A Globally Mass Conservative Nonlinear Reduced Basis Method for Parabolic Free Boundary Problems

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MoRePaS IV

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Outline

1. Reduced Basis Methods for Advection Dominated Problems.

2. A Globally Mass Conservative Nonlinear Reduced Basis Method for Parabolic Free Boundary Problems.

Reduced Basis Methods for Advection Dominated Problems

Parametric Model Order Reduction

Consider time-dependent parametric problems

$$\Phi : \mathcal{P} \to X([0, T]; V_h), \qquad s : X([0, T]; V_h) \to \mathbb{R}^S$$

where

- $\mathcal{P} \subset \mathbb{R}^P$ parameter domain.
- V_h “truth” solution state space, $\dim V_h \gg 0$.
- Φ maps parameters to solutions (*hard* to compute).
- s maps state vectors to quantities of interest.

Objective

Compute

$$s \circ \Phi : \mathbb{R}^P \to X([0, T]; V_h) \to \mathbb{R}^S$$

for *many* $\mu \in \mathcal{P}$ or *quickly* for unknown single $\mu \in \mathcal{P}$.

Reduced Basis Methods: Three Basic Ideas

Objective

Compute

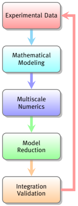
$$s \circ \Phi : \mathbb{R}^P \to X([0, T]; V_h) \to \mathbb{R}^S$$

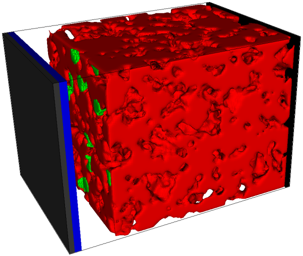
When Φ, s sufficiently smooth, quickly computable low-dimensional approximation of $s \circ \Phi$ should exist.

- **Idea 1:** State space projection:
  - Define approximation $\Phi_N : \mathcal{P} \to X([0, T]; V_N)$, $N := \dim V_N \ll \dim V_h$, via (Petrov-)Galerkin projection.
  - Approximate $s \circ \Phi \approx s \circ \Phi_N$.
- **Idea 2:** Construct V_N from PODs of solution snapshots $\Phi(\mu_1), \dots, \Phi(\mu_k)$.
- **Idea 3:** Select $\mu_1, \dots, \mu_k$ iteratively via greedy search over $\mathcal{P}$ using quickly computable surrogate $\eta(\Phi_N(\mu), \mu) \geq \|\Phi(\mu) - \Phi_N(\mu)\|$ (POD-Greedy).

+ Hyper-reduction technique (EIM, DEIM, GEIM, Gappy POD, ...)

Example: RB Approximation of Li-Ion Battery Models





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

Full order model:

- 2.920.000 DOFs
- Simulation time: $\approx$ 13h

Reduced order model:

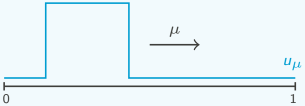
- Snapshots: 3
- $\dim V_N = 145$
- Rel. err.: $< 1.5 \cdot 10^{-3}$
- Reduction time: $\approx$ 9h
- Simulation time: $\approx$ 5m
- Speedup: **154**

Trouble with Advection Dominated Problems

Typically slow decay of Kolmogorov N-widths d_N of the solution manifold, but RB will only work well for rapid decay!

$$d_N := \inf_{\substack{V_N \subseteq V_h \\ \dim V_N \leq N}} \sup_{\substack{u \in \Phi(\mathcal{P}) \\ t \in [0,T]}} \|u(t) - P_{V_N}(u(t))\|.$$

Basic example



$$\partial_t u(t,x) + \mu \cdot \partial_x u_\mu(t,x) = 0$$
$$u_\mu(0,x) = u_0(x),\ u_\mu(0,t) = u_\mu(1,t)$$
$$\mu, x, t \in [0,1]$$

Here: $d_N \sim N^{-1/2}$ w.r.t. $L^2([0,1])$.

However: We can describe solution easily as

$$u_\mu(t,x) = u_0(x - \mu \cdot t \mod 1).$$

Nonlinear Approximation

General Idea

Write $u_\mu(t,x)$ as

$$u_\mu(t,x) = g_\mu(t).v_\mu(t,x)$$

dynamics of u_μ
large variation in time

shape of u_μ
small variation in time

where $\mathcal{V}$ function space, $v_\mu(t) \in \mathcal{V}$ and $g_\mu(t)$ is element of Lie group G acting on $\mathcal{V}$.

