Westfälische
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Hierarchical Approximate POD

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living.knowledge
WWU Münster

LMS-EPSRC Symposion
Model Order Reduction

Durham
August 15, 2017

Reduced Basis Methods and POD

RB for Nonlinear Evolution Equations

Full order problem

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

$$\partial_t u_\mu(t) + \mathcal{L}_\mu(u_\mu(t)) = 0, \quad u_\mu(0) = u_0,$$

where $\mathcal{L}_\mu : \mathcal{P} \times V_h \to V_h$ is a nonlinear finite volume operator.

Reduced order problem

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.

$$\partial_t u_{\mu,N}(t) + P_{V_N}(\mathcal{L}_\mu(u_{\mu,N}(t))) = 0, \quad u_{\mu,N}(0) = P_{V_N}(u_0),$$

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

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

- Still expensive to evaluate projected operator $P_{V_N} \circ \mathcal{L}_\mu : V_N \longrightarrow V_h \longrightarrow V_N$
  $\Longrightarrow$ use hyper-reduction (e.g. empirical interpolation).

Basis Generation

Offline phase

Basis for V_N is computed from **solution snapshots** $u_{\mu_s}(t)$ of full order problem via:

- Proper Orthogonal Decomposition (POD)
- POD-Greedy (= greedy search in μ + POD in t)

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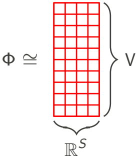
POD (a.k.a. PCA, Karhunen–Loève decomposition)

Given Hilbert space V, $\mathcal{S} := \{v_1, \dots, v_S\} \subset V$, the k-th POD mode of $\mathcal{S}$ is the k-th left-singular vector of the mapping

$$\Phi : \mathbb{R}^S \to V, \quad e_s \to \Phi(e_s) := v_s$$



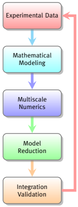
Optimality of POD

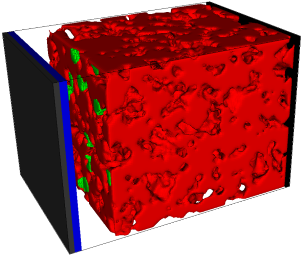
Let V_N be the linear span of first N POD modes, then:

$$\sum_{s \in \mathcal{S}} \|s - P_{V_N}(s)\|^2 = \sum_{m=N+1}^{|\mathcal{S}|} \sigma_m^2 = \min_{\substack{X \subset V \\ \dim X \leq N}} \sum_{s \in \mathcal{S}} \|s - P_X(s)\|^2$$

Stephan Rave (stephan.rave@wwu.de)

Example: RB Approximation of Li-Ion Battery Models



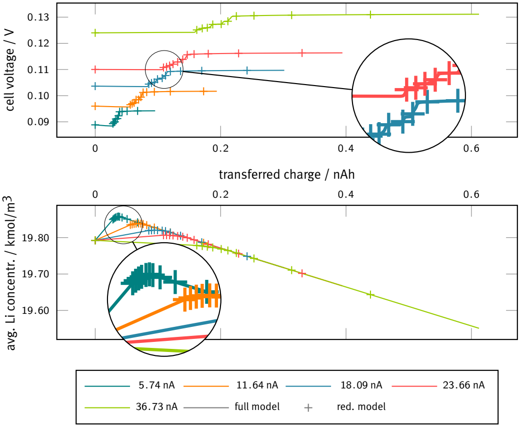


MULTIBAT: Gain understanding of degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.

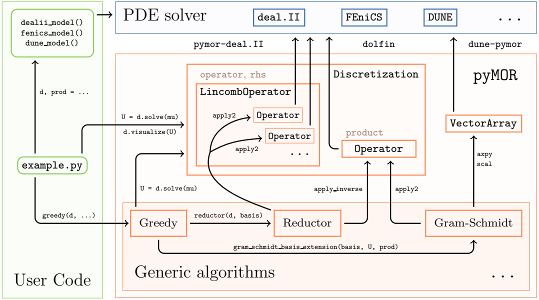
- Focus: Li-Plating.
- Li-plating initiated at interface between active particles and electrolyte.
- Need microscale models which resolve active particle geometry.
- Huge nonlinear discrete models.

