Registration-based model reduction of parameterized PDEs with sharp gradients

Tommaso Taddei Inria, MEMPHIS Team Trieste, SIAM Colloguia, June 18th 2020





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Objective

Parameterized Model Order Reduction (pMOR) for PDEs

The goal of pMOR is to reduce the **marginal** cost associated with the solution to parameterized problems.

pMOR is motivated by *real-time* and *many-query* problems design and optimization, UQ, control

Parameterized Model Order Reduction (pMOR) for PDEs

The goal of pMOR is to reduce the **marginal** cost associated with the solution to parameterized problems.

pMOR is motivated by *real-time* and *many-query* problems design and optimization, UQ, control

Given the **manifold** $\mathcal{M} = \{u_{\mu} : \mu \in \mathcal{P}\} \subset \mathcal{X}$, where $\mathcal{P} \subset \mathbb{R}^{P}$ is a compact set, and $(\mathcal{X}, \|\cdot\|)$ is an Hilbert space over $\Omega \subset \mathbb{R}^{d}$,

the goal of pMOR is to determine a **low-rank approx**imation \hat{u}_{μ} of u_{μ} that can be rapidly computed for any $\mu \in \mathcal{P}$.

pMOR: general recipe

Pb: find $u_{\mu} \in \mathcal{X} : A_{\mu}(u_{\mu}, v) = F(v)$ $\forall v \in \mathcal{Y} \ \mu \in \mathcal{P}$ **Approx:** $\hat{u}_{\mu} = \sum_{n=1}^{N} \widehat{\alpha}_{\mu}^{n} \zeta_{n}, \qquad \widehat{\alpha}^{n} : \mathcal{P} \to \mathbb{R}, \ \zeta_{n} \in \mathcal{X}$



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Offline stage: (performed once) compute $u_{\mu^1}, \ldots, u_{\mu^{n_{\text{train}}}}$ using a FE (or FV...) solver; construct $\{\zeta_n\}_{n=1}^N$ and define $\mathcal{Z}_N = \operatorname{span}\{\zeta_n\}_{n=1}^N$.

Online stage: (performed for any new $\bar{\mu} \in \mathcal{P}$) estimate the solution coefficients $\widehat{\alpha}_{\bar{\mu}}^1, \ldots, \widehat{\alpha}_{\bar{\mu}}^N$. estimate $\|\hat{u}_{\bar{\mu}} - u_{\bar{\mu}}\|$.

 $N \ll N_{\rm hf} = {
m dofs} \ {
m of} \ {
m the} \ {
m Full} \ {
m Order} \ {
m Model} \ \left({
m FOM} \atop {
m FE,...}
ight)$

pMOR: challenges

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Offline stage: (performed once) compute u_{μ1},..., u_{μⁿtrain} using a FE (or FV...) solver;
1. construct {ζ_n}^N_{n=1} and define Z_N = span{ζ_n}^N_{n=1}.

Online stage: (performed for any new $\bar{\mu} \in \mathcal{P}$)

- 2. estimate the solution coefficients $\widehat{\alpha}_{\overline{\mu}}^1, \ldots, \widehat{\alpha}_{\overline{\mu}}^N$.
- 3. estimate $\|\hat{u}_{\bar{\mu}} u_{\bar{\mu}}\|$.

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Successful applications of pMOR methods

Past and current research on pMOR focuses on

- 1. data compression
- 2. generalization
- 3. a posteriori error estimation



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 $egin{array}{c} \mathcal{Z}_{\mathsf{N}} \ \mathcal{Z}_{\mathsf{N}} &\Rightarrow \widehat{oldsymbol{lpha}}_{ar{\mu}} \ \| \widehat{oldsymbol{u}}_{ar{\mu}} - oldsymbol{u}_{ar{\mu}} \| \end{array}$

PR-scRBE: Patera, Huynh, Knezevic, Akselos S.A.
Port-Reduced static condensation RB Element method component-based structures, solid mechanics.

LRB-Ms: Ohlberger, Schindler, Localized RB Multiscale method multiscale problems, porous media.

Akselos is a software company that provides a commercial implementation of $\mathsf{PR}\text{-scRBE}$.

Data compression

Challenges: turbulence (wide spectrum of scales), approximation of shocks, boundary/internal layers...

nonlinear approximation procedures.

