Registration-based model reduction of parameterized PDEs

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Joint work with L Zhang (Inria)

Collaborators:[1]

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Sponsors:

IdEx Bordeaux (projet émergence)	2020 - 2021
EDF	2020 - 2021
ANDRA	2019 - 2022

[1] TT would also like to thank Y Maday, P Mounoud, AT Patera and M Yano for fruitful discussions.

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.

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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 approximation** $\widehat{U}_\mu$ of U_μ that can be rapidly computed for any $\mu \in \mathcal{P}$.

pMOR: general recipe

Pb: find $U_\mu \in \mathcal{X} : R_\mu(U_\mu, v) = 0, \qquad \forall\, v \in \mathcal{Y},\ \mu \in \mathcal{P}$

Approx: $\widehat{U}_\mu = \mathrm{Z}(\widehat{\boldsymbol{\alpha}}_\mu), \qquad \mathrm{Z} : \mathbb{R}^n \to \mathcal{X},\ \widehat{\boldsymbol{\alpha}} : \mathcal{P} \to \mathbb{R}^n$

Offline stage: (performed once)

compute high-fidelity estimates of U, $\{U_{\mu^k}^{\mathrm{hf}}\}_{k=1}^{n_{\mathrm{train}}}$;

determine the low-rank approximation $\mathrm{Z} : \mathbb{R}^n \to \mathcal{X}$.

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

solve a reduced-order model (ROM) to estimate $\widehat{\boldsymbol{\alpha}}_{\mu'}$;

estimate the error $\|\widehat{U}_{\mu'} - U_{\mu'}\|$.

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pMOR literature: Patera, Maday, Farhat, Quarteroni, Ohlberger,...

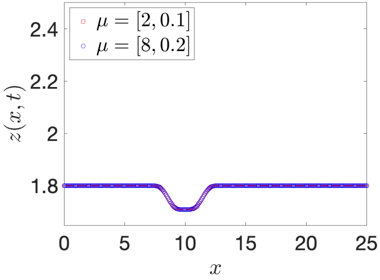
Recent review: Handbook on MOR, De Gruyter, 2021.

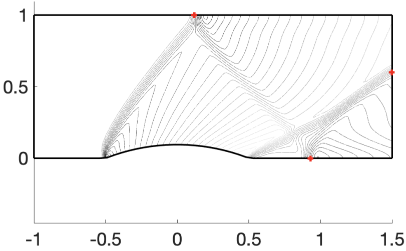
Problem of interest: hyperbolic conservation laws

Goal: model reduction for hyperbolic systems of PDEs.

In this talk, we consider:

- 1D shallow water equations over a bump with parametric inflow;
- 2D compressible Euler equations with varying free-stream velocity over a parametric bump.

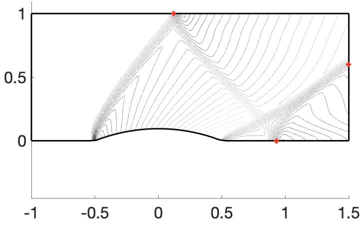




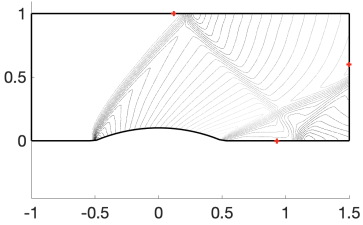
Major challenges

Application of pMOR to hyperbolic PDEs presents unique challenges.

1. CFD simulations are expensive $\Rightarrow$ ROMs need to be trained using few snapshots. small data pb
2. Linear approximations are inadequate for transport.
3. Mesh should be refined close to shocks; ROMs must be defined over a common mesh.



$\mathrm{Mach} = 1.7$



$\mathrm{Mach} = 1.8$

Objective of this work

Devise a registration-based projection-based multi-fidelity MOR approach for parameterized conservation laws.

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Devise a registration-based projection-based multi-fidelity MOR approach for parameterized conservation laws.

Registration: given snapshots $\{U^{\mathrm{hf}}_{\mu^k}\}_k$, seek a mapping $\Phi : \Omega \times \mathcal{P} \to \Omega$ to align moving structures in a reference configuration.

Projection-based MOR provides a rigorous framework to build the ROM for $\widehat{\boldsymbol{\alpha}}_\mu$.