Example: Numerical Results

- 2.920.000 DOFs
- Snapshots: 3
- $\dim V_N = 98 + 47$
- $M = 710 + 774$
- Rel. err.: $< 1.5 \cdot 10^{-3}$
- Full model: $\approx$ 13h
- Reduction: $\approx$ 9h
- Red. model: $\approx$ 5m
- Speedup: **154**



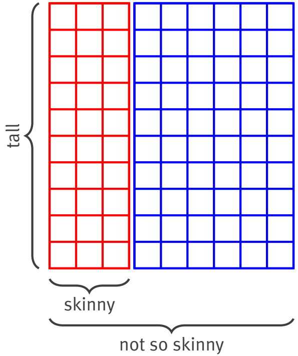
pyMOR – Model Order Reduction with Python



- Quick prototyping with Python.
- Seamless integration with high-performance PDE solvers including FEniCS, deal.II, NGSolve, DUNE.
- Out of box MPI support for reduction algs. and PDE solvers.
- BSD-licensed, fork us on Github!

HAPOD – Hierarchical Approximate POD

Are your tall and skinny matrices not so skinny anymore?



POD of large snapshot sets:

- large computational effort
- hard to parallelize
- data $>$ RAM $\Longrightarrow$ disaster

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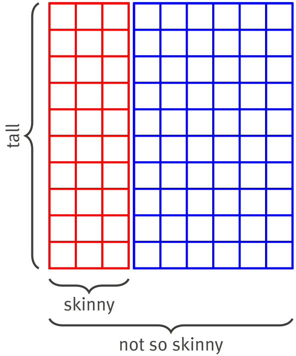

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Solution: PODs of PODs!

Disclaimer

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- Others have done it before – often well-hidden in a paper on entirely different topic.
  We are aware of:
  [Abu-Khzam, Samatova, Ostrouchov, Langston, 2002], [Brands, Mergheim, Steinmann, 2016], [Macua, Belanovic, Zazo, 2010], [Wang, Birdwell, 2004], [Qu, Ostrouchov, Samatova, Geist, 2002], [Paul-Dubois-Taine, Amsallem, 2015], [Iwen, Ong, 2017]

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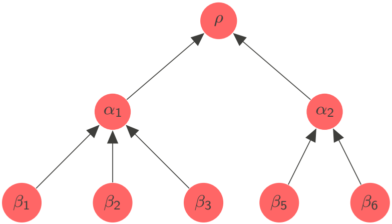
- Our contributions:
  1. Formalization for arbitrary trees of worker nodes.
  2. Extensive theoretical analysis.
  3. A recipe for selecting local truncation thresholds.
  4. Extensive numerical experiments.

- Can be trivially extended to low-rank approximation of snapshot matrix by keeping track of right-singular vectors.

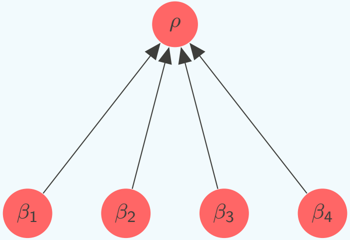
HAPOD – Hierarchical Approximate POD



- Input: Assign snapshot vectors to leaf nodes β_i as input.
- At each node:
  1. Perform POD of input vectors with given local ℓ^2-error tolerance.
  2. Scale POD modes by singular values.
  3. Send scaled modes to parent node as input.
- Output: POD modes at root node ρ.

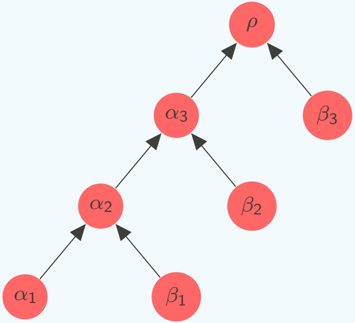
HAPOD – Special Cases

Distributed HAPOD



- Distributed, communication avoiding POD computation.

Incremental HAPOD



- On-the-fly compression of large trajectories.