Generalization

Challenges: fragility of Galerkin models, nonlinearities. stabilized formulations; hyper-reduction.

Error estimation

Challenge: need for estimates of averaged QOIs. time-averaged error indicators.

Aim of this talk: focus on data compression

Abstract goal: given snapshots $\{u^k\}_{k=1}^{n_{\text{train}}}$, determine a low-rank approximation of $u : \mathcal{P} \to \mathcal{X}$.

Key feature: registration.

Related questions: not covered in this talk. 1. Adaptive sampling; choice of $\{\mu^k\}_k$

2. Online prediction of u_{μ} for given $\mu \in \mathcal{P}$.

Taddei; A registration method for model order reduction: data compression and geometry reduction; SISC, 2020.

Taddei, Zhang; *Space-time registration-based model reduction of parameterized one-dimensional hyperbolic PDEs;* submitted, 2020.

lollo, Taddei, Zhang; *Registration-based model reduction in complex two-dimensional geometries;* in preparation, 2020.

Registration-based data compression

Seek approximations s.t. $\widehat{u}_{\mu} := Z_N \,\widehat{\alpha}_{\mu} = \sum_{\substack{n=1 \ n=1}}^{N} (\widehat{\alpha}_{\mu})_n \zeta_n.$ Z_N is learned through the snapshots $\{u_{\mu^k}\}_{k=1}^{n_{\text{train}}} \subset \mathcal{M}.$ $\operatorname{strong/weak-Greedy, POD....}$ Seek approximations s.t. $\widehat{u}_{\mu} := Z_N \widehat{\alpha}_{\mu} = \sum (\widehat{\alpha}_{\mu})_n \zeta_n$.

 Z_N is learned through the snapshots $\{u_{\mu^k}\}_{k=1}^{n_{\text{train}}} \subset \mathcal{M}$. strong/weak-Greedy, POD,...

n=1

Notation: $Z_N = \operatorname{span} \{\zeta_n\}_{n=1}^N$ reduced space; $Z_N : \alpha \mapsto \sum_n \alpha_n \zeta_n$ reduced operator.

Linear compression methods naturally fit within the standard **variational framework**.

 $\begin{array}{l} \mathcal{A}_{\mu}\left(Z_{N}\,\widehat{\boldsymbol{\alpha}}_{\mu},Z_{N}\boldsymbol{\alpha}\,\right) \,=\, \mathcal{F}(Z_{N}\boldsymbol{\alpha}) \quad \forall\,\boldsymbol{\alpha}\in\mathbb{R}^{N}\\ & \quad \text{Galerkin projection.} \end{array}$

Proper orthogonal decomposition (Lumley, Sirovich,...)

- $\left[Z_N, \{\boldsymbol{\alpha}^k\}_k\right] = \text{POD}\left(\{u^k\}_k, (\cdot, \cdot), N\right), \qquad Z_N \boldsymbol{\alpha}^k = \Pi_{\mathcal{Z}_N} u^k$
- Method of snapshots (Sirovich, 1987)
- 1. Compute the Gramian matrix $C \in \mathbb{R}^{n_{\text{train}} \times n_{\text{train}}}$,
 - $\mathsf{C}_{k,k'} = \left(u^k, u^{k'}\right)$
- 2. Solve the eigenproblem: $\mathbf{C}\boldsymbol{\zeta}_n = \lambda_n \boldsymbol{\zeta}_n, \ \lambda_1 \geq \lambda_2 \geq \dots$
- 3. Return the linear operator $Z_N = [\zeta_1, \ldots, \zeta_N]$, where

$$\zeta_n = \sum_{k=1}^{N} (\zeta_n)_k u^k, \|\zeta_1\| = \ldots = \|\zeta_N\| = 1,$$

and

$$\{\boldsymbol{\alpha}^k\}_{k=1}^{n_{\text{train}}}, \text{ s.t. } (\boldsymbol{\alpha}^k)_n := (\zeta_n, u^k), n = 1, \dots, N.$$

Proper orthogonal decomposition (Lumley, Sirovich,...)

Equivalence with other methods: SVD, Karhunen–Loève expansion, principal component analysis.

