WWU MÜNSTER

APPLIED MATHEMATICS MÜNSTER

Reduced Order Modeling of a Free Boundary Osmotic Cell Swelling Problem with Exact Mass Conservation

Christoph Lehrenfeld, Stephan Rave

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

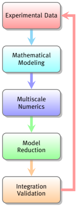
$$s \circ \Phi : \mathbb{R}^P \to X([0,T]; V_h) \to \mathbb{R}^S$$

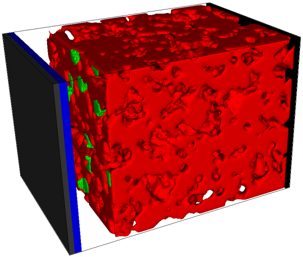
When Φ, s sufficiently smooth, quickly computable low-dimensional approximation of $s \circ \Phi$ should exist.

- **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 $\Phi(\mu_1), \ldots, \Phi(\mu_k)$.
- **Idea 3:** Select $\mu_1, \ldots, \mu_k$ 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.

FOM:

- 2.920.000 DOFs
- Simulation time: $\approx$ 15.5h

ROM:

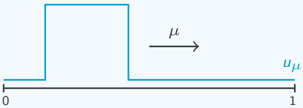
- Snapshots: 3
- dim $V_N = 245$
- Rel. err.: $< 4.5 \cdot 10^{-3}$
- Reduction time: $\approx$ 14h
- Simulation time: $\approx$ 8m
- Speedup: 120

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. $L^2([0,1])$.

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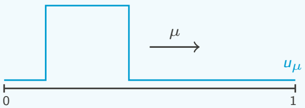

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Here: $d_N \sim N^{-1/2}$ w.r.t. $L^2([0,1])$.

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 $u_\mu(t,x)$!

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- 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:

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

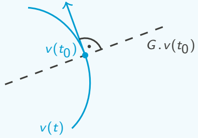
frozen PDAE

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

reconstruction equation

Orthogonality phase condition

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



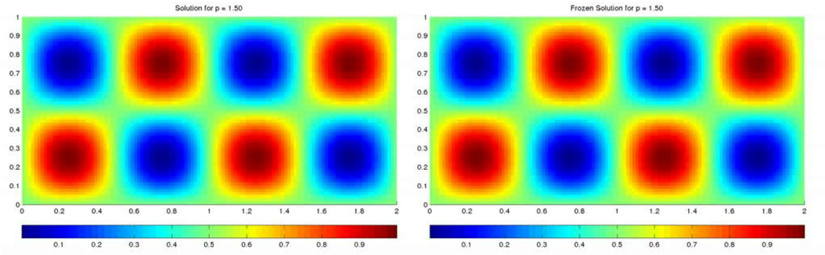
Test Problem

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.



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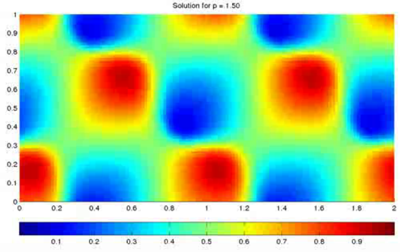
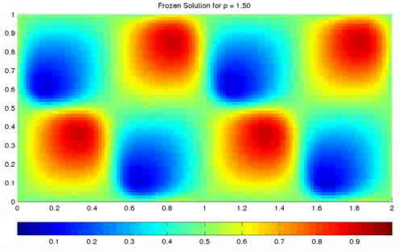




Combining RB with the Method of Freezing

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

Solve

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

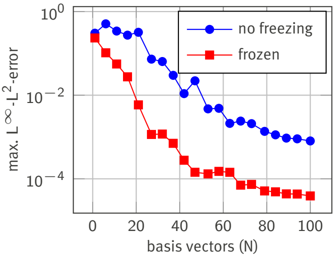
and

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

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

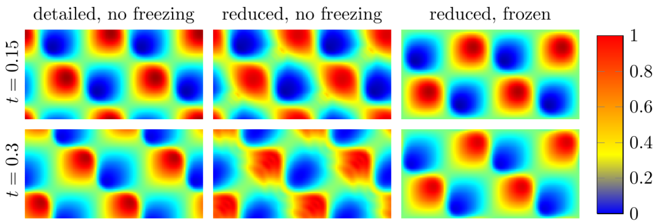


Left:

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

Bottom:

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



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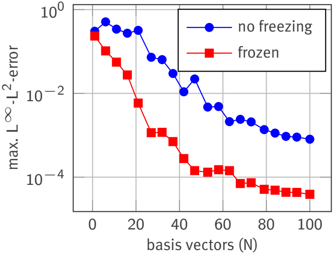

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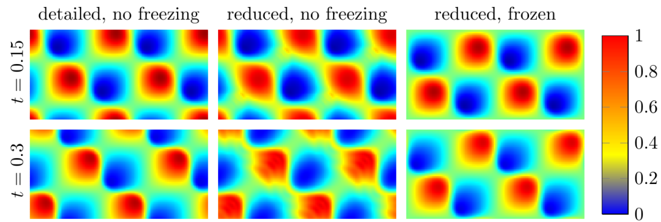

Freezing of multiple waves?

See Harshit Bansal's talk at 11:05, Room 532!

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 $u_{\text{ext}}, \alpha, \beta, \gamma \in \mathbb{R}$, the **concentration** $u(t)$ and **normal velocity** w_Γ of $\partial\Omega(t)$ 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).
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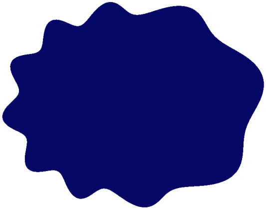

- u_0: constant concentration in $\Omega(t)^c$
- κ: mean curvature of $\partial\Omega(t)$
- α: diffusivity of u
- $-\beta\kappa$: surface tension
- $\gamma(u - u_{ext})$: osmotic pressure

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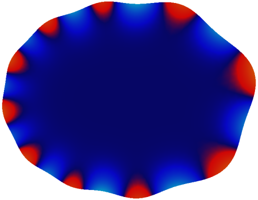

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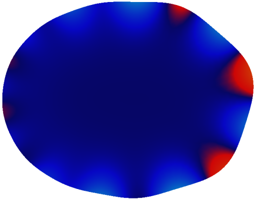

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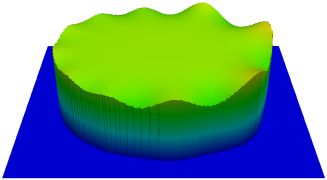
Eulerian Approximation

- Consider $u(t) \in L^2(\Omega(t)) \hookrightarrow L^2(\mathbb{R}^d)$ as joint approximation space.



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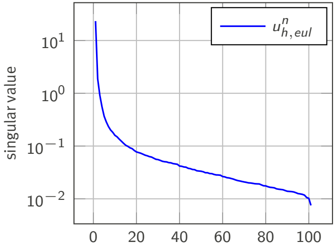
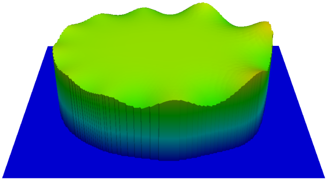
- Consider $u(t) \in L^2(\Omega(t)) \hookrightarrow L^2(\mathbb{R}^d)$ as joint approximation space.
- moving domain boundary
  $\Longrightarrow$ moving discontinuity in $u(t)$
  $\Longrightarrow$ slow singular value decay





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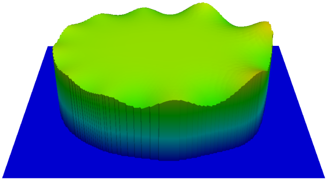

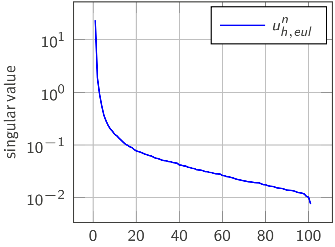

Idea

Use nonlinear transformation

$$u(t)[\Psi(t)[x]]$$

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:

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1. Compute boundary velocity:

$$\int_{\hat{\Gamma}} J_\Gamma^{n-1} \hat{\mathbf{w}}_{\Gamma,h}^{n-1} \cdot \hat{\mathbf{s}}_h \, d\mathbf{s} + \beta \Delta t \int_{\hat{\Gamma}} J_\Gamma^{n-1} \left(\mathbf{P} \cdot (\mathbf{F}^{n-1})^{-T} \cdot \nabla \hat{\mathbf{w}}_{\Gamma,h}^{n-1} \right) : \left((\mathbf{F}^{n-1})^{-T} \nabla \hat{\mathbf{s}}_h \right) d\mathbf{s}$$
$$= -\beta \int_{\hat{\Gamma}} J_\Gamma^{n-1} \mathbf{P} : (\mathbf{F}^{n-1})^{-T} \nabla_{\hat{\Gamma}} \hat{\mathbf{s}}_h \, d\mathbf{s} + \gamma \int_{\hat{\Gamma}} J_\Gamma^{n-1} (\hat{u}_h - u_{\mathrm{ext}}) \hat{\mathbf{s}}_h \cdot ((\mathbf{F}^{n-1})^{-T} \hat{\mathbf{n}}) \, d\mathbf{s}.$$

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2. Extend velocity to interior via harmonic extension:

$$-\operatorname{div}[h_{\mathcal{T}}^{-1} (\nabla \hat{\mathbf{w}}_h^{n-1} + (\nabla \hat{\mathbf{w}}_h^{n-1})^T)] = 0 \quad \text{in } \hat{\Omega}, \qquad \hat{\mathbf{w}}_h^{n-1} = \hat{\mathbf{w}}_{\Gamma,h}^{n-1} \quad \text{on } \partial\hat{\Omega}.$$

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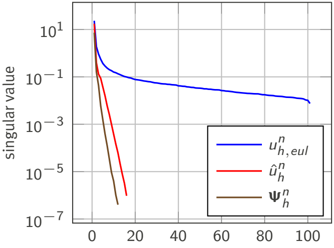
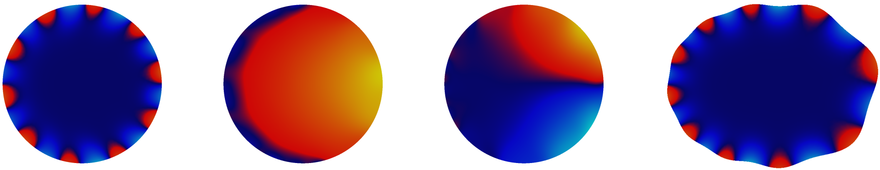
3. Update deformation field:
$$\boldsymbol{\Psi}_h^n = \boldsymbol{\Psi}_h^{n-1} + \Delta t \hat{\mathbf{w}}_h^{n-1}.$$
4. Update concentration field:
$$\int_{\hat{\Omega}} J^n \, \hat{u}_h^n \hat{v}_h \, d\mathbf{x} + \Delta t \int_{\hat{\Omega}} J^n \, \hat{u}_h^n \, \hat{\mathbf{w}}_h^{n-1} \cdot ((\mathbf{F}^n)^{-T} \cdot \nabla \hat{v}_h) d\mathbf{x}$$
$$+ \alpha \Delta t \int_{\hat{\Omega}} J^n \left((\mathbf{F}^n)^{-T} \nabla \hat{u}_h^n\right) \cdot \left((\mathbf{F}^n)^{-T} \nabla \hat{v}_h\right) d\mathbf{x} = \int_{\hat{\Omega}} J^{n-1} \, \hat{u}_h^{n-1} \hat{v}_h \, d\mathbf{x}.$$