- $v_\mu(t,x)$ should be easier to approximate by a linear space than $u_\mu(t,x)$!
- Related/other approaches: [Rowley, Marsden, 2000] [Gerbeau, Lombardi, 2014] [Iollo, Lombardi, 2014] [Carlberg, 2015] [Taddei, Perotto, Quarteroni, 2015] [Reiss, Schulze, Sesterhenn, Mehrmann, 2015] [Cagniart, Maday, Stamm, 2016] [Nair, Balajewicz, 2017] [Welper, 2017] [Rim, Moe, LeVeque, 2018] …

Method of Freezing [Beyn, Thümmler, 2004], [Rowley et. al., 2000, 2003]

Definition (Method of Freezing)

With initial conditions $v_\mu(0) = u(0),\ g_\mu(0) = e$, solve:

$$\begin{gathered}\partial_t v_\mu(t) + \mathcal{L}_\mu(v_\mu(t)) + \mathfrak{g}_\mu(t).v_\mu(t) = 0 \\ \Phi(v_\mu(t), \mathfrak{g}_\mu(t)) = 0\end{gathered}$$

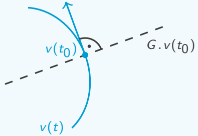
frozen PDAE

$$\mathfrak{g}_\mu(t) = g(t)_\mu^{-1}\partial_t g_\mu(t)$$

reconstruction equation

Orthogonality phase condition

$$\begin{aligned}\Phi(v,\mathfrak{g}) = 0 \ &:\Longleftrightarrow \partial_t v(t) \perp G.v(t) \\ &\Longleftrightarrow (\mathcal{L}(v) + \mathfrak{g}.v,\ \mathfrak{h}.v) = 0 \quad \forall \mathfrak{h} \in G\end{aligned}$$



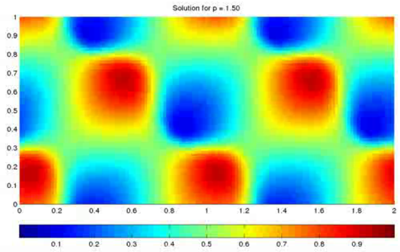
Test Problem

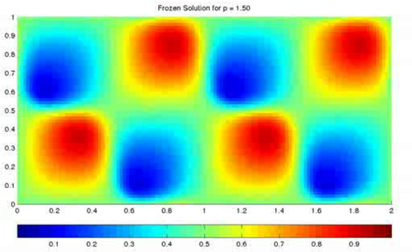
2D Burgers-type problem

Solve on $\Omega = [0,2] \times [0,1]$ with periodic boundaries, $t \in [0, 0.3]$, $\vec{v} \in \mathbb{R}^2$ and $\mu \in [1,2]$:

$$\partial_t u + \nabla \cdot (\vec{v} \cdot u^\mu) = 0$$
$$u(0, x_1, x_2) = 1/2(1 + \sin(2\pi x_1)\sin(2\pi x_2))$$

Let $G := \mathbb{R}^2$ act on u by periodic shifts.





Combining RB with the Method of Freezing

FrozenRB-Scheme for 2D-shifts [Ohlberger, R, 2013]

Solve

$$\partial_t v_{\mu(t),N} + P_{V_N} \circ \mathcal{I}_M[\mathcal{L}_\mu](v_{\mu,N}(t)) - \mathfrak{g}_{\mu(t),N} \cdot (P_{V_N} \circ \nabla)(v_{\mu,N}(t)) = 0$$
$$\left[(\partial_{x_i} v_{\mu,N},\, \partial_{x_j} v_{\mu,N})\right]_{i,j} \cdot \left[\mathfrak{g}_{\mu,N}\right]_j = \left[(\mathcal{I}_M[\mathcal{L}_\mu](v_\mu),\, \partial_{x_i} v_{\mu,N})\right]_i$$

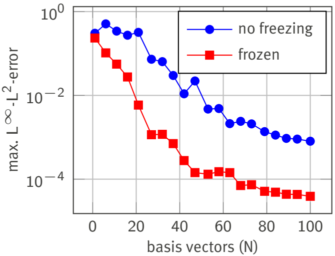
and

$$\partial_t g_\mu(t) = \mathfrak{g}_\mu(t)$$

with initial conditions $v_\mu(0) = u(0)$, $g_\mu(0) = (0,0)^T$.