Optimality:¹ The space \mathcal{Z}_N satisfies

 $n_{\rm train}$

$$\mathcal{Z}_N \in \arg \inf_{\mathcal{W} \subset \mathcal{X}, \dim(\mathcal{W}) = N} \sum_{k=1}^{n_{\mathrm{train}}} \|\Pi_{\mathcal{W}^{\perp}} u^k\|^2.$$

Furthermore, $\sum_{n=1}^{n_{\text{train}}} \|\Pi_{\mathcal{Z}_{N}^{\perp}} u^{k}\|^{2} = \sum_{n=1}^{n_{\text{train}}} \lambda_{n}$.

n=N+1

Practical performance: if $u \in C^{\infty}(\mathcal{P}; \mathcal{X})$, the eigenvalues λ_n are expected to decay exponentially².

¹Volkwein, 2011. Schmidt-Eckart-Young theorem. ²See Cohen, DeVore, Schwab, 2010 for the analysis.

k=1

Inadequacy of linear compression methods

Consider the parametric field $u_{\mu}(x) = \operatorname{sign} (x - \mu), x \in \Omega = (0, 1), \mu \in \mathcal{P} = \left[\frac{1}{3}, \frac{2}{3}\right].$ Then, $\inf_{\mathcal{W} \subset \mathcal{X}, \dim(\mathcal{W}) = N} \sup_{\mu \in \mathcal{P}} \|\Pi_{\mathcal{W}^{\perp}} u_{\mu}\|_{L^{2}(\Omega)} = \mathcal{O}\left(N^{-1/2}\right).$

Linear methods are ill-suited to deal with traveling fronts.

Taddei, Perotto, Quarteroni, 2015; Ohlberger, Rave, 2015.

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we have that $u_{\mu} \circ \Phi_{\mu} = \mathrm{sign}\left(2X - 1\right)$ is μ -independent .

 \Rightarrow Registration-based nonlinear compression

Taddei, Perotto, Quarteroni, 2015; Ohlberger, Rave, 2015.

We seek approximations of the form

 $u_{\mu} \approx \widehat{u}_{\mu} \circ \underline{\Phi}_{\mu}^{-1}$ where $\widehat{u}_{\mu} = Z_N \widehat{\alpha}_{\mu}$, $\underline{\Phi}_{\mu} = \mathrm{id} + W_M \widehat{a}_{\mu}$. The mapping $\underline{\Phi}_{\mu}$ should be a bijection in Ω for all $\mu \in \mathcal{P}$ and should make the mapped manifold

 $\widetilde{\mathcal{M}} := \left\{ u_{\mu} \circ \underline{\Phi}_{\mu} : \mu \in \mathcal{P} \right\}$

more amenable for linear compression methods (e.g., POD).

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A few references:

Ohlberger, Rave, 2013; Iollo, Lombardi, 2014; Taddei, Perotto, Quarteroni, 2015; Mojgani, Balajewicz, 2017; Mowlavi, Sapsis, 2018.

Overview

Objective develop a *general* registration-based generalization of POD.

 $\begin{bmatrix} Z_N, \{\boldsymbol{\alpha}^k\}_k \end{bmatrix} = \text{POD}\left(\{u^k\}_k, (\cdot, \cdot), N\right) \Rightarrow \\ \begin{bmatrix} Z_N, W_M, \{\boldsymbol{\alpha}^k\}_k, \{\mathbf{a}^k\}_k \end{bmatrix} = \text{RePOD}\left(\{u^k\}_k, (\cdot, \cdot), N, M\right).$

Agenda:

- 1. Registration for $\Omega = (0, 1)^2$.
- 2. Application to 1D shallow water equations.
- 3. Beyond rectangular domains.
- 3. Conclusions and perspectives.

General = independent of the underlying PDE model.

Generalization

Task: given Z_N , W_M , how can we compute α_{μ} , \mathbf{a}_{μ} ?