HAPOD – Some Notation

Trees

$\mathcal{T}$	the tree
$\rho_\mathcal{T}$	root node
$\mathcal{N}_\mathcal{T}(\alpha)$	nodes of $\mathcal{T}$ below or equal node α
$\mathcal{L}_\mathcal{T}$	leafs of $\mathcal{T}$
$L_\mathcal{T}$	depth of $\mathcal{T}$

HAPOD

$\mathcal{S}$	snapshot set
$D : \mathcal{S} \to \mathcal{L}_\mathcal{T}$	snapshot to leaf assignment
$\varepsilon_\mathcal{T}(\alpha)$	error tolerance at α
$\lvert \mathrm{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon_\mathcal{T}](\alpha) \rvert$	number of HAPOD modes at α
$\lvert \mathrm{POD}(\mathcal{S}, \varepsilon) \rvert$	number of POD modes for error tolerance ε
P_α	orth. proj. onto HAPOD modes at α
$\widetilde{\mathcal{S}}_\alpha$	snapshots at leafs below α

HAPOD – Theoretical Analysis

Theorem (Error bound[1])

$$\sum_{s\in\widetilde{\mathcal{S}}_\alpha} \|s - P_\alpha(s)\|^2 \leq \sum_{\gamma\in\mathcal{N}_\mathcal{T}(\alpha)} \varepsilon_\mathcal{T}(\gamma)^2.$$

[1] For special cases in appendix of [Paul-Dubois-Taine, Amsallem, 2015].

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Theorem (Mode bound)

$$\left|\mathrm{HAPOD}[\mathcal{S},\mathcal{T},D,\varepsilon_\mathcal{T}](\alpha)\right| \leq \left|\mathrm{POD}\left(\widetilde{\mathcal{S}}_\alpha, \varepsilon_\mathcal{T}(\alpha)\right)\right|.$$

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But how to choose $\varepsilon_\mathcal{T}$ in practice?

- Prescribe error tolerance ε^* for final HAPOD modes.
- Balance quality of HAPOD space (number of additional modes) and computational efficiency ($\omega \in [0, 1]$).
- Number of input snapshots should be irrelevant for error measure (might be even unknown a priori). Hence, control ℓ^2-*mean* error $\frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} \|s - P_{\rho_\mathcal{T}}(s)\|^2$.

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HAPOD – Theoretical Analysis

Theorem (ℓ^2-mean error and mode bounds)

Choose local POD error tolerances $\varepsilon_{\mathcal{T}}(\alpha)$ *for* ℓ^2*-approximation error as:*

$$\varepsilon_{\mathcal{T}}(\rho_{\mathcal{T}}) := \sqrt{|S|} \cdot \omega \cdot \varepsilon^*, \qquad \varepsilon_{\mathcal{T}}(\alpha) := \sqrt{\widetilde{\mathcal{S}}_\alpha} \cdot (L_{\mathcal{T}} - 1)^{-1/2} \cdot \sqrt{1 - \omega^2} \cdot \varepsilon^*.$$

Then:

$$\frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} \|s - P_{\rho_{\mathcal{T}}}(s)\|^2 \leq \varepsilon^{*2} \quad \textit{and} \quad |\,\mathrm{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon_{\mathcal{T}}]| \leq |\overline{\mathrm{POD}}(\mathcal{S}, \omega \cdot \varepsilon^*)|,$$

where $\overline{\mathrm{POD}}(\mathcal{S}, \varepsilon) := \mathrm{POD}(\mathcal{S}, |\mathcal{S}| \cdot \varepsilon)$.

Moreover:

$$\begin{aligned} |\,\mathrm{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon_{\mathcal{T}}](\alpha)| &\leq |\overline{\mathrm{POD}}(\widetilde{\mathcal{S}}_\alpha, (L_{\mathcal{T}} - 1)^{-1/2} \cdot \sqrt{1 - \omega^2} \cdot \epsilon^*)| \\ &\leq \min_{N \in \mathbb{N}}(d_N(\mathcal{S}) \leq (L_{\mathcal{T}} - 1)^{-1/2} \cdot \sqrt{1 - \omega^2} \cdot \epsilon^*). \end{aligned}$$

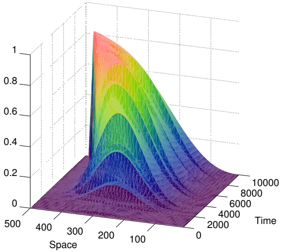
Incremental HAPOD Example

Compress state trajectory of forced inviscid Burgers equation:

$$
\begin{aligned}
\partial_t z(x,t) + z(x,t) \cdot \partial_x z(x,t) &= u(t) \exp(-\frac{1}{20}(x - \frac{1}{2})^2), & (x,t) &\in (0,1) \times (0,1), \\
z(x,0) &= 0, & x &\in [0,1], \\
z(0,t) &= 0, & t &\in [0,1],
\end{aligned}
$$

where $u(t) \in [0, 1/5]$ iid. for 0.1% random timesteps, otherwise 0.