- EI-Greedy, POD-Greedy algorithms for basis generation.
- Full offline/online decomposition.
- No additional evaluations of nonlinearity.

Results for the Burgers Problem

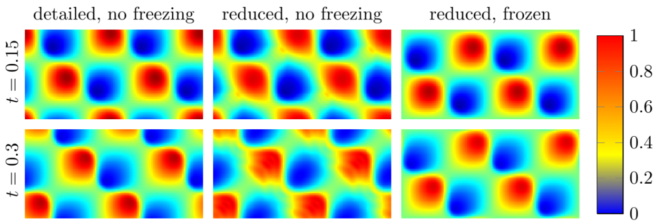


Left:

- $1.9 \cdot N$ interpolation points.
- Test set: 100 random μ.

Bottom:

- $\dim V_N = 20$, 38 interpolation points.
- $\mu = 1.5$.



Freezing of multiple waves?

See Harshit Bansal's poster!

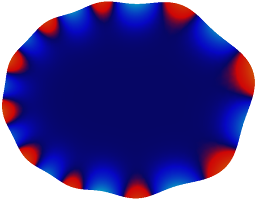
A Globally Mass Conservative Nonlinear Reduced Basis Method for Parabolic Free Boundary Problems

A Free Boundary Problem

Osmotic cell swelling model [Lippoth, Prokert, 2012]

Given $\Omega(0) \subset \mathbb{R}^d$, $u(0) \in H^1(\Omega(0))$ and coefficients $u_0, \alpha, \beta, \gamma \in \mathbb{R}$, the **concentration** $u(t)$ and **normal velocity** $\mathcal{V}_n$ of $\partial\Omega(t)$ is given by:

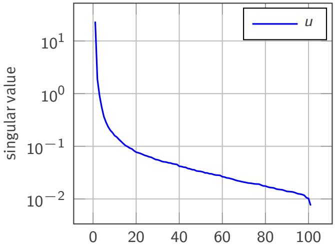
$$\begin{aligned} \partial_t u - \alpha \Delta u &= 0 && \text{in } \Omega(t) \\ \mathcal{V}_n u + \alpha \partial_n u &= 0 && \text{on } \partial\Omega(t) \\ -\beta H + \gamma(u - u_0) &= \mathcal{V}_n && \text{on } \partial\Omega(t) \end{aligned}$$

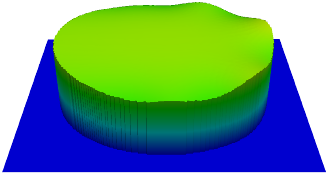


- u_0: constant concentration in $\Omega(t)^c$
- H: mean curvature of $\partial\Omega(t)$
- α: diffusivity of u
- $-\beta H$: surface tension
- $\gamma(u - u_0)$: osmotic pressure

Eulerian Approximation

- Consider $u(t) \in L^2(\Omega(t)) \hookrightarrow L^2(\mathbb{R}^d)$ as joint approximation space.
- moving domain boundary
  $\Longrightarrow$ moving discontinuity in $u(t)$
  $\Longrightarrow$ slow singular value decay





Idea

Use nonlinear transformation

$$\Psi(t).u(t)(x) := u(t)[\Psi(t)[x]]$$

to freeze boundary $\Gamma(t)$ in space.

- Fix reference domain

$$\hat{\Omega} := \Psi(t)^{-1}(\Omega(t)).$$

ALE Formulation

Fix reference domain $\widehat{\Omega}$ and introduce deformation field $\Psi(t)$ s.t. $\Psi(t)(\widehat{\Omega}) = \Omega(t)$.
Pulling back the equations to $\hat{\Omega}$ leads to the following time-discretization scheme:

1. Compute boundary velocity:
$$\int_{\hat{\Gamma}} J_\Gamma \hat{V}_\Gamma^{n-1} \cdot \hat{s}\, ds + \Delta t \int_{\hat{\Gamma}} J_\Gamma \beta\left((F^{n-1})^{-T} \nabla_{\hat{\Gamma}} \hat{V}_\Gamma^{n-1}\right) : \left((F^{n-1})^{-T} \nabla_{\hat{\Gamma}} \hat{s}\right) ds$$
$$= \int_{\hat{\Gamma}} \beta(P : (F^{n-1})^{-T} \nabla_{\hat{\Gamma}} \hat{s} + \gamma(\hat{u} - u_{\text{ext}})\hat{s} \cdot ((F^{n-1})^{-T} \hat{\nu}))\, ds.$$