Generalization

Task: given Z_N, W_M , how can we compute $\alpha_{\mu}, \mathbf{a}_{\mu}$? Consider the problem: find $u_{\mu} \in \mathcal{X} = H_0^1(\Omega)$ s.t. $\int_{\Omega} \underline{\underline{K}}_{\mu} \nabla u_{\mu} \cdot \nabla v d\underline{x} = \int_{\Omega} f_{\mu} v \ d\underline{x} \ \forall \ v \in \mathcal{X}.$ Then, $\tilde{u}_{\mu} = u_{\mu} \circ \underline{\Phi}_{\mu}$ solves $(\underline{\underline{G}}_{\mu} = \nabla \underline{\Phi}_{\mu}, g_{\mu} = \det(\underline{\underline{G}}_{\mu}))$ $\int_{\Omega} \underline{\widetilde{K}}_{\mu} \nabla \widetilde{u}_{\mu} \cdot \nabla v d\underline{x} = \int_{\Omega} \widetilde{f}_{\mu} v \ d\underline{x} \ \forall \ v \in \mathcal{X},$ with $\underline{\underline{\breve{K}}}_{\mu} = g_{\mu} \underline{\underline{\underline{G}}}_{\mu}^{-1} \left(\underline{\underline{K}}_{\mu} \circ \underline{\underline{\Phi}}_{\mu} \right) \underline{\underline{\underline{G}}}_{\mu}^{-T}$ and $\widetilde{f}_{\mu} = g_{\mu} \left(f_{\mu} \circ \underline{\underline{\Phi}}_{\mu} \right)$.

Generalization

Task: given Z_N, W_M , how can we compute $\alpha_{\mu}, \mathbf{a}_{\mu}$? Consider the problem: find $u_{\mu} \in \mathcal{X} = H_0^1(\Omega)$ s.t. $\int_{\Omega} \underline{\underline{K}}_{\mu} \nabla u_{\mu} \cdot \nabla v d\underline{x} = \int_{\Omega} f_{\mu} v \ d\underline{x} \ \forall \ v \in \mathcal{X}.$ Then, $\tilde{u}_{\mu} = u_{\mu} \circ \underline{\Phi}_{\mu}$ solves $(\underline{\underline{G}}_{\mu} = \nabla \underline{\Phi}_{\mu}, g_{\mu} = \det(\underline{\underline{G}}_{\mu}))$ $\int_{\Omega} \underline{\widetilde{K}}_{\mu} \nabla \widetilde{u}_{\mu} \cdot \nabla v d\underline{x} = \int_{\Omega} \widetilde{f}_{\mu} v \ d\underline{x} \ \forall \ v \in \mathcal{X},$ with $\underline{\widetilde{K}}_{\mu} = g_{\mu} \underline{\underline{G}}_{\mu}^{-1} \left(\underline{\underline{K}}_{\mu} \circ \underline{\Phi}_{\mu} \right) \underline{\underline{G}}_{\mu}^{-T}$ and $\widetilde{f}_{\mu} = g_{\mu} \left(f_{\mu} \circ \underline{\Phi}_{\mu} \right)$. Projection-based methods can be used for the

approximation of \tilde{u}_{μ} as is.

Simultaneous approximation of mapping and solution is also possible. Zahr, Persson, 2018 (DG framework). 16

Registration for $\Omega=(0,1)^2$

Inputs: solution snapshots $\{u^k\}_k$.

Outputs: $Z_N, W_M, \{\alpha^k\}_k, \{\mathbf{a}^k\}_k \text{ s.t. } u^k \circ \underline{\Phi}^k \approx \widehat{u}^k,$ $\underline{\Phi}^k = \mathrm{id} + \underline{\varphi}^k, \ \underline{\varphi}^k = W_M \mathbf{a}^k, \ \widehat{u}^k = Z_N \alpha^k.$

1. Characterize a set of admissible mappings.

2. **Optimization-based registration.** Given Z_N and u^k , determine Φ^k .

3. **Parametric registration.** Use 2 to simultaneously build Z_N and the mappings $\{\underline{\Phi}^k\}_k$.

A class of admissible mappings: theoretical rationale

Consider $\underline{\Phi} = i\mathbf{d} + \underline{\varphi}$ where $\underline{\varphi} \in C^1$, $\underline{\varphi} \cdot \underline{n}\Big|_{\partial\Omega} = 0$. Then, $\underline{\Phi}$ is bijective in Ω if $\inf_{\underline{x}\in\Omega} g(\underline{x}) := \det(\nabla \underline{\Phi}(\underline{x})) > 0$.

Condition $\underline{\varphi} \cdot \underline{n} \Big|_{\partial \Omega} = 0$ allows tangential displacements.