LSPG projection	Carlberg et al., 2011
Element-wise empirical quadrature	Farhat et al., 2015; Yano, 2019.

Multi-fidelity training offers a systematic framework to reduce offline costs.

Agenda of the talk

1. Registration.
2. Projection-based model reduction.
3. Multi-fidelity training.
4. Numerical results.
    - Euler equations past a bump.
    - Shallow water equations.
5. Analysis: expressivity of nonlinear approximations.
6. Conclusions.

Registration

- Spectral (element) maps
- Optimization statement
- Parametric registration (Greedy+POD)

General plan

Task: given $\{U_{\mu^k}\}_{k=1}^{n_{\rm train}}$, compute $\Phi : \Omega \times \mathcal{P} \to \mathbb{R}^d$.

1. Choose approximation $\mathcal{N} : \mathcal{A}_{\rm bj} \subset \mathbb{R}^M \to {\rm Lip}(\Omega; \mathbb{R}^d)$.

   Desiderata: high expressive power;
   easy to enforce bijectivity.

2. Compute $\Phi^k = \mathcal{N}(\mathbf{a}_{\rm hf}^k)$ for $k = 1, 2, \ldots, n_{\rm train}$.

   Solution to minimization pb.

3. Apply POD to obtain $\Phi^k \approx \mathcal{N}(\mathbf{W}\mathbf{a}^k)$,

   $\mathbf{a}^k \in \mathbb{R}^m$, $m \ll M$.

4. Use regression algorithm (e.g., RBF) to learn

   $\mu \in \mathcal{P} \mapsto \widehat{\mathbf{a}}_\mu \in \mathbb{R}^m \quad \Rightarrow \Phi_\mu := \mathcal{N}(\mathbf{W}\widehat{\mathbf{a}}_\mu)$.

Taddei, SISC 2020; Taddei, Zhang, M2AN, 2021.
Taddei, Zhang, *submitted*, 2021.

Registration

- Spectral (element) maps
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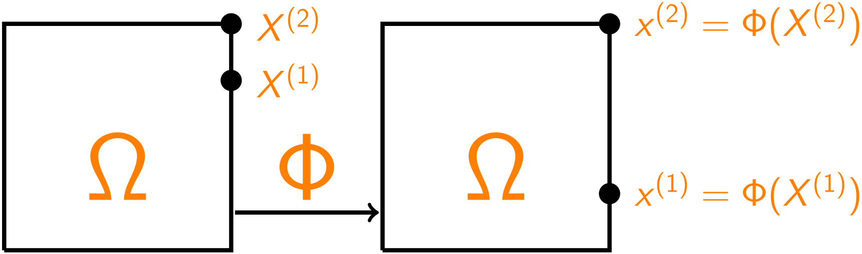
Choice of $\mathcal{N}$ for $\Omega = (0,1)^2$: spectral maps

Thm: Consider $\Phi = \mathtt{id} + \varphi$ where $\varphi \in C^1$, $\varphi \cdot n\big|_{\partial\Omega} = 0$.

Then, Φ is bijective in Ω if $\inf_{x \in \Omega} g(x) = \det(\nabla\Phi(x)) > 0$.

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



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Then, Φ is bijective in Ω if $\inf_{x\in\Omega} g(x) = \det(\nabla\Phi(x)) > 0$.

Choice of $\mathcal{N}$: set $\mathcal{N}(\mathbf{a}) = \mathtt{id} + \sum_{i=1}^{M} (\mathbf{a})_i \varphi_i$, where $\varphi_1, \ldots, \varphi_M$ are tensorized polynomials, $\varphi_i \cdot n\big|_{\partial\Omega} = 0$.

Bijectivity: define the admissible class of mappings

$$\mathcal{A}_{\mathrm{bj}} := \left\{ \mathbf{a} \in \mathbb{R}^M : \inf_{x\in\Omega} g(x;\mathbf{a}) = \det\left(\nabla\mathcal{N}(\mathbf{a})\right) > 0 \right\}$$

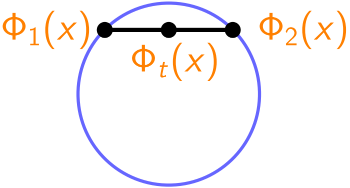
and the proxy $\mathcal{A}'_{\mathrm{bj}} := \left\{ \mathbf{a} \in \mathbb{R}^M : \mathcal{C}(\mathbf{a}) \le \delta \right\}$ with

$$\mathcal{C}(\mathbf{a}) := \int_\Omega \exp\left(\frac{\epsilon - g(x;\mathbf{a})}{C_{\exp}}\right) + \exp\left(\frac{g(x;\mathbf{a}) - 1/\epsilon}{C_{\exp}}\right) dx.$$

Limitation of affine mappings for non-rectangular domains

Example: $\Omega = \mathcal{B}_{R=1}(0)$, consider bijections Φ_1, Φ_2 and assume that $\Phi_1(x) \neq \Phi_2(x)$ at $x \in \partial\Omega$.

