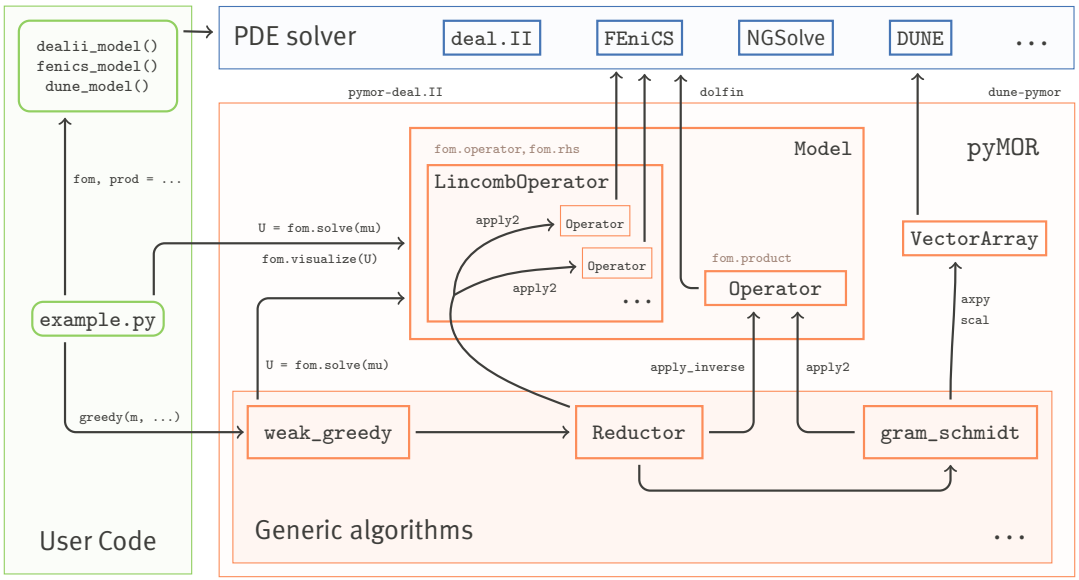
pyMOR – Model Order Reduction with Python

Goal

One library for algorithm development *and* large-scale applications.

- Started late 2012, 20k lines of Python code, 6k single commits.
- BSD-licensed, fork us on GitHub!
- Quick prototyping with Python 3.
- Comes with small `NumPy`/`SciPy`-based discretization toolkit for getting started quickly.
- Seamless integration with high-performance PDE solvers.

Generic Algorithms and Interfaces for MOR



- `VectorArray`, `Operator`, `Model` classes represent objects in solver's memory.
- No communication of high-dimensional data.
- Tight, low-level integration with external solver.
- No MOR-specific code in solver.

Implemented Algorithms

- Gram-Schmidt, POD, HAPOD.
- Greedy basis generation with different extension algorithms.
- Automatic (Petrov-)Galerkin projection of arbitrarily nested affine combinations of operators.
- Interpolation of arbitrary (nonlinear) operators, EI-Greedy, DEIM.
- A posteriori error estimation.
- System theory methods: balanced truncation, IRKA, ...
- Iterative linear solvers, eigenvalue computation, Newton algorithm, time-stepping algorithms.
- New! Non-intrusive MOR using artificial neural networks.

RB Software Design Comparison

	via disk	in solver	low-dim	pyMOR
large (e.g. matrix-free) problems				
empirical interpolation				
reusability w. new solver				
reusability w. new MOR alg.				
MOR alg. easy to implement				
easy to maintain				
MOR and solver dev. decoupled				

RB Software Design Comparison

	via disk	in solver	low-dim	pyMOR
large (e.g. matrix-free) problems	☹	☺	☺	☺
empirical interpolation	☹	☺	😐	☺
reusability w. new solver	☺	☹	😐	☺
reusability w. new MOR alg.	☺	☺	😐	☺
MOR alg. easy to implement	☺	😐	☹	😐
easy to maintain	☺	😐	☹	☺
MOR and solver dev. decoupled	☺	☹	☹	☺

Some things you can do with pyMOR

FEniCS Support

- Directly interfaces FEniCS
  LA backend, no copies needed.
- Use same MOR code as with builtin
  discretization toolkit!
- Builtin support for empirical
  interpolation.
- Thermal block demo:
  30 SLOC FEniCS +
  15 SLOC wrapping for pyMOR.
- Easily increase FEM order, etc.