Consider $\underline{\Phi} = \mathrm{id} + \underline{\varphi}$ where $\underline{\varphi} \in C^1$, $\underline{\varphi} \cdot \underline{n}\Big|_{\partial\Omega} = 0$. Then, $\underline{\Phi}$ is bijective in Ω if $\inf_{\underline{x}\in\Omega} g(\underline{x}) := \det(\nabla \underline{\Phi}(\underline{x})) > 0$.

We consider a space of tensorized polynomials of degree J + 1, that is $\underline{\varphi} \in \mathcal{W}_{hf}$, $\dim(\mathcal{W}_{hf}) = M_{hf} = 2J^2$.

We replace the constraint $\inf_{\underline{x}\in\Omega} g(\underline{x}) > 0$ with $\mathcal{C}(\varphi) :=$

$$\int_{\Omega} \exp\left(\frac{\epsilon - g(\underline{x})}{C_{\exp}}\right) + \exp\left(\frac{g(\underline{x}) - 1/\epsilon}{C_{\exp}}\right) \ d\underline{x} - \delta \le 0,$$

which provides a sufficient condition for bijectivity, for $\exp(\frac{\epsilon}{C_{\exp}}) \gg 1$ and moderate $\|\nabla g\|_{L^{\infty}(\Omega)}$.

Optimization-based registration

Given the target $u \in \mathcal{X}$, the spaces $\mathcal{Z}_N \subset L^2(\Omega)$, $\mathcal{W}_M \subset \mathcal{W}_{hf}$, we seek $\underline{\Phi} = \mathrm{id} + \varphi$ to minimize

$$\left(\min_{\psi\in\mathcal{Z}_N}\|u\circ\underline{\Phi}-\psi\|_{L^2(\Omega)}^2\right) + \xi \left|\underline{\varphi}\right|_{H^2(\Omega)}^2,$$

subject to $\mathcal{C}(\underline{\varphi}) \leq 0$.

Optimization-based registration

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$$\left(\min_{\psi\in\mathcal{Z}_{N}}\|u\circ\underline{\Phi}-\psi\|_{L^{2}(\Omega)}^{2}\right)+\xi\left|\underline{\varphi}\right|_{H^{2}(\Omega)}^{2},$$

subject to $\mathcal{C}(\underline{\varphi}) \leq 0$.

 $f(\underline{\Phi}; u) := \min_{\psi \in \mathcal{Z}_{N}} \|u \circ \underline{\Phi} - \psi\|_{L^{2}(\Omega)}^{2}$ proximity measure measures approximability of the target in the mapped domain.

 $\xi \left| \underline{\varphi} \right|_{H^2(\Omega)}^2$ is a regularization term to bound gradient and Hessian of $\underline{\varphi}$ (and thus ∇g).

Parametric registration $\{\underline{\Phi}^{\star,k}\}_k, \mathcal{Z}_N \leftarrow \{u^k\}_k, \mathcal{Z}_{N_0}, \mathcal{W}_{\mathrm{hf}}$

1. Set
$$\mathcal{Z}_{N=N_0} = \mathcal{Z}_{N_0}$$
, $\mathcal{W}_M = \mathcal{W}_{hf}$.
For $N = N_0, \dots, N_{max} - 1$
2. $[\underline{\varphi}^{\star,k}, f_{N,M}^{\star,k}] = \text{registration} (u^k, \mathcal{Z}_N, \mathcal{W}_M)$
 $k = 1, \dots, n_{\text{train}}$.
3. $[\mathcal{W}_M, \{\mathbf{a}^k\}_k] = \text{POD} (\{\underline{\varphi}^{\star,k}\}_{k=1}^{n_{\text{train}}}, tol_{\text{pod}}, (\cdot, \cdot)_{\star})$
if $\max_k f_{N,M}^{\star,k} < \text{tol}$, break
else
4. $\mathcal{Z}_{N+1} = \mathcal{Z}_N \cup \text{span} \{u_{u^{k^\star}} \circ \Phi^{\star,k^\star}\}$

 $k^{\star} = rg \max_k \mathfrak{f}_{N,M}^{\star,k}$

EndIf

EndFor

$$\mathfrak{f}_{N,M}^{\star,k} = \mathfrak{f}(\underline{\Phi}^{\star}; u^{k}) := \min_{\psi \in \mathcal{Z}_{N}} \| u^{k} \circ \underline{\Phi} - \psi \|_{L^{2}(\Omega)}^{2}$$

Parametric registration: remarks

The Greedy procedure simultaneously constructs the space \mathcal{Z}_N and the mappings $\{\Phi\}_k$.