Then, $\Phi_t := t\Phi_1 + (1-t)\Phi_2$ is not a bijection in Ω for any $t \in (0, 1)$.



Conclusion: affine mappings — $\mathcal{N}(\mathbf{a}) = \mathtt{id} + W_M\mathbf{a}$ — cannot properly capture finite deformations over non-straight edges.

Special case: annular domains. Taddei, Zhang, 2021.

Partitioned approach based on spectral element maps (I)

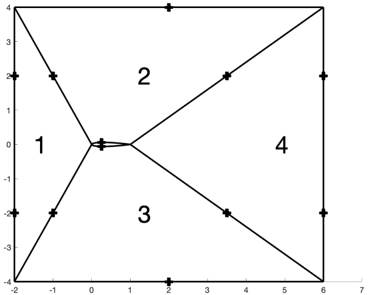
Introduce a partition of Ω, $\{\Omega_q\}_{q=1}^{N_{\rm dd}}$ such that Ω_q is isomorphic to $\widehat{\Omega} = (0,1)^2$. Define mappings $\Psi_q : \widehat{\Omega} \to \Omega_q$ (e.g., Gordon-Hall maps), $q = 1, \ldots, N_{\rm dd}$.

Consider mappings of the form

$$\mathcal{N}(\cdot) = \sum_{q=1}^{N_{\rm dd}} \Psi_q \circ \Phi_q \circ \Psi_q^{-1} \mathbb{1}_{\Omega_q}$$

where

$$\Phi_q = \mathtt{id} + W_M^q \mathbf{a} : \widehat{\Omega} \to \widehat{\Omega}.$$



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

Partitioned approach based on spectral element maps (II)

- Local bijectivity is equivalent to bijectivity of Φ_q in $\widehat{\Omega}$.

  admissible class naturally defined.

- Implementation borrows several elements from classic isoparametric spectral element discretizations.

  KZ Korczak, AT Patera, 1986.

- **Parameterized geometries:** Consider $\Psi_q : \widehat{\Omega} \times \mathcal{P} \to \mathbb{R}^2$, and define $\bar{\mu} \in \mathcal{P}$, $\Omega_q = \Omega_{q,\bar{\mu}}$. Then,

$$\mathcal{N}_\mu(\mathbf{a}) = \sum_{q=1}^{N_{\mathrm{dd}}} \Psi_{q,\mu} \circ \Phi_q(\mathbf{a}) \circ {\Psi_{q,\bar{\mu}}}^{-1} \, \mathbb{1}_{\Omega_q} : \Omega_{\bar{\mu}} \to \Omega_\mu.$$

$\Psi^{-1}_{1,\bar{\mu}}, \ldots, \Psi^{-1}_{N_{\mathrm{dd}},\bar{\mu}}$ can be precomputed offline.

Registration

- Spectral (element) maps
- Optimization statement
- Parametric registration (Greedy+POD)

Define the mesh $\mathcal{T}_{\mathrm{hf}} = \left(\{x_j^{\mathrm{hf}}\}_j, \mathtt{T}\right)$, with nodes $\{x_j^{\mathrm{hf}}\}_j$ and connectivity matrix $\mathtt{T}$, and the associated FE space $\mathcal{X}_{\mathrm{hf}}$.

Given $w \in \mathcal{X}_{\mathrm{hf}}$, denote by $\mathbf{w} \in \mathbb{R}^N$ the associated vector representation.

Given $\Phi : \Omega \to \Omega$, define the mapped mesh $\Phi\left(\mathcal{T}_{\mathrm{hf}}\right) = \left(\{\Phi\left(x_j^{\mathrm{hf}}\right)\}_j, \mathtt{T}\right)$.