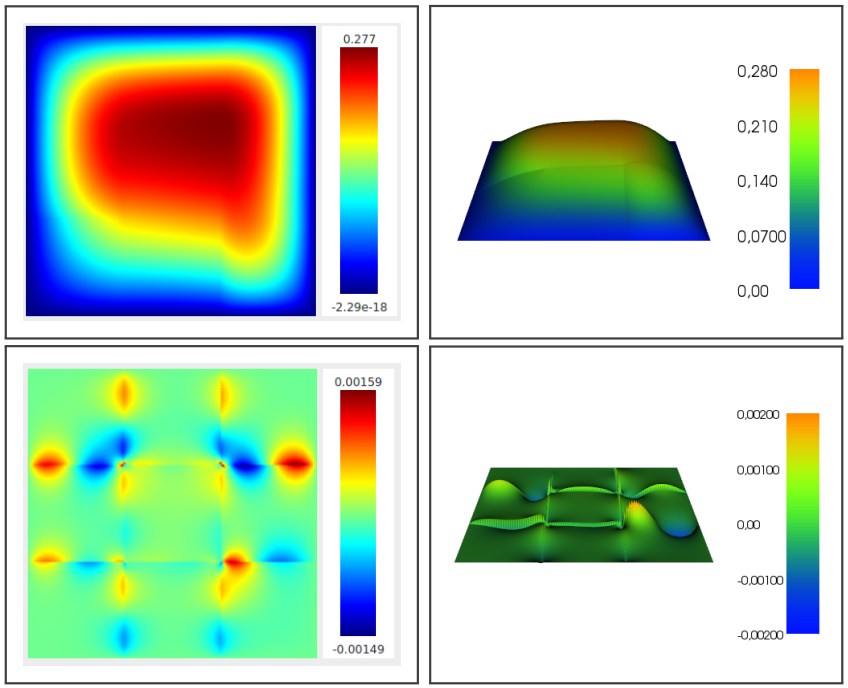


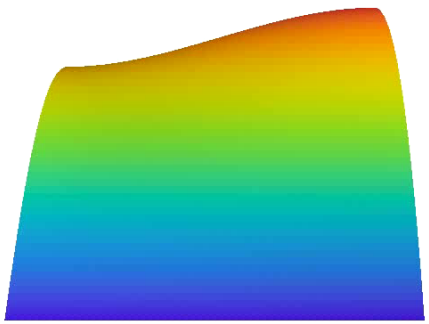
Figure: 3x3 thermal block problem
top: red. solution, bottom: red. error
left: pyMOR solver, right: FEniCS solver

Empirical Interpolation with FEniCS

Nonlinear Poisson problem from FEniCS docs (for $\mu = 1$)

$$
\begin{aligned}
-\nabla \cdot \left\{ (1 + \mu u^2(x, y)) \cdot \nabla u(x, y) \right\} &= x \cdot \sin(y) && \text{for } x, y \in (0, 1) \\
u(x, y) &= 1 && \text{for } x = 1 \\
\nabla u(x, y) \cdot n &= 0 && \text{otherwise}
\end{aligned}
$$

- `mesh = UnitSquareMesh(100, 100); V = FunctionSpace(mesh, "CG", 2).`
- Time for solution: ≈ 3.4 s.
- $\mu \in [1, 1000]$, RB size: 2, EI DOFs: 5, rel. error $\approx 10^{-6}$.