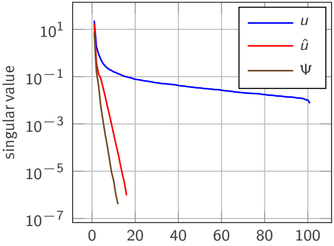
2. Extend velocity to interior via harmonic extension:
$$\int_{\hat{\Gamma}} \frac{1}{h}(\nabla \hat{V}^{n-1} + (\nabla \hat{V}^{n-1})^T) : (\nabla \hat{s} + (\nabla \hat{s})^T)\, dx = 0, \qquad \hat{V}^{n-1} = \hat{V}_\Gamma^{n-1} \quad \text{on } \partial\hat{\Omega}.$$

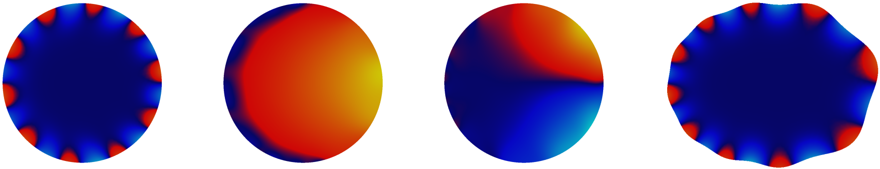
3. Update deformation field:
$$\Psi^n = \Psi^{n-1} + \Delta t \hat{V}^{n-1}.$$

4. Update concentration field:
$$\int_{\hat{\Omega}} J^n\, \hat{u}^n \hat{v}\, dx + \Delta t \int_{\hat{\Omega}} J^n\, \hat{u}^n\, V_h^{n-1} \cdot ((F^n)^{-T} \nabla \hat{v}) dx$$
$$+ \Delta t \int_{\hat{\Omega}} J^n\, \alpha\, ((F^n)^{-T} \nabla \hat{u}^n) \cdot ((F^n)^{-T} \nabla \hat{v})\, dx = \int_{\hat{\Omega}} J^{n-1}\, \hat{u}^{n-1} \hat{v}\, dx.$$

ALE Formulation

- Rapid singular value decay of both concentration and deformation fields.
- After space discretization this corresponds to moving-mesh approach (ALE), where $\Psi^n(v)$ is the trajectory of the vertex v.
- In contrast to “parameterized domain problems”, the domain deformation Ψ^n is part of the equation system.





$\hat{u}^n$ Ψ^n_1 Ψ^n_2 reconstruction

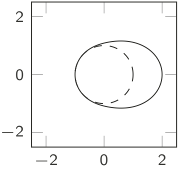
Nonlinear RBM for Free Boundary Problems

Use standard RB machinery to construct ROM:

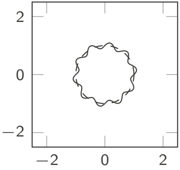
- Compute low-rank approximation spaces for $\hat{u}^n$, Ψ^n, $\hat{V}_\Gamma^n$ via POD. (Could also use POD-Greedy).
- Use EIM to approximate coefficient functions, vectors, tensors depending nonlinearly on Ψ^n.
- Similar to [Ballarin, Rozza, 2016] in context of FSI.

Numerical Experiment

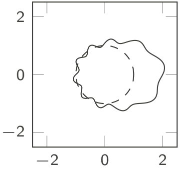
- Parameterization:
  - $\alpha \in [0.1, 1]$
  - $\beta \in [0.01, 0.1]$
  - $\delta_1, \delta_2 \in [0, 1]$
- Snapshots: 3^4
- FOM: 3988 + 7976 DOFS