Definition. Φ is $\mathcal{T}_{\mathrm{hf}}$-*bijective* if the element mappings

$$\Psi_{k,\Phi}^{\mathrm{hf}}(x) = \sum_{i=1}^{n_{\mathrm{lp}}} \Phi(x_{i,k}^{\mathrm{hf}})\hat{\phi}_i(x)$$

are invertible.

Optimization statement (I)

Informal statement

Given snapshots $\{U^k := U_{\mu^k}\}_k$ and the approximation $\mathcal{N} : \mathbb{R}^M \to \mathrm{Lip}(\Omega; \mathbb{R}^d)$, we seek $\mathbf{a}^k \in \mathbb{R}^M$ to minimize

$$\min_{\zeta \in \mathcal{Z}_n} \|U^k \circ \Phi^k - \zeta\|^2_{L^2(\Omega)}$$ over all bijective maps.

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Challenges

- $\Phi^k(\mathcal{T}_{\mathrm{hf}})$ should be a proper mesh of Ω.
- the choice of $\mathcal{Z}_n$ is inherently coupled with the problem of finding Φ. more on this later.

Optimization statement(II)

Given the target $U \in \mathcal{X}$, the space $\mathcal{Z}_n \subset \mathcal{X}$, and $\mathcal{N}$,
we seek $\Phi = \mathcal{N}(\mathbf{a})$ to minimize

$$\left(\min_{\psi \in \mathcal{Z}_n} \| U \circ \Phi - \psi \|^2_{L^2(\Omega)} \right) + \xi \, \| \mathbf{A}^{1/2}_{\mathrm{stab}} \mathbf{a} \|_2^2 + \xi' \, \mathfrak{R}_{\mathrm{msh}}(\Phi),$$

subject to $\mathcal{C}(\Phi) \le 0$.

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

$\mathfrak{f}(\Phi; u) := \min_{\psi \in \mathcal{Z}_n} \| U \circ \Phi - \psi \|^2_{L^2(\Omega)}$ **proximity measure**

measures approximability of the target in the mapped domain.

$\| \mathbf{A}^{1/2}_{\mathrm{stab}} \mathbf{a} \|_2 = \sum_q \left| \Phi_q \right|^2_{H^2(\widehat{\Omega})}$ is a regularization term to bound gradient and Hessian of Φ (and thus ∇g).

Given the target $U \in \mathcal{X}$, the space $\mathcal{Z}_n \subset \mathcal{X}$, and $\mathcal{N}$, we seek $\Phi = \mathcal{N}(\mathbf{a})$ to minimize

$$\left(\min_{\psi \in \mathcal{Z}_n} \| U \circ \Phi - \psi \|_{L^2(\Omega)}^2 \right) + \xi \, \| \mathbf{A}_{\mathrm{stab}}^{1/2} \mathbf{a} \|_2^2 + \xi' \, \mathfrak{R}_{\mathrm{msh}}(\Phi),$$

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

Mesh distortion penalization: Zahr, Persson, 2018

$$\mathfrak{R}_{\mathrm{msh}}(\Phi) = \sum_{k=1}^{N_{\mathrm{e}}} |\mathtt{D}_k| \exp\left(\frac{\| \nabla \Psi_{k,\Phi}^{\mathrm{hf}} \|_{\mathrm{F}}^2}{|\det(\nabla \Psi_{k,\Phi}^{\mathrm{hf}})|} - \mathfrak{f}_{\mathrm{msh,max}} \right)$$

enforces *discrete bijectivity* wrt $\mathcal{T}_{\mathrm{hf}}$.

Registration sensor

Pre-processing U improves performance and facilitates registration $\Rightarrow$

replace U with registration sensor $\mathfrak{s}(U) \in [L^2(\widehat{\Omega})]^{N_{\mathrm{dd}}}$.

$\mathfrak{s}(U)$ should "highlight" moving features that are troubling for linear approximations. $\leftrightarrow$ sensors for shock-capturing.

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Euler eqs: $\mathfrak{s}(U) = \mathrm{Ma}$.

We define $\mathfrak{s}(U)$ over a structured mesh to speed up registration.