If $\mathcal{W}_{hf} = \emptyset$ (no registration), \Rightarrow Strong Greedy.

In practice, the algorithm is applied to the modified snapshots $\{s^k = \mathfrak{s}(u^k)\}_k$ where $\mathfrak{s} : \mathcal{X} \to L^2(\Omega)$ is a **registration sensor.** more on s later.

 $\Rightarrow \text{ We cannot use the algorithm to build } \mathcal{Z}_{N}. \text{ Instead,} \\ \left[Z_{N}, \{\boldsymbol{\alpha}^{k}\}_{k}\right] = \text{POD}\left(\{u^{k} \circ \underline{\Phi}^{\star,k}\}_{k}, (\cdot, \cdot), N\right),$

POD reduction inside the for loop preserves the condition $\underline{\varphi} \in \mathcal{W}_M \Rightarrow \underline{\varphi} \cdot \underline{n}|_{\partial\Omega} = 0$; reduces dramatically the cost of subsequent iterations.

Application to 1D shallow water equations

Problem statement

Consider the problem: find u = [h, q]' such that $\begin{cases} \partial_t \underline{u} + \partial_x \underline{f}(\underline{u}) = -gh\partial_x b\underline{e}_2, \quad (x, t) \in \Omega = (0, L) \times (0, T) \\ q(0, t) = q_{\mathrm{in}, \mu}(t), \quad h(L, t) = 2, \quad \underline{u}(x, 0) = \underline{u}_0(x), \end{cases}$ with $\underline{f}(\underline{u}) = [q, \frac{q^2}{h} + \frac{g}{2}h^2]^T$, $b(x) = -0.2 + e^{-0.125(x-10)^4}$, $q_{\mathrm{in},\mu}(t) = q_0 \left(1 + \mu_1 t e^{-\frac{1}{2\mu_2^2}(t-0.05)^2}\right), \quad q_0 = 4.4,$ \underline{u}_0 is the steady-state solution obtained for $q_{\text{in},\mu} \equiv q_0$. $\mu = [\mu_1, \mu_2] \in \mathcal{P} = [2, 8] \times [0.1, 0.2].$

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The problem shares relevant features with **dam-break studies** with non-constant bathymetry.

Behavior of the free surface z = h + b

Application of the registration procedure

We train our model based on $n_{\text{train}} = 10^2$ samples; we assess performance based on $n_{\text{test}} = 20$ samples. We consider the **registration sensor** $\mathfrak{s}(u) = h$.

We initialize the template space $\mathcal{T}_{N_0=2} = \operatorname{span}\{h_0, h_{\overline{\mu}}\}$, we set $\xi = 10^{-4}$, $M_{\mathrm{hf}} = 128$, $tol_{\mathrm{pod}} = 10^{-4} \implies M = 5$

Application of the registration procedure

- We train our model based on $n_{\text{train}} = 10^2$ samples; we assess performance based on $n_{\text{test}} = 20$ samples.
- We consider the **registration sensor** $\mathfrak{s}(\underline{u}) = h$.
- We initialize the template space $\mathcal{T}_{N_0=2} = \operatorname{span}\{h_0, h_{\overline{\mu}}\}$, we set $\xi = 10^{-4}$, $M_{\text{hf}} = 128$, $tol_{\text{pod}} = 10^{-4} \Rightarrow M = 5$
- **Generalization** (for out-of-sample μ)
 - Mapping coefficients: RBF-based regression. Wendland, 2004.
 - **Solution coefficients:** Petrov-Galerkin proj + EQ. Farhat et al. 2015; Yano, 2019.

Taddei, Zhang, 2020 (submitted).

Behavior of the registered free surface z = h + b

Performance of the registration procedure



Performance of the ROM



Beyond rectangular domains

Example: $\Omega = \mathcal{B}_{R=1}(\underline{0})$, consider bijections $\underline{\Phi}_1$, $\underline{\Phi}_2$ and assume that $\underline{\Phi}_1(\underline{x}) \neq \underline{\Phi}_2(\underline{x})$ at $\underline{x} \in \partial \Omega$.