- Upwind finite difference scheme on uniform mesh with $N = 500$ nodes.
- 10^4 explicit Euler steps.
- 100 sub-PODs, $\omega = 0.75$.
- All computations on Raspberry Pi 1B single board computer (512MB RAM).



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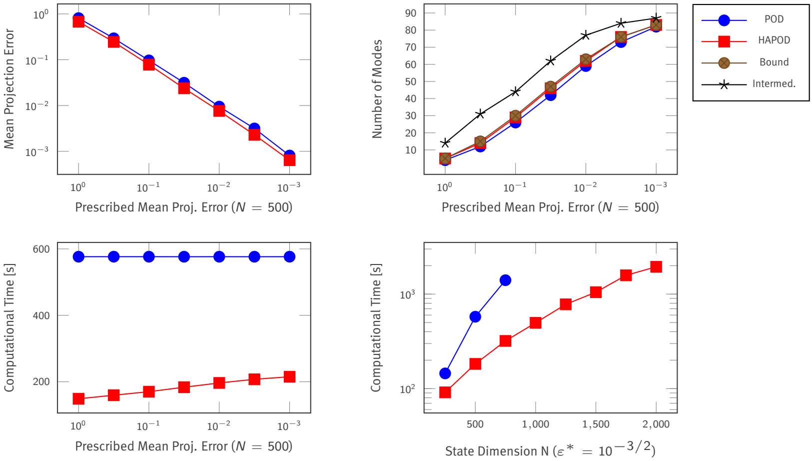
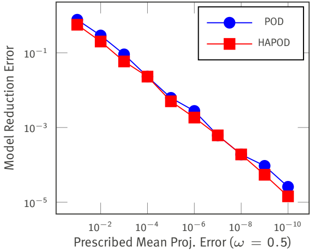


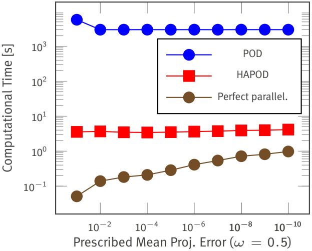
Distributed HAPOD Example

Distributed computation and POD of empirical cross Gramian:

$$\widehat{W}_{X,ij} := \sum_{m=1}^{M} \int_0^\infty \langle x_i^m(t), y_m^j(t) \rangle \, \mathrm{d}t \in \mathbb{R}^{N \times N} \qquad (\rightarrow \text{C.Himpe's talk})$$

- 'Synthetic' benchmark model[2] from MORWiki with parameter $\theta = \frac{1}{10}$.
- Partition $\widehat{W}_X$ into 100 slices of size 10.000×100.



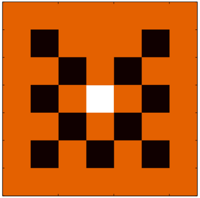


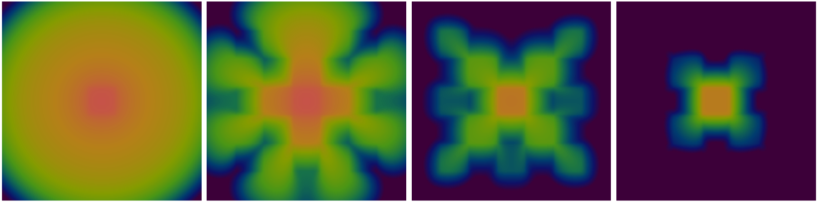
[2] See: `http://modelreduction.org/index.php/Synthetic_parametric_model`

HAPOD – HPC Example

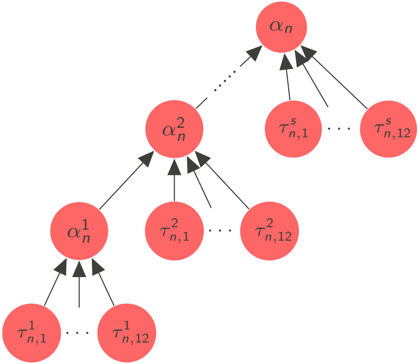
2D neutron transport equation:

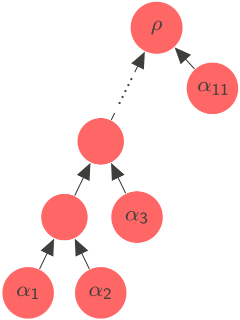
- Moment closure/FV approximation.
- Varying absorbtion and scattering coefficients.
- Distributed snapshot and HAPOD computation on PALMA cluster (125 cores).





