Westfälische
Wilhelms-Universität
Münster

# HAPOD
# Fast and Simple Distributed POD Computation

Christian Himpe, Tobias Leibner and Stephan Rave

living.knowledge
WWU Münster

GAMM Jahrestagung

Weimar
March 9, 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 $V_N$.

# 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 $V_N$.

- 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 $\mu$ + POD in $t$)

# Basis Generation

## Offline phase

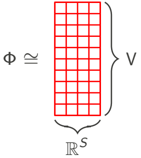
Basis for $V_N$ is computed from **solution snapshots** $u_{\mu_s}(t)$ of full order problem via:

- Proper Orthogonal Decomposition (POD)
- POD-Greedy (= greedy search in $\mu$ + POD in $t$)

## 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:

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

# Example: RB Approximation of Li-Ion Battery Models

ulm university universität ulm

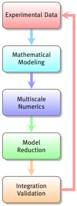
Institute of Technical Thermodynamics

**MULTIBAT**

SPONSORED BY THE Federal Ministry of Education and Research

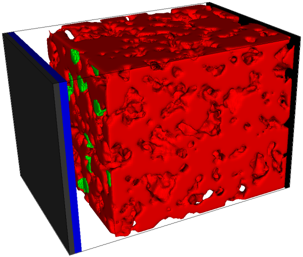
Fraunhofer ITWM

Westfälische Wilhelms-Universität Münster



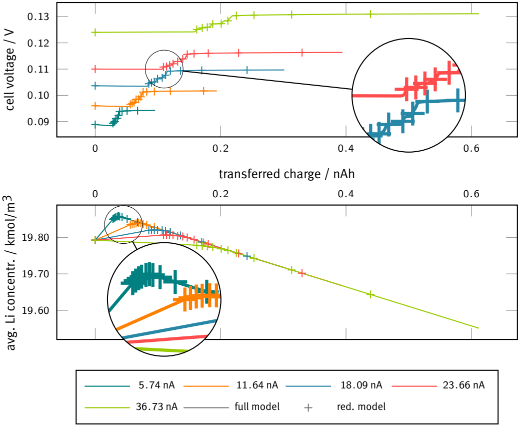

**MULTIBAT:** Gain understanding of degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.

- 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.

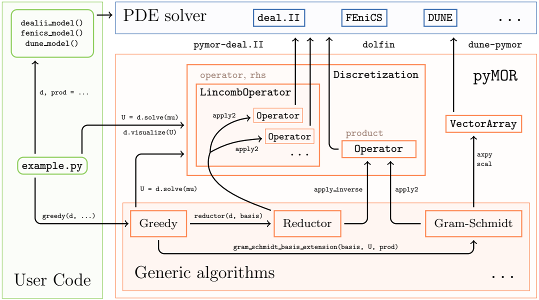


# Example: Numerical Results

- 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**



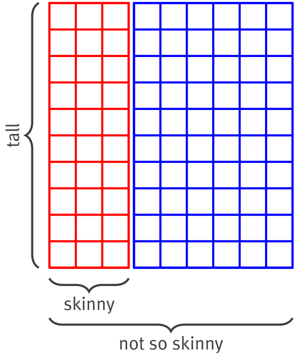
# pyMOR – Model Order Reduction with Python




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

# HAPOD – Hierarchical Approximate POD

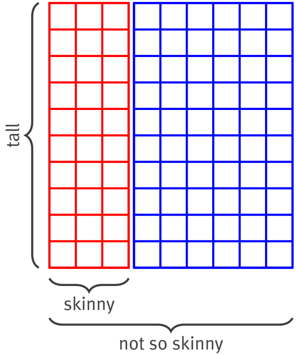
# Are your tall and skinny matrices not so skinny anymore?