- Local operator evaluation implemented using `dolfin.SubMesh`.
- Speedup: 80.
- See `fenics_nonlinear` demo.

deal.II Support

- `pymor-deall.II` support module

  `https://github.com/pymor/pymor-deal.II`

- Python bindings for
  - `dealii::Vector`,
  - `dealii::SparseMatrix`.
- pyMOR wrapper classes.
- MOR demo for linear elasticity example from tutorial.

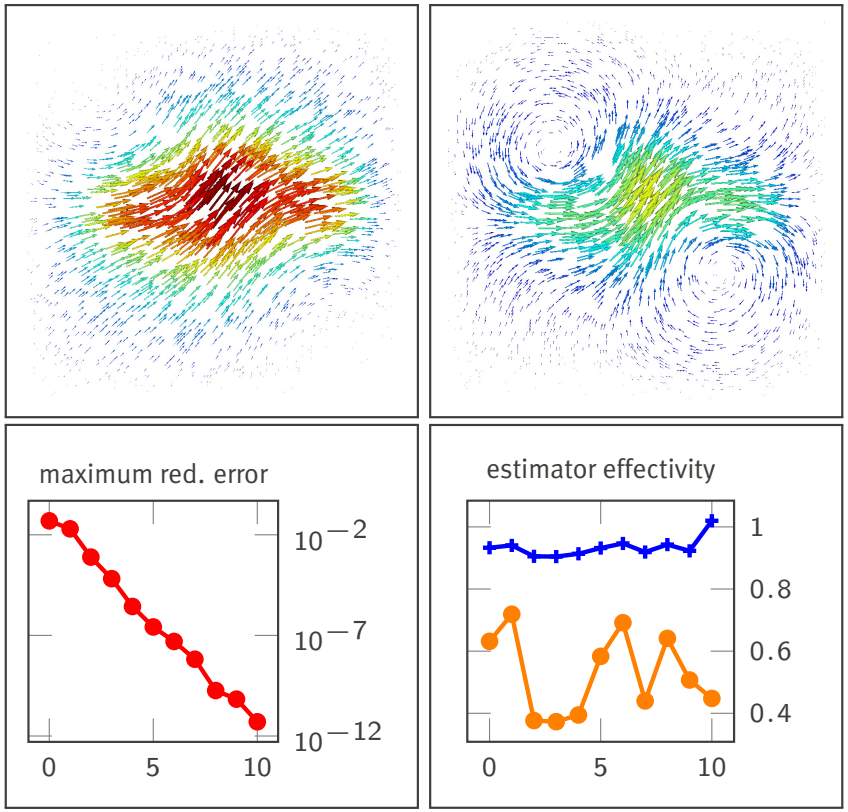


Figure: top: Solutions for $(\mu, \lambda) = (1, 1)$ and $(\mu, \lambda) = (1, 10)$, bottom: red. errs. and max./min. estimator effectivities vs. dim V_N.

NGSolve Support

- Based on `NGS-Py` Python bindings for NGSolve.
- pyMOR wrappers for vector and matrix classes.
- 3d thermal block demo included.
- Joint work with
  Christoph Lehrenfeld.