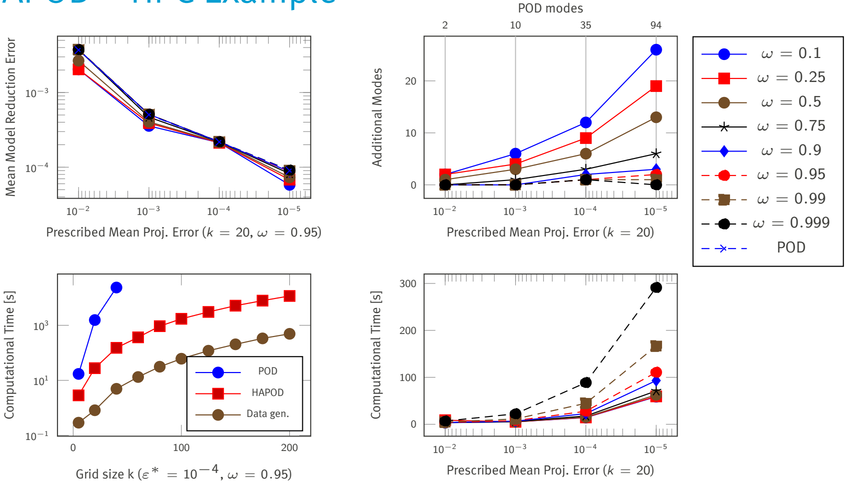
HAPOD – HPC Example



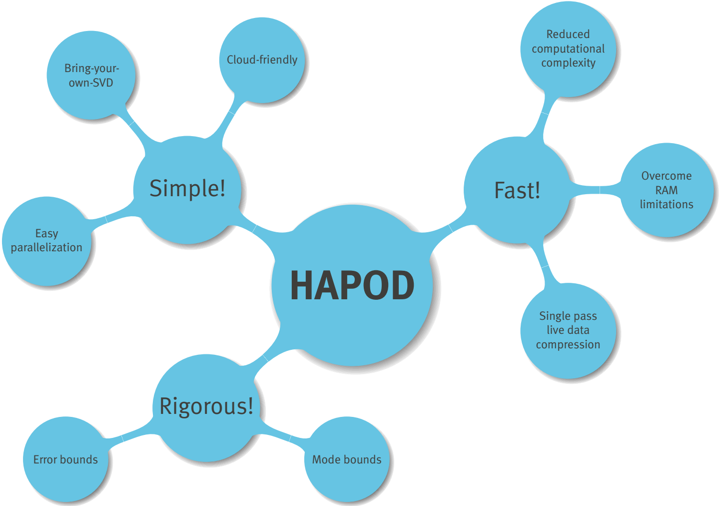


- HAPOD on compute node n. Time steps are split into s slices. Each processor core computes one slice at a time, performs POD and sends resulting modes to main MPI rank on the node.
- Incremental HAPOD is performed on MPI rank 0 with modes collected on each node.

HAPOD – HPC Example



- $\approx 39.000 \cdot k^3$ doubles of snapshot data (≈ 2.5 terabyte for $k = 200$).


HAPOD
Simple!
Bring-your-own-SVD
Cloud-friendly
Easy parallelization
Fast!
Reduced computational complexity
Overcome RAM limitations
Single pass live data compression
Rigorous!
Error bounds
Mode bounds

Thank you for your attention!

C. Himpe, T. Leibner, S. Rave, Hierarchical Approximate Proper Orthogonal Decomposition
arXiv:1607.05210

My homepage
`http://stephanrave.de/`

pyMOR – Generic Algorithms and Interfaces for Model Order Reduction
SIAM J. Sci. Comput., 38(5), pp. S194–S216
`pip install git+https://github.com/pymor/pymor@hapod`

MULTIBAT: Unified Workflow for fast electrochemical 3D simulations of lithium-ion cells combining virtual stochastic microstructures, electrochemical degradation models and model order reduction
arXiv:1704.04139