POD of large snapshot sets:

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

# Are your tall and skinny matrices not so skinny anymore?

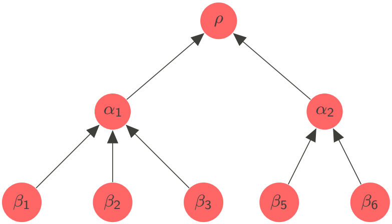



POD of large snapshot sets:

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

**Solution:** PODs of PODs!

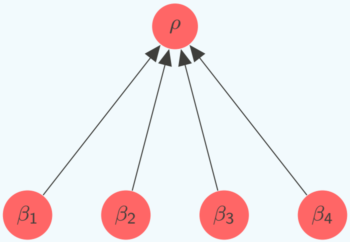
# HAPOD – Hierarchical Approximate POD




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

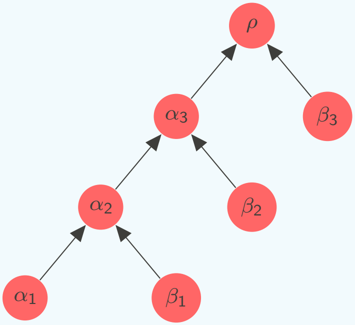
# HAPOD – Special Cases

## Distributed HAPOD




- Distributed, communication avoiding POD computation.

## Live HAPOD




- On-the-fly compression of large trajectories.

# HAPOD – Theoretical Analysis

## Theorem (Error and mode bounds)

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

$$\varepsilon_\mathcal{T}(\rho) := \frac{\sqrt{|S|}}{\sqrt{\mathcal{I}_\rho}} \cdot \omega \cdot \varepsilon^*, \qquad \varepsilon_\mathcal{T}(\alpha) := \frac{\sqrt{|S_\alpha|}}{\sqrt{\mathcal{I}_\alpha \cdot (L-1)}} \cdot \sqrt{1-\omega^2} \cdot \varepsilon^*.$$

*Then:*

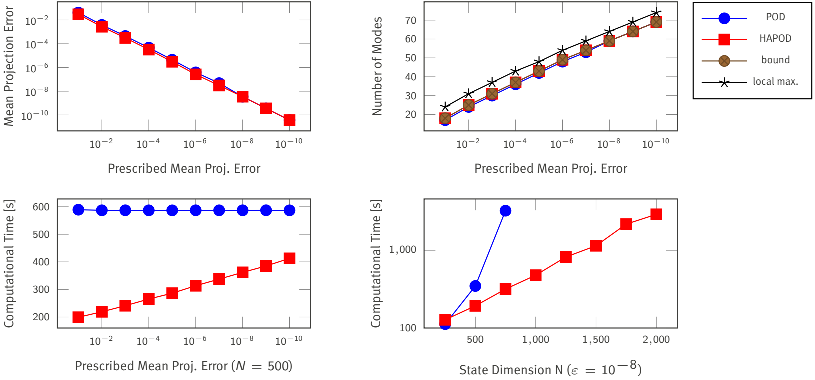
$$\frac{1}{|\mathcal{S}|}\sum_{s\in\mathcal{S}} \|s - P(s)\|^2 \leq (\varepsilon^*)^2 \quad \textit{and} \quad |\,\mathrm{HAPOD}[\mathcal{S}, \varepsilon_\mathcal{T}]| \leq |\,\mathrm{POD}(\mathcal{S}, \omega\cdot\varepsilon^*)|.$$

*Moreover:*

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

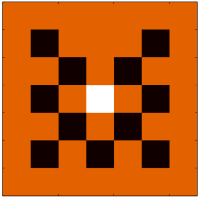
# Live HAPOD Example

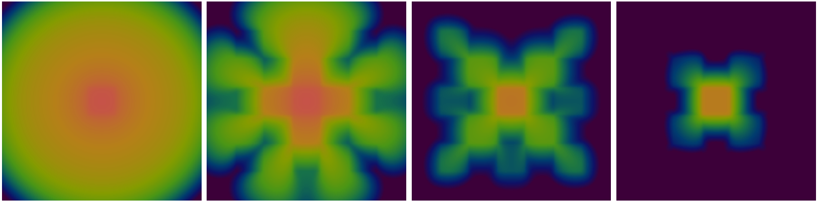
- State space trajectory of ‘synthetic’ MORWiki benchmark model excited with random input (100 $\times$ 100 time steps).
- All computations on Raspberry Pi 1B single board computer.



