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Nonlinear Model Order Reduction for Problems with Moving Discontinuities

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CASA Colloquium

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Outline

- Reduced Basis Methods for Nonlinear Evolution Equations: Trouble with Advection Dominated Problems.
- The FrozenRB scheme. (Joint work with Mario Ohlberger.)
- Nonlinear MOR via Lagrangian Formulation. (Joint work in progress with Christoph Lehrenfeld.)

Reduced Basis Methods

Parametric Model Order Reduction

Consider time-dependent parametric problems

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

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

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

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

Reduced Basis Methods: Three Basic Ideas

Objective

Compute

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

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

- **Idea 1:** State space projection:
  - Define approximation $\Phi_N : \mathcal{P} \to L^\infty([0, T]; V_N)$, $N := \dim V_N \ll \dim V_h$, via 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).

RB for Nonlinear Evolution Equations

Full order problem

Find $\Phi(\mu) := u_\mu \in L^\infty([0, T]; V_h)$ such that

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

where $\mathcal{L}_\mu : \mathcal{P} \times V_h \to V_h$ is a parametric (nonlinear) Finite Volume operator.

Reduced order problem

For given $V_N \subset V_h$, find $\Phi_N(\mu) := u_{\mu,N} \in L^\infty([0, T]; V_N)$ such that

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

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

Empirical Operator Interpolation (a.k.a. DEIM, EIM)

Problem: Still expensive to evaluate

$$P_{V_N} \circ \mathcal{L}_\mu : V_N \longrightarrow V_h \longrightarrow V_N.$$

Solution:

- Use locality of finite volume operators:

$$\text{to evaluate } M \text{ DOFs of } \mathcal{L}_\mu(u) \text{ we need } M' \leq C \cdot M \text{ DOFs of } u.$$

- Approximate

$$\mathcal{L}_\mu \approx \mathcal{I}_M[\mathcal{L}_\mu] := I_M \circ \mathcal{L}_{M,\mu} \circ R_{M'},$$

  where

$R_{M'} \colon V_h \to \mathbb{R}^{M'}$	restriction to M' DOFs needed for evaluation
$\mathcal{L}_{M,\mu} \colon \mathbb{R}^{M'} \to \mathbb{R}^M$	$\mathcal{L}_\mu$ restricted to M interpolation DOFs
$I_M \colon \mathbb{R}^M \to V_h$	linear combination with interpolation basis

- Use greedy algorithm to determine DOFs and interpolation basis from operator evaluations on appropriate solution trajectories.

Full Reduction

Reduced order problem (with EI)

Find $\Phi_N(\mu) := u_{\mu,N} \in L^\infty([0, T]; V_N)$ such that

$$\partial_t u_{\mu,N}(t) + \{(P_{V_N} \circ I_M) \circ \mathcal{L}_{M,\mu} \circ R_{M'}\}(u_{\mu,N}(t)) = 0, \quad u_{\mu,N}(0) = P_{V_N}(u_0).$$

Offline/Online decomposition

- Precompute the linear operators $P_{V_N} \circ I_M$ and $R_{M'}$ w.r.t. basis of V_N.
- Effort to evaluate $(P_{V_N} \circ I_M) \circ \mathcal{L}_{M,\mu} \circ R_{M'}$ w.r.t. this basis:

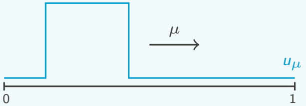
$$\mathcal{O}(MN) + \mathcal{O}(M) + \mathcal{O}(MN).$$

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

The FrozenRB scheme

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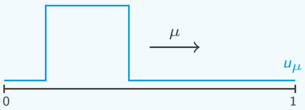

$$\partial_t u(t,x) + \mu \cdot \partial_x u_\mu(t,x) = 0$$
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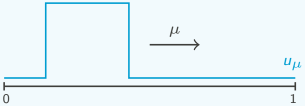

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Here: $d_N \sim N^{-1/2}$ w.r.t. $L^2([0,1])$.