Then, $\underline{\Phi}_t := t\underline{\Phi}_1 + (1-t)\underline{\Phi}_2$ is not a bijection in Ω for any $t \in (0, 1)$.

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Conclusion: affine mappings — $\underline{\Phi} = id + W_M a$ — cannot properly capture finite deformations over non-straight edges.

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Conclusion: affine mappings — $\underline{\Phi} = id + W_M a$ — cannot properly capture finite deformations over

non-straight edges.

Question: how can we characterize admissible mappings?

Model problem: potential flow past an airfoil

Consider the problem: $-\Delta u_{\mu} = 0$ in Ω , $u_{\mu}|_{\partial\Omega} = h_{\mu}$, $\mu = [\mu_1, \mu_2], \ \Omega = \Omega_{\text{box}} \setminus \Omega_{\text{naca}}$.



Define G_{naca} s.t. $\partial \Omega_{\text{naca}} = \{ \underline{x} : G_{\text{naca}}(\underline{x}) = 0 \}.$

Strategy 1: constrained approach (I)

We consider mappings $\underline{\Phi} = \mathtt{id} + \varphi$ over Ω_{box} such that

- 1. $\underline{\varphi} \cdot \underline{n}|_{\partial\Omega_{\mathrm{box}}} = 0$, $\mathcal{C}(\underline{\varphi}) \leq 0$ same as before
- 2. $\sum_{i} |G_{\text{naca}}(\underline{\Phi}(\underline{x}_{i}))|^{2} tol \leq 0.$ new 3. $\underline{\Phi}(\underline{x}_{i}^{\text{fix}}) = \underline{x}_{i}^{\text{fix}}.$ new

Constraints in 1. enforce bijectivity in Ω_{box} .

Constraint in 2. controls $\max_{\underline{x}\in\partial\Omega} \operatorname{dist}(\underline{\Phi}(\underline{x}),\partial\Omega)$.

Constraint in 2 is nonlinear and non-convex \Rightarrow similar per-iteration cost

Constraint in 3. deals with "difficult points".

 $\underline{x}_{1}^{\text{fix}} = [0, 0], [1, 0].$

The additional constraints should ultimately control the Hausdorff distance $\operatorname{dist}_{\operatorname{H}}(\underline{\Phi}(\partial\Omega), \partial\Omega) =$

 $\max\left\{\max_{\underline{x}\in\partial\Omega}\operatorname{dist}\left(\underline{\Phi}(\underline{x}),\partial\Omega\right), \ \max_{\underline{x}\in\partial\Omega}\operatorname{dist}\left(\underline{x},\underline{\Phi}(\partial\Omega)\right)\right\}.$

Theoretical rationale: under proper assumptions on the domain Ω and the mapping $\underline{\Phi}$, we can control $\operatorname{dist}_{\mathrm{H}}(\underline{\Phi}(\partial\Omega), \partial\Omega)$ in terms of $\max_{\underline{x}\in\partial\Omega}\operatorname{dist}(\underline{\Phi}(\underline{x}), \partial\Omega)$.

Observation: constraint 3 plays a decisive role when there are corners.

Iollo, Taddei, Zhang, (in preparation)

Strategy 2: partitioned approach (I)

Introduce a partition of Ω , $\{\Omega_q\}_{q=1}^{N_{\rm dd}}$ such that Ω_q is isomorphic to $\widehat{\Omega} = (0, 1)^2$.



 $\underline{\Phi}$ should be (i) globally continuous, and (ii) locally bijective, $\underline{\Phi}(\Omega_q) = \Omega_q$, $q = 1, \dots, N_{dd}$.

Local bijectivity is equivalent to bijectivity of $\underline{\Phi}_q$ in $\overline{\Omega}$. admissible class naturally defined.

Implementation borrows several elements from classic isoparametric spectral element discretizations. KZ Korczak, AT Patera, 1986. Local bijectivity is equivalent to bijectivity of $\underline{\Phi}_q$ in $\overline{\Omega}$. admissible class naturally defined.