$\delta_1 = 1, \delta_2 = 0$

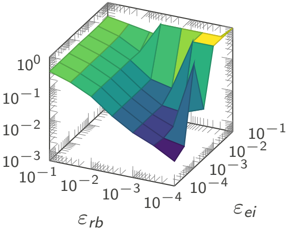


$\delta_1 = 0, \delta_2 = 1$

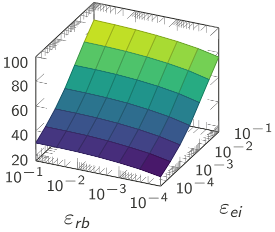


$\delta_1 = 1, \delta_2 = 1$

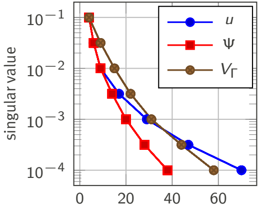
Rel. L^∞–L^∞–H^1 Error in u



Model Reduction Speedup



Basis Sizes



Global Mass Conservation

Concentration update

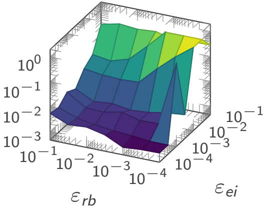
$$\int_{\hat\Omega} J^n\ \hat u^n \hat v\ dx + \Delta t \int_{\hat\Omega} J^n\ \hat u^n\ V_h^{n-1} \cdot ((F^n)^{-T} \nabla \hat v) dx$$
$$+ \Delta t \int_{\hat\Omega} J^n\ \alpha\ ((F^n)^{-T} \nabla \hat u^n) \cdot ((F^n)^{-T} \nabla \hat v)\ dx = \int_{\hat\Omega} J^{n-1}\ \hat u^{n-1} \hat v\ dx.$$

- Testing with $\hat v \equiv 1$ yields:

$$\int_{\Omega^n} u^n\ dx = \int_{\hat\Omega} J^n\ \hat u^n\ dx + 0 + 0 = \int_{\hat\Omega} J^{n-1}\ \hat u^n = \int_{\Omega^{n-1}} u^{n-1}\ dx$$

- Mass conservation is preserved by RB projection by adding 1 to RB for u^n.
- Inexact assembly of mass matrix due to EI destroys mass conservation.

Rel. Mass Conservation Error



Global Mass Conservation with EI

- Note that in 2D:

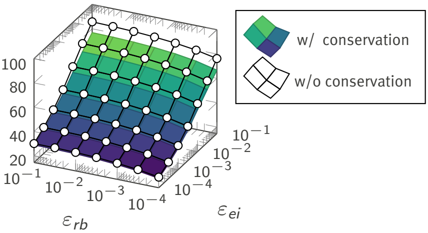
$$\int_{\hat\Omega} J^n\, \hat u^n \hat v = m(\Psi^n, \Psi^n, \hat u^n, \hat v),$$

where

$$m(\Phi^n, \Psi^n, \hat u^n, \hat v) = \int_{\hat\Omega} \partial_x \Phi^n_x \cdot \partial_y \Psi^n_y \cdot \hat u^n \cdot \hat v + \partial_x \Phi^n_y \cdot \partial_y \Psi^n_x \cdot \hat u^n \cdot \hat v \; dx.$$

- Could assemble mass matrix 4-tensor exactly.
- Relatively expensive.
  (dim RB = 30 $\Longrightarrow$ 6MB for reduced tensor)
- 5-tensor in 3D!
- Better approach:
  1. Assemble mass matrix using EI.
  2. Assemble 3-tensor $m(\Phi^n, \Psi^n, \hat u^n, 1)$ exactly and set corresponding row of mass matrix.

Model Reduction Speedup



Outlook: Remeshing

Strongly anisotropic mesh deformations in ALE schemes lead to:

- bad approximation spaces.
- ill-conditioned system matrices.

Possible MOR approach:

- In FOM: Locally adapt mesh $\hat{\mathcal{T}}_h$ on $\hat{\Omega}$ s.t. $\Psi^n(\hat{\mathcal{T}}_h)$ has good shape regularity properties.
- Solve extension problem for $\hat{V}_\Gamma^n$ on Ω^n instead of $\hat{\Omega}$.
- Use "RB for AFEM" methods to construct ROM [Ullmann, Rotkvic, Lang, 2016] [Yano 2016] [Ali, Steih, Urban, 2017] [Hinze, Gräßle, 2017].
- Deformation-dependent norms?
- Dictionary-based approaches?

Thank you for your attention!

Ohlberger, R, *Nonlinear reduced basis approximation of parameterized evolution equations via the method of freezing*, C. R. Math. Acad. Sci. Paris, 351 (2013).

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Milk, R, Schindler, *pyMOR – Generic Algorithms and Interfaces for Model Order Reduction* SIAM J. Sci. Comput., 38(5), 2016.
`http://www.pymor.org/`

My homepage (with FrozenRB code)
`http://stephanrave.de/`