ALE Formulation

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





$\hat{u}_h^n$ $\mathbf{\Psi}_{h1}^n$ $\mathbf{\Psi}_{h2}^n$ reconstruction

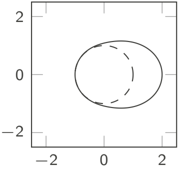
Nonlinear RBM for Free Boundary Problems

Use standard RB machinery to construct ROM:

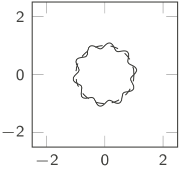
- Compute low-rank approximation spaces for $\hat{u}_h^n$, $\mathbf{\Psi}_h^n$, $\hat{\mathbf{w}}_{\Gamma,h}^n$ via POD.
  (Could also use POD-GREEDY).
- Use EIM to approximate coefficient functions, vectors, tensors depending nonlinearly on $\mathbf{\Psi}_h^n$.
- Similar to [Ballarin, Rozza, 2016] in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

Numerical Experiment

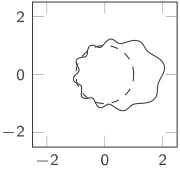
- Parameterization:
  - $\alpha \in [0.1, 1]$
  - $\beta \in [0.001, 0.1]$
  - $\delta_1, \delta_2 \in [0, 1]$
- Snapshots: 3^4
- FOM: 3988 + 7976 DOFS



$\delta_1 = 1, \delta_2 = 0$

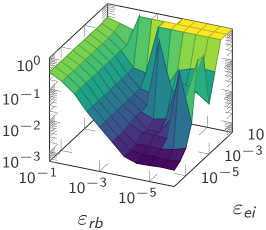


$\delta_1 = 0, \delta_2 = 1$

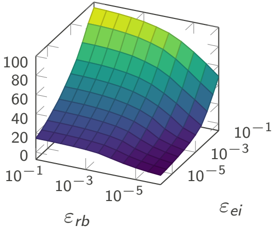


$\delta_1 = 1, \delta_2 = 1$

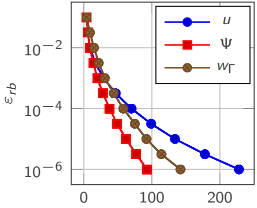
Rel. L^∞–L^∞–H^1 Error in u



Model Reduction Speedup



Basis Sizes



Global Mass Conservation

Concentration update

$$\int_{\hat{\Omega}} J^n \, \hat{u}_h^n \hat{v}_h \, d\mathbf{x} + \Delta t \int_{\hat{\Omega}} J^n \, \hat{u}_h^n \, \hat{\mathbf{w}}_h^{n-1} \cdot ((\mathbf{F}^n)^{-T} \cdot \nabla \hat{v}_h) d\mathbf{x}$$
$$+ \alpha \, \Delta t \int_{\hat{\Omega}} J^n \, ((\mathbf{F}^n)^{-T} \nabla \hat{u}_h^n) \cdot ((\mathbf{F}^n)^{-T} \nabla \hat{v}_h) \, d\mathbf{x} = \int_{\hat{\Omega}} J^{n-1} \, \hat{u}_h^{n-1} \hat{v}_h \, d\mathbf{x}.$$

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Concentration update

$$\int_{\hat\Omega} J^n\, \hat u_h^n \hat v_h\, d\mathbf{x} + \Delta t \int_{\hat\Omega} J^n\, \hat u_h^n\, \hat{\mathbf{w}}_h^{n-1} \cdot ((\mathbf{F}^n)^{-T} \cdot \nabla \hat v_h) d\mathbf{x}$$
$$+ \alpha\, \Delta t \int_{\hat\Omega} J^n\, ((\mathbf{F}^n)^{-T} \nabla \hat u_h^n) \cdot ((\mathbf{F}^n)^{-T} \nabla \hat v_h)\, d\mathbf{x} = \int_{\hat\Omega} J^{n-1}\, \hat u_h^{n-1} \hat v_h\, d\mathbf{x}.$$