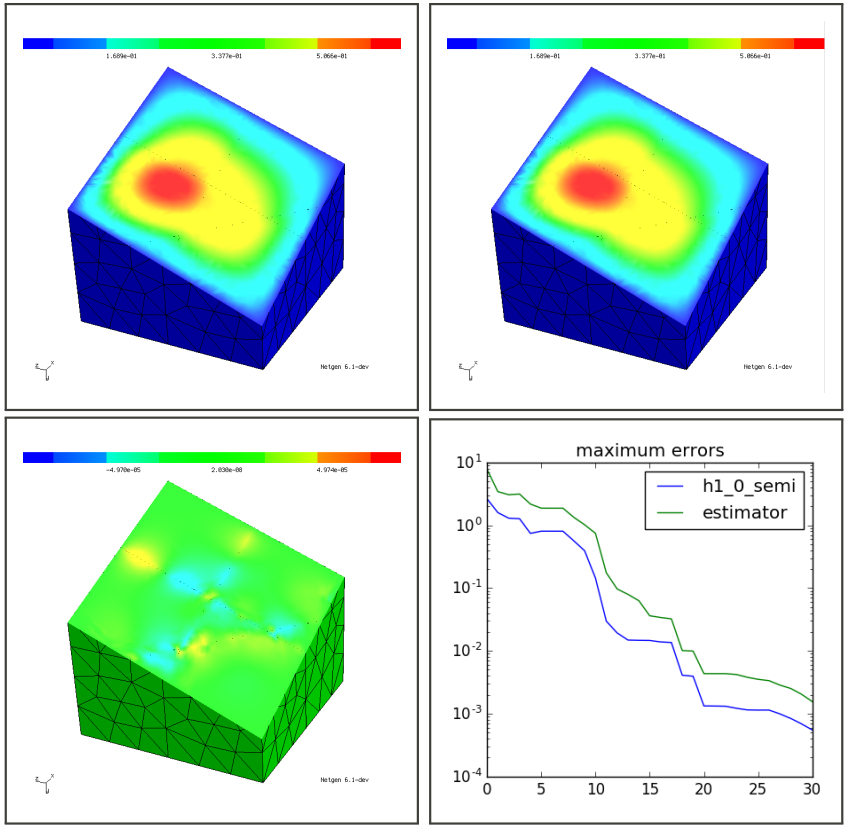


Figure: 3d thermal block problem
top: full/red. sol., bottom: err. for worst approx. μ and max. red. error vs. dim V_N.

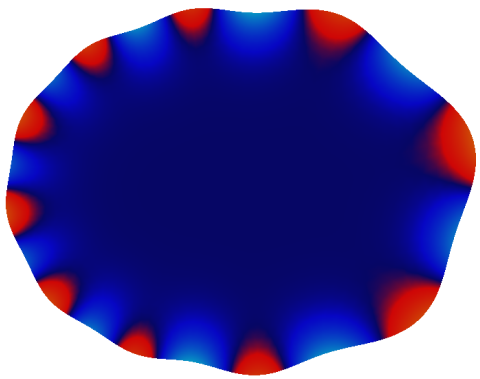
MOR for an NGSolve Free Boundary Problem

[Lehrenfeld, R, 19]

Osmotic cell swelling model [Lippoth, Prokert, 2012]

Given $\Omega(0) \subset \mathbb{R}^d$, $u(0) \in H^1(\Omega(0))$ and coefficients $u_{\text{ext}}, \alpha, \beta, \gamma \in \mathbb{R}$, the **concentration** $u(t)$ and **normal velocity** w_Γ of $\Gamma(t)$ is given by:

$$\begin{aligned} \partial_t u - \alpha \Delta u &= 0 && \text{in } \Omega(t), \\ w_\Gamma u + \alpha \partial_{\mathbf{n}} u &= 0 && \text{on } \Gamma(t), \\ -\beta\kappa + \gamma(u - u_{\text{ext}}) &= w_\Gamma && \text{on } \Gamma(t). \end{aligned}$$



- ALE formulation $\rightarrow$ diffusion coeffs nonlinear in deformation field Ψ
- Empirical interpolation w.r.t. Ψ.

Tools for interfacing MPI parallel solvers

- Automatically make sequential bindings MPI aware.
- Reduce HPC-Cluster models without thinking about MPI at all.
- Interactively debug MPI parallel solvers.