However: We can describe solution easily as

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

Nonlinear Approximation

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

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

Nonlinear Approximation

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

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

- **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 than $u_\mu(t, x)$!

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

- Consider Lie group G acting on $\mathcal{V}$ and evolution equation of the form:

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

- Substituting the *ansatz* $u_\mu(t) = g_\mu(t).v_\mu(t)$ leads to:

$$\partial_t v_\mu(t) + g_\mu(t)^{-1}.\,\mathcal{L}_\mu(g_\mu(t).v_\mu(t)) + \mathfrak{g}_\mu(t).v_\mu(t) = 0$$
$$\mathfrak{g}_\mu(t) = g_\mu(t)^{-1}\partial_t g_\mu(t).$$

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- Have $\dim(G)$ additional degrees of freedom.
  $\rightarrow$ Add additional algebraic constraint (phase condition):

$$\Phi(v_\mu(t), \mathfrak{g}_\mu(t)) = 0.$$

- Further assume invariance of $\mathcal{L}_\mu$ under action of G:

$$h^{-1}.\,\mathcal{L}_\mu(h.w) = \mathcal{L}_\mu(w) \quad \forall h \in G, w \in \mathcal{V}.$$

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:

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

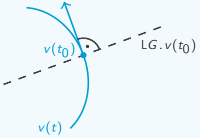
frozen PDAE

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

reconstruction equation

Orthogonality phase condition

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



Example: 2D-Shifts

Consider $G = \mathbb{R}^2$, $LG = \mathbb{R}^2$ acting via

$$g.u(x) := u(x-g), \quad x \in \mathbb{R}^2$$
$$\mathfrak{g}.u = -\mathfrak{g} \cdot \nabla u$$

The Method of Freezing for 2D-shifts

Solve

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

and

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

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

Test Problem

2D Burgers-type problem

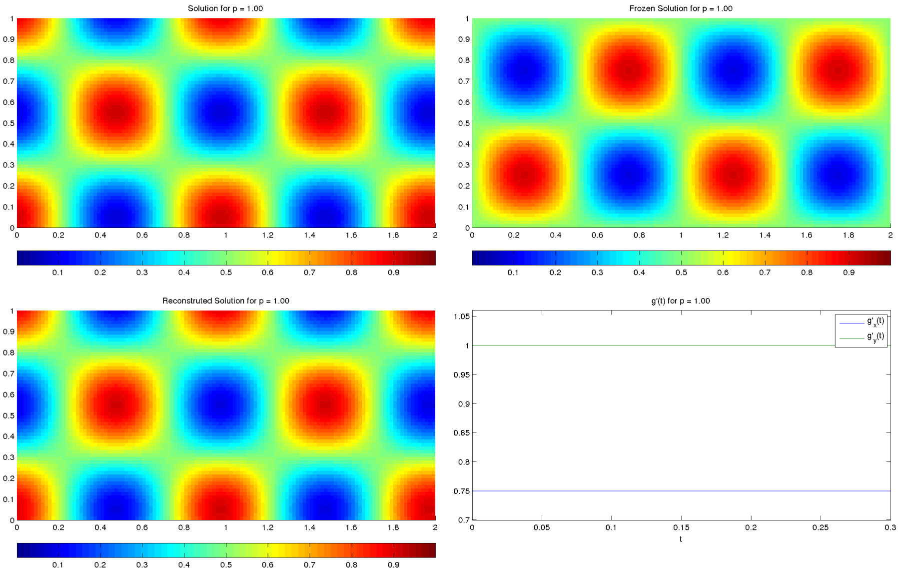
Solve on $\Omega = [0, 2] \times [0, 1]$:

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

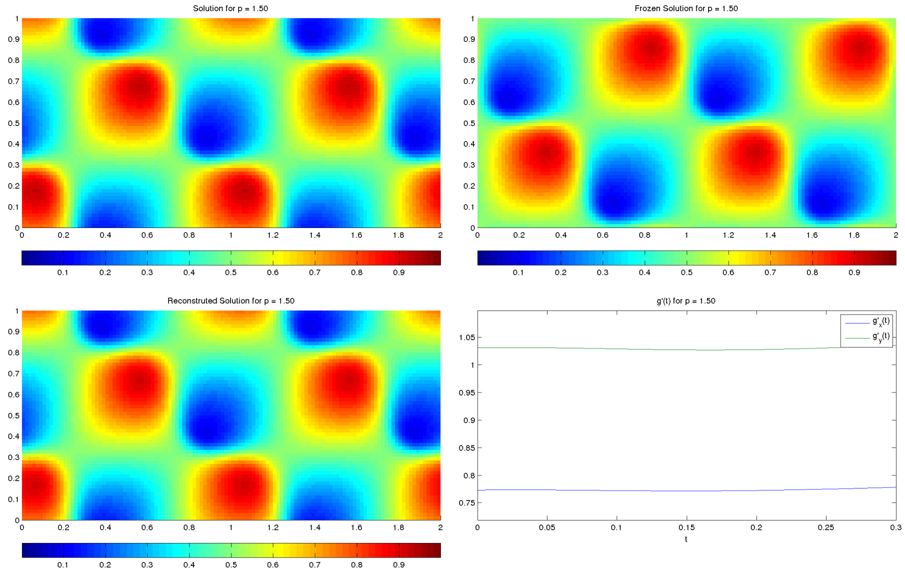
for $t \in [0, 0.3]$, $\vec{v} \in \mathbb{R}$ with periodic boundary conditions and $\mu \in \mathcal{P} = [1, 2]$.

- Finite volume (Lax-Friedrichs) space discretization on 240 x 120 grid.
- Explicit Euler time-stepping (200 time steps).
- Same problem as in [Drohmann, Haasdonk, Ohlberger, 2012].
- (The following videos are actually computed on a 120 x 60 grid.)

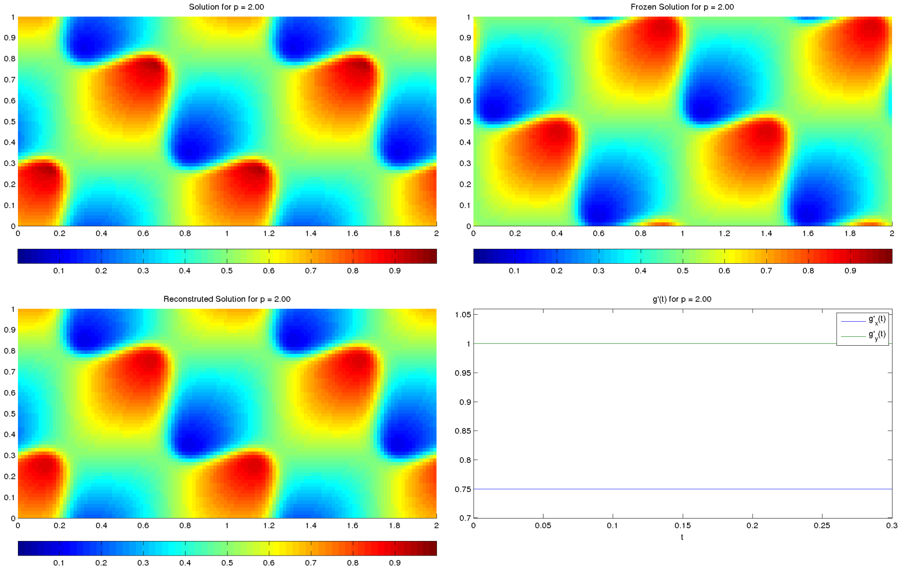
Frozen vs. Non-frozen Solution $(\mu = 1, \vec{v} = (0.75, 1)^T)$