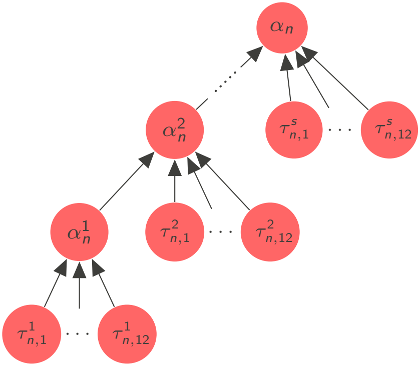
# HAPOD – HPC Example

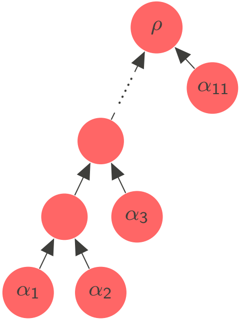
- 2D neutron transport equation.
- Moment closure/FV approximation.
- Varying absorbtion and scattering coefficients.
- Distributed snapshot and HAPOD computation on PALMA cluster (125 cores).





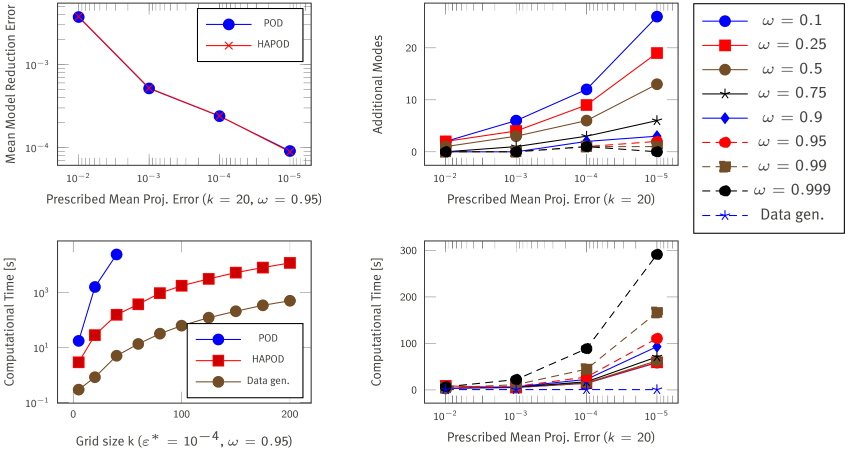
# HAPOD – HPC Example



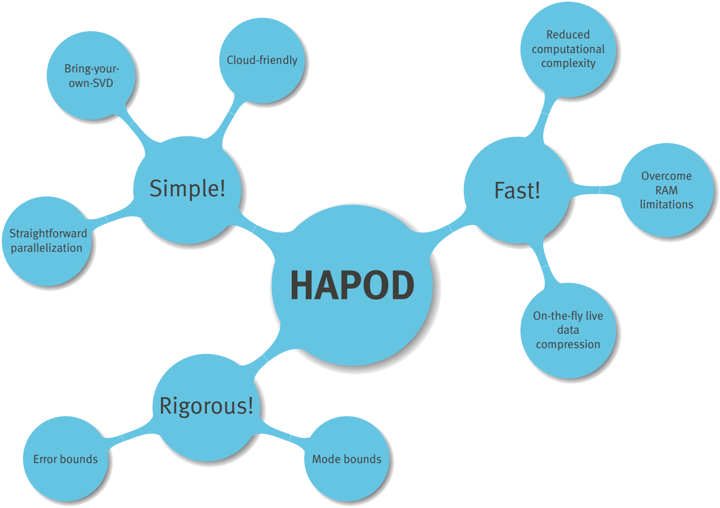




- HAPOD on compute node $n$. Time steps are split into $s$ slices. Each processor core computes one slice at a time, performs POD and sends resulting modes to main MPI rank on the node.
- Live HAPOD is performed on MPI rank 0 with modes collected on each node.

# HAPOD – HPC Example




- $\approx 39.000 \cdot k^3$ doubles per trajectory ($\approx 2.5$ terabyte for $k = 200$).


HAPOD
Simple!
Bring-your-own-SVD
Cloud-friendly
Straightforward parallelization
Fast!
Reduced computational complexity
Overcome RAM limitations
On-the-fly 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
`http://www.pymor.org/`

MULTIBAT: Unified Workflow for fast electrochemical 3D simulations of lithium-ion cells combining virtual stochastic microstructures, electrochemical degradation models and model order reduction (submitted)
`http://j.mp/multibat`