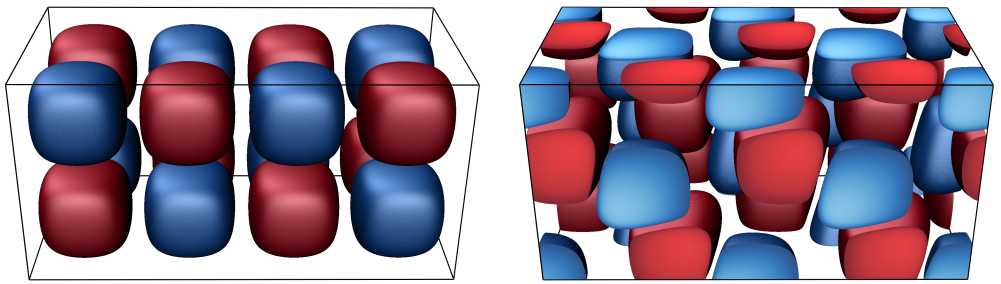


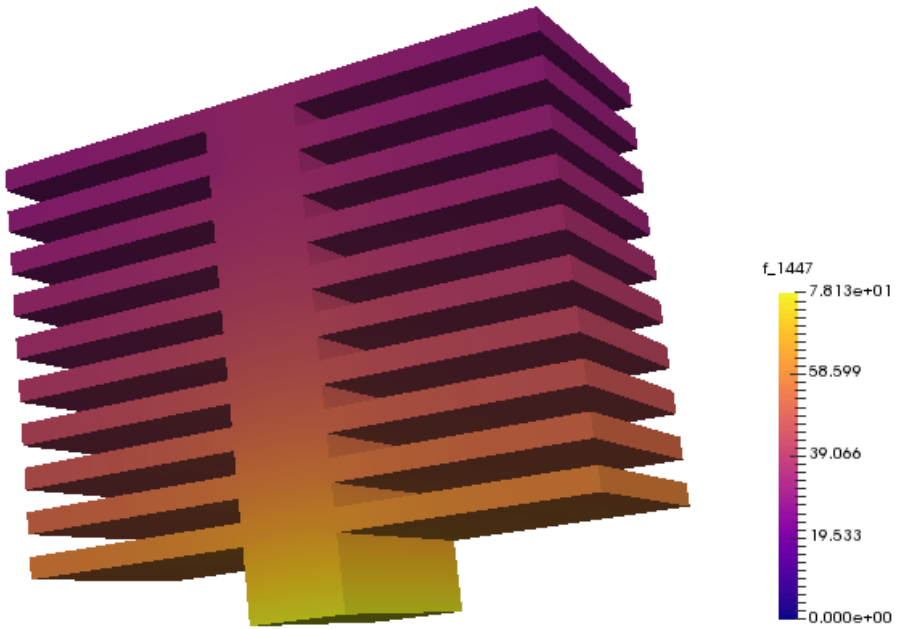
Figure: FV solution of 3D Burgers-type equation ($27.6 \cdot 10^6$ DOFs, 600 time steps) using Dune.

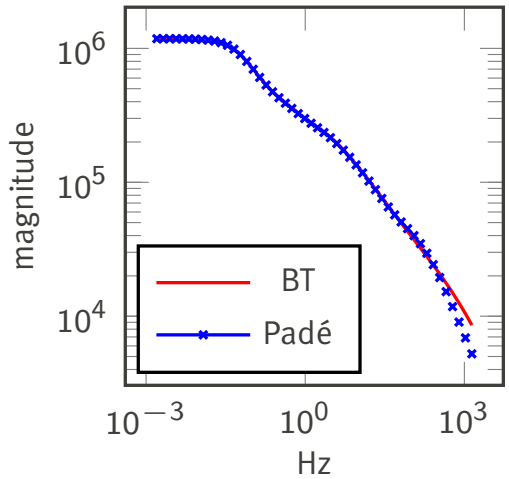
Table: Time (s) needed for solution using DUNE / DUNE with pyMOR timestepping.