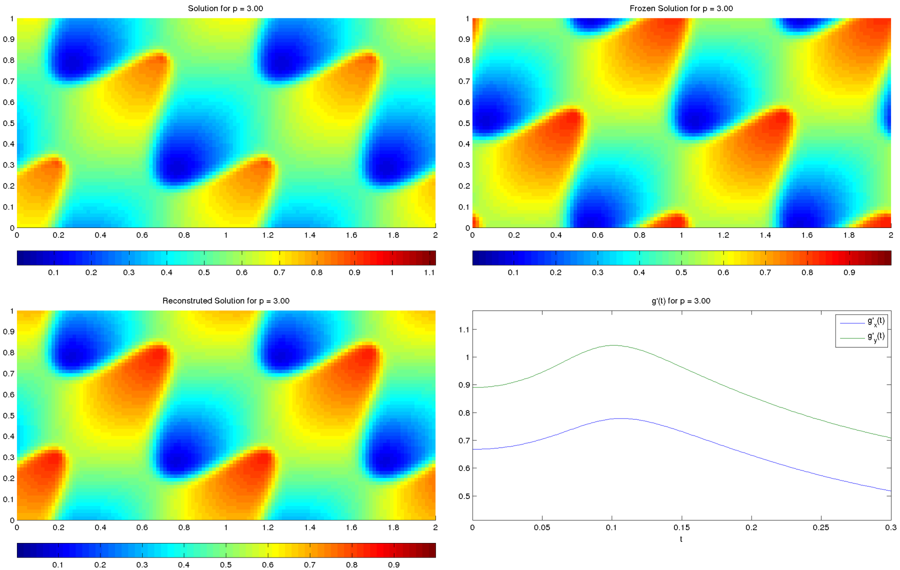
Frozen vs. Non-frozen Solution $(\mu = 1.5, \vec{v} = (0.75, 1)^T)$



Frozen vs. Non-frozen Solution $(\mu = 2, \vec{v} = (0.75, 1)^T)$



Frozen vs. Non-frozen Solution $(\mu = 3, \vec{v} = (0.75, 1)^T)$



Combining RB with the Method of Freezing

Combining RB with the Method of Freezing

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

Solve

$$\partial_t v_{\mu(t),N} + P_{V_N} \circ \mathcal{I}_M[\mathcal{L}_\mu](v_{\mu,N}(t)) - \mathfrak{g}_{\mu(t),N} \cdot (P_{V_N} \circ \nabla)(v_{\mu,N}(t)) = 0$$

$$\left[(\partial_{x_i} v_{\mu,N},\, \partial_{x_j} v_{\mu,N})\right]_{i,j} \cdot \left[\mathfrak{g}_{\mu,N}\right]_j = \left[(\mathcal{I}_M[\mathcal{L}_\mu](v_\mu),\, \partial_{x_i} v_{\mu,N})\right]_i$$

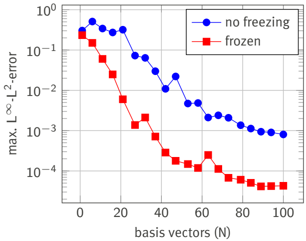
and

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

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 (small overhead).

Results for the Burgers Problem $(\vec{v} = (1,1)^T)$

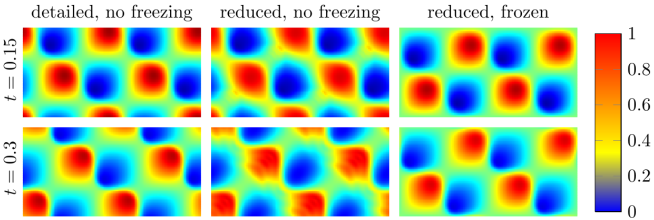


Left:

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

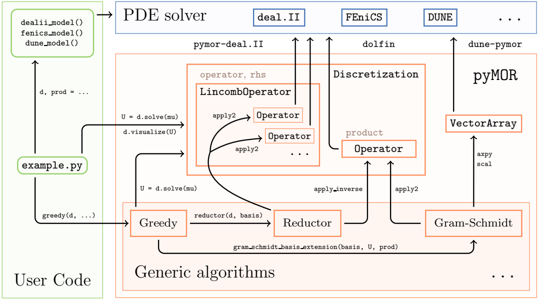
Bottom:

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



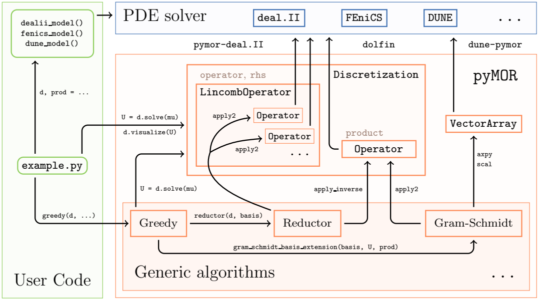
Advertisement Break

pyMOR – Model 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!

pyMOR – Model Reduction with Python



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pyMOR – RB Approximation of Li-Ion Battery Models

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MULTIBAT

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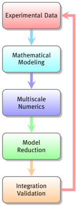

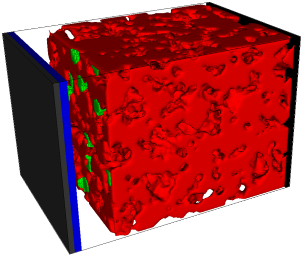

MULTIBAT: Gain understanding of degradation processes in rechargeable Li-Ion Batteries through mathematical modeling and simulation.

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

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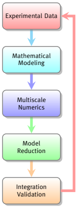

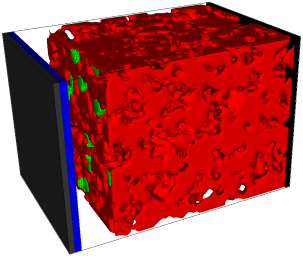

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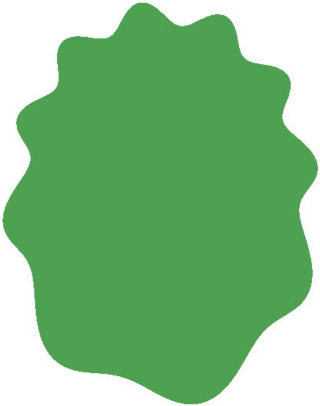
- Focus: Li-Plating.
- Li-plating initiated at interface between active particles and electrolyte.
- Need large microscale models which resolve active particle geometry.
- **New project coming!**

NOW HIRING

Nonlinear MOR via Lagrangian Formulation

A Free Boundary Problem

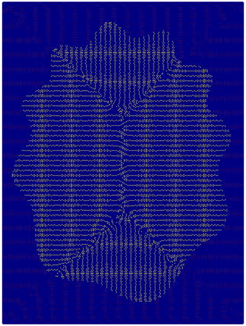


Osmotic cell swelling model

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

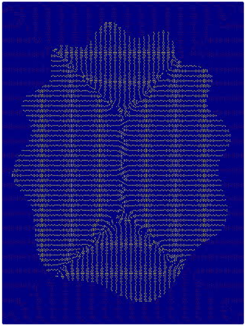
- u: concentration field
- u_0: concentration in outside
- $\mathcal{V}_n$: normal velocity of $\partial\Omega(t)$
- κ: curvature of $\partial\Omega(t)$

Eulerian Approximation in $L^2(\mathbb{R}^2)$

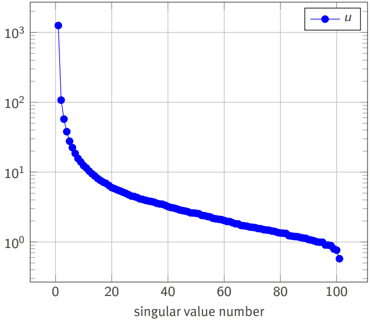


- Could consider $u(t) \in L^2(\Omega(t)) \hookrightarrow L^2(\mathbb{R}^2)$ to define joint approximation space.