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

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

Global Mass Conservation

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$$\int_{\hat\Omega} J^n\, \hat u_h^n \hat v_h\, dx + \Delta t \int_{\hat\Omega} J^n\, \hat u_h^n\, \hat{\mathbf{w}}_h^{n-1} \cdot ((\mathbf{F}^n)^{-T} \cdot \nabla \hat v_h) dx$$
$$+ \alpha\, \Delta t \int_{\hat\Omega} J^n\, ((\mathbf{F}^n)^{-T} \nabla \hat u_h^n) \cdot ((\mathbf{F}^n)^{-T} \nabla \hat v_h)\, dx = \int_{\hat\Omega} J^{n-1}\, \hat u_h^{n-1} \hat v_h\, dx.$$

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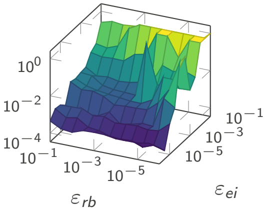
- Mass conservation is preserved by RB projection by adding 1 to RB for u_h^n.
- Inexact assembly of mass matrix due to EI destroys mass conservation.

Rel. Mass Conservation Error



Global Mass Conservation with EI

- Note that in 2D:

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

  where

$$m(\Phi_h^n, \mathbf{\Psi}_h^n, \hat{u}_h^n, \hat{v}_h) = \int_{\hat{\Omega}} \partial_x \Phi_{h_x}^n \cdot \partial_y \mathbf{\Psi}_{h_y}^n \cdot \hat{u}_h^n \cdot \hat{v}_h + \partial_x \Phi_{h_y}^n \cdot \partial_y \mathbf{\Psi}_{h_x}^n \cdot \hat{u}_h^n \cdot \hat{v}_h \, dx.$$

Global Mass Conservation with EI

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$$m(\Phi_h^n, \boldsymbol{\Psi}_h^n, \hat u_h^n, \hat v_h) = \int_{\hat\Omega} \partial_x \Phi_{h\,x}^n \cdot \partial_y \boldsymbol{\Psi}_{h\,y}^n \cdot \hat u_h^n \cdot \hat v_h + \partial_x \Phi_{h\,y}^n \cdot \partial_y \boldsymbol{\Psi}_{h\,x}^n \cdot \hat u_h^n \cdot \hat v_h \, dx.$$
- Could assemble mass matrix 4-tensor exactly.
- Relatively expensive.
(dim RB = 30 $\Longrightarrow$ 6MB for reduced tensor)
- 5-tensor in 3D!

Global Mass Conservation with EI

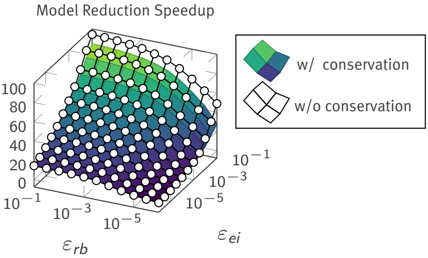
- Note that in 2D:

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

  where

$$m(\Phi_h^n, \mathbf{\Psi}_h^n, \hat{u}_h^n, \hat{v}_h) = \int_{\hat{\Omega}} \partial_x \Phi_{hx}^n \cdot \partial_y \mathbf{\Psi}_{hy}^n \cdot \hat{u}_h^n \cdot \hat{v}_h + \partial_x \Phi_{hy}^n \cdot \partial_y \mathbf{\Psi}_{hx}^n \cdot \hat{u}_h^n \cdot \hat{v}_h \, dx.$$

- 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 $m(\Phi_h^n, \mathbf{\Psi}_h^n, \hat{u}_h^n, 1)$ exactly and set corresponding row of mass matrix.



Thank you for your attention!

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Ohlberger, R, *Reduced Basis Methods: Success, Limitations and Future Challenges*, Proceedings of ALGORITMY 2016.

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/`

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. $\mathbf{\Psi}_h^n(\hat{\mathcal{T}}_h)$ has good shape regularity properties.
- Solve extension problem for $\hat{\mathbf{w}}_{\Gamma,h}^n$ 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?