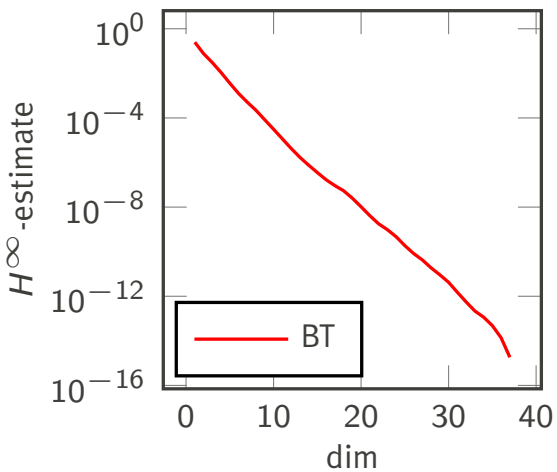
MPI ranks	1	2	3	6	12	24	48	96	192
DUNE	17076	8519	5727	2969	1525	775	395	202	107
pyMOR	17742	8904	6014	3139	1606	816	418	213	120
overhead	3.9%	4.5%	5.0%	5.7%	5.3%	5.3%	6.0%	5.4%	11.8%

System-Theoretic MOR with FEniCS

- MPI distributed heatsink model with FEniCS
- Heat conduction with Robin boundary
- Input: heat flow at base
- Output: temperature at base
- MOR: Balanced truncation and Padé approximation







System-Theoretic MOR with FEniCS – Implementation

Model assembly with FEniCS

```
def discretize():
    domain = ...
    mesh = ms.generate_mesh(domain, RESOLUTION)
    subdomain_data = ...

    V = df.FunctionSpace(mesh, 'P', 1)
    u = df.TrialFunction(V)
    v = df.TestFunction(V)
    ds = df.Measure('ds', domain=mesh, subdomain_data=boundary_markers)

    A = df.assemble(- df.Constant(100.) * df.inner(df.grad(u), df.grad(v)) * df.dx
    - df.Constant(0.1) * u * v * ds(1))
    B = df.assemble(df.Constant(1000.) * v * ds(2))
    E = df.assemble(u * v * df.dx)
```

System-Theoretic MOR with FEniCS – Implementation

pyMOR wrapping

```
# def discretize (cont.)
    # monkey patch apply_inverse_adjoint, assuming symmetriy
    FenicsMatrixOperator.apply_inverse_adjoint = FenicsMatrixOperator.apply_inverse

    space = FenicsVectorSpace(V)
    A = FenicsMatrixOperator(A, V, V)
    B = VectorOperator(space.make_array([B]))
    C = B.H
    E = FenicsMatrixOperator(E, V, V)
    fom = LTIModel(A, B, C, None, E)
    return fom
```

System-Theoretic MOR with FEniCS – Implementation

pyMOR wrapping

```
# def discretize (cont.)
    # monkey patch apply_inverse_adjoint, assuming symmetriy
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    C = B.H
    E = FenicsMatrixOperator(E, V, V)
    fom = LTIModel(A, B, C, None, E)
    return fom
```

MPI wrapping

```
from pymor.tools import mpi
if mpi.parallel:
    from pymor.models.mpi import mpi_wrap_model
    fom = mpi_wrap_model(discretize, use_with=True)
else:
    fom = discretize()
```

System-Theoretic MOR with FEniCS – Implementation

Balanced Truncation

```
reductor = BTReductor(fom)
bt_rom = reductor.reduce(10)

bt_rom.mag_plot(np.logspace(-2, 4, 100), Hz=True)
```

Padé approximation

```
k = 10
V = arnoldi(fom.A, fom.E, fom.B, [0] * r)
W = arnoldi(fom.A, fom.E, fom.C, [0] * r, trans=True)
pade_rom = LTIPGReductor(fom, W, V, False).reduce()

pade_rom.mag_plot(np.logspace(-2, 4, 100), Hz=True)
```

Thank you for your attention!

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SIAM J. Sci. Comput., 38(5), 2016.
`http://www.pymor.org/`

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