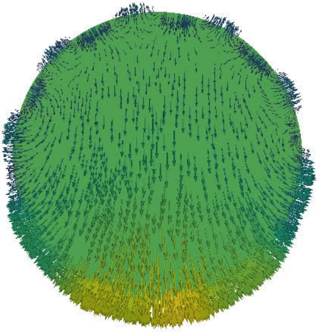
Eulerian Approximation in $L^2(\mathbb{R}^2)$



- Could consider $u(t) \in L^2(\Omega(t)) \hookrightarrow L^2(\mathbb{R}^2)$ to define joint approximation space.
- However, moving domain boundary leads to slow singular value decay of solution trajectory:



Lagrangian Formulation



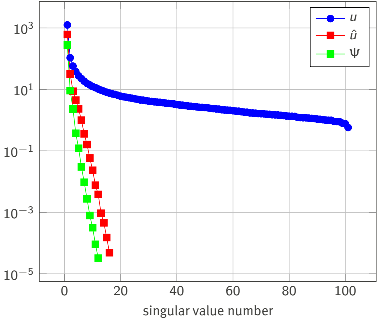
- Fix reference domain $\widehat{\Omega}$ and introduce deformation field $\Psi(t)$ s.t. $\Psi(t)(\widehat{\Omega}) = \Omega(t)$.
- Time-discrete concentration equation on $\widehat{\Omega}$,

$$\int_{\hat{\Omega}} J_{n+1}\hat{u}_{n+1}\hat{v}\,dx + \Delta t \int_{\hat{\Omega}} J_{n+1}\partial_t\Psi_{n+1}\cdot(\partial_x\Psi_{n+1}^{-T}\cdot\nabla_{\hat{x}}\hat{v})\hat{u}_{n+1}dx \\ + \Delta t\int_{\hat{\Omega}} \alpha J_{n+1}(\partial_x\Psi_{n+1}^{-T}\nabla_{\hat{x}}u)\cdot(\partial_x\Psi_{n+1}^{-T}\nabla_{\hat{x}}\hat{v})\,dx = \int_{\hat{\Omega}} J_n\hat{u}_n\hat{v}\,dx,$$

  where $J_n := |\det(\partial_x\Psi_n)|$.
- Compute updated Ψ_{n+1} on $\partial\widehat{\Omega}$, and extend to $\widehat{\Omega}$ via harmonic extension.

- After space discretization this corresponds to moving-mesh approach ($\to$ ALE), where $\Psi(t)(v)$ is the trajectory of the vertex v.

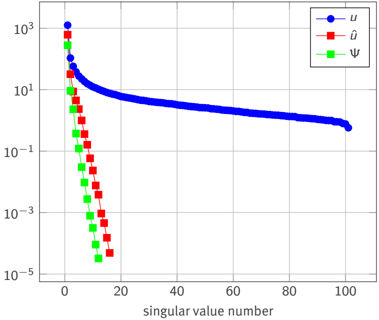
Nonlinear MOR via Lagrangian Formulation



Lagrangian ROM construction:

- Both trajectories $\hat{u}(t)$, $\Psi(t)$ are smooth and exhibit fast singular value decay.
- Compute low-rank approximation spaces $V_{\hat{u}}$, V_Ψ via POD.
- Note: V_Ψ acts nonlinearly on $V_{\hat{u}}$.
- Use EIM to approximate nonlinearities in coefficient functions.

Nonlinear MOR via Lagrangian Formulation



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Preliminary MOR results:

- $\mu \in \mathbb{R}^3$ (2D initial conditions + diffusivity)
- FOM: 3988 / 5592 DOFs
- ROM: 38 / 24 DOFs
- 40 / 42 / 21 / 20 / 2 / 33 EI points
- max rel. space-time error: $3 \cdot 10^{-3}$
- Speedup: 64

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