Implementation borrows several elements from classic isoparametric spectral element discretizations. KZ Korczak, AT Patera, 1986.

Pro: possibility to approximate exactly the geometry with polynomials of moderate order.

Con: local bijectivity implies global bijectivity but it is a much stronger condition \Rightarrow limited approximation power.

Consider $n_{\text{train}} = 50$ snapshots for training and $n_{\text{test}} = 100$ snapshots for testing.

Consider a fully non-intrusive approach (RBF regression for $\hat{\alpha}_{\mu}, \hat{\mathbf{a}}_{\mu}$).

We measure performance using

$$egin{aligned} & E^{ ext{geo}}_{\Phi}(\mu) = \max_{i \in \mathcal{I}_{ ext{naca}}} \left| \mathcal{G}_{ ext{naca}} \left(\underline{\Phi}_{\mu}(\underline{x}^{ ext{hf}}_{i})
ight)
ight|, \ & E^{ ext{sol}}_{\Phi}(\mu) = rac{\|u_{\mu} - \widehat{u}_{\mu} \circ \underline{\Phi}^{-1}_{\mu}\|_{H^{1}(\Omega)}}{\|u_{\mu}\|_{H^{1}(\Omega)}}. \end{aligned}$$

 $\{\underline{x}_i^{\text{hf}}\}_{i \in \mathcal{I}_{\text{naca}}}$ nodes of the FE mesh on the airfoil.

Numerical results: geometrical error





Conclusions and perspectives

We propose a **general** = independent of the underlying PDE model registration-based compression strategy for pMOR, $u_{\mu} \approx \widehat{u}_{\mu} \circ \underline{\Phi}_{\mu}^{-1}$ with $\widehat{u}_{\mu} = Z_N \alpha_{\mu}$ and $\underline{\Phi}_{\mu} = \text{id} + W_M a_{\mu}$

We illustrate the application to one-dimensional systems of hyperbolic PDEs (shallow-water equations).

We illustrate the extension to non-rectangular domains (potential flow).

Several theoretical and methodological challenges need to be addressed.

- 1. Development of fully-intrusive schemes for the simultaneous prediction of $\widehat{\alpha}_{\mu}$ and \widehat{a}_{μ} . Link with Zahr, Persson, JCP, 2018.
- Investigation of performance for relevant problems. in CFD self-similarity, transport.
- 3. Mathematical analysis.

for what problems shall registration help?

Geometry reduction

Given the parameterized domains $\{\Omega_{\mu}\}_{\mu\in\mathcal{P}}\subset\mathbb{R}^{d}$, the goal of **geometry reduction** is to determine a **low-rank mapping** $\underline{\Phi}$ and a domain $\widehat{\Omega}$ such that $\underline{\Phi}_{\mu}$ is invertible in $\widehat{\Omega}$ and $\underline{\Phi}_{\mu}(\widehat{\Omega}) \approx \Omega_{\mu}, \quad \forall \mu \in \mathcal{P}.$

pMOR techniques in parameterized domains:AE Løvgren, Y Maday, and EM Rønquist. M2AN, 2006;G Rozza, DBP Huynh, AT Patera, ARCME, 2008;A Manzoni, A Quarteroni, G Rozza, IJNME, 2012.

and many others. 43

Geometry reduction

Given the parameterized domains $\{\Omega_{\mu}\}_{\mu\in\mathcal{P}}\subset\mathbb{R}^{d}$, the goal of **geometry reduction** is to determine a **low-rank mapping** ϕ and a domain Ω such that $\underline{\Phi}_{\mu}$ is invertible in $\widehat{\Omega}$ and $\underline{\Phi}_{\mu}(\widehat{\Omega}) \approx \Omega_{\mu}$, $\forall \mu \in \mathcal{P}$. This is equivalent to reducing $\mathcal{M}^{\text{geo}} := \{ u_{\mu} := \mathbb{1}_{\Omega_{\mu}} \}_{\mu \in \mathcal{P}}$ to a singleton $\hat{u} = \mathbb{1}_{\hat{0}}$. Joint work with F Ballarin, E Delgado, A Mola, and G Rozza.

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CEMRACS 2021

Data Assimilation and Model Reduction in high-dimensional problems

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Thank you for your attention!

Please visit math.u-bordeaux.fr/~ttaddei/ for further information.