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$$\mathfrak{f}(\Phi^{\star,k}; U) = \min_{\psi \in \mathcal{S}_n} \|\mathfrak{s}(U) \circ \Phi^{\star,k} - \psi\|^2_{L^2(\widehat{\Omega})},$$

$\mathcal{S}_n$ = template space

Registration

- Spectral (element) maps
- Optimization statement
- Parametric registration (Greedy+POD)

Parametric registration $\{\Phi^{\star,k}\}_k \leftarrow \{U^k\}_k, \mathcal{S}_{n_0}, \mathcal{N}$

1. Set $\mathcal{S}_{n=n_0} = \mathcal{S}_{n_0}$, $\mathbf{W}_m = \mathbb{1}_M$.

For $\quad n = n_0, \ldots, n_{\max} - 1$

2. $[\mathbf{a}^{\star,k}, \mathfrak{f}^{\star,k}_{n,m}] = \texttt{registration}\left(U^k, \mathcal{S}_n, \mathcal{N}(\mathbf{W}_m \bullet)\right)$
$k = 1, \ldots, n_{\mathrm{train}}$.

3. $[\mathbf{W}_m, \ \{\mathbf{a}^k\}_k] = \texttt{POD}\left(\{\mathbf{a}^{\star,k}\}_{k=1}^{n_{\mathrm{train}}}, tol_{\mathrm{pod}}, (\cdot,\cdot)_\star\right)$

if $\quad \max_k \mathfrak{f}^{\star,k}_{n,m} < \texttt{tol}, \quad$ break

else

4. $\mathcal{S}_{n+1} = \mathcal{S}_n \cup \mathrm{span}\{\mathfrak{s}(U_{\mu^{k^\star}}) \circ \Phi^{\star,k^\star}\}$
$k^\star = \arg\max_k \mathfrak{f}^{\star,k}_{n,m}$.

EndIf

EndFor

$$\mathfrak{f}^{\star,k}_{n,m} = \mathfrak{f}(\Phi^{\star,k}; u^k) := \min_{\psi \in \mathcal{S}_n} \|\mathfrak{s}(U^k) \circ \Phi^{\star,k} - \psi\|^2_{L^2(\widehat{\Omega})}$$

Parametric registration: remarks

- The Greedy procedure iteratively constructs the space $\mathcal{S}_n$ and the mappings $\{\Phi\}_k$.

  If $\mathcal{N} = \mathtt{id}$ (no registration) $\Rightarrow$ Strong Greedy.

- The algorithm is applied to the sensor $s(U)$ $\Rightarrow$ it cannot be employed to build the reduced space for U.

- POD reduction inside the for loop

  preserves the structure of the map,

$$\mathcal{N}(\mathbf{a}) = \sum_{q=1}^{N_{\mathrm{dd}}} \Psi_q \circ \Phi_q \circ \Psi_q^{-1} \mathbb{1}_{\Omega_q}, \quad \Phi_q = \mathtt{id} + W_M^q \mathbf{a}$$

  reduces dramatically the cost of subsequent iterations.

Projection-based model order reduction

Lagrangian methods approximate the solution U_μ as:

$$U_\mu \approx \sum_{i=1}^{n} (\widehat{\boldsymbol{\alpha}}_\mu)_i \, \zeta_i \circ \boldsymbol{\Phi}_\mu^{-1}.$$

In FE/FV framework, this translates to

$$\mu \in \mathcal{P} \mapsto \left(\boldsymbol{\Phi}_\mu(\mathcal{T}_{\mathrm{hf}}), \; \widehat{\mathbf{U}}_\mu = \mathbf{Z}\widehat{\boldsymbol{\alpha}}_\mu \right)$$

Lagrangian (or registration-based) methods for pMOR

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If $\boldsymbol{\Phi} : \Omega \times \mathcal{P} \to \Omega$ is given, Lagrangian methods correspond to *linear methods in parameterized domains*:

well-understood problem;

simple to implement in FE/FV framework.

Treatment of parameterized geometries

Two paradigms (cf. Taddei, Zhang, Arxiv, 2020):

- Map-then-discretize (MtD): mesh fixed; PDE modified;
- Discretize-then-map (DtM): mesh modified; PDE fixed.

Example: Laplace: $-\Delta U = 0, \; U|_{\partial \Phi_\mu(\Omega)} = g$.

Define the residual $R_\mu^{\mathrm{eq}}(u, v) = \sum_{k=1}^{N_\mathrm{e}} \rho_k^{\mathrm{eq}} r_\mu^k(u, v)$.

MtD: $r_\mu^k(u, v) = \int_{\mathtt{D}_k} \det(\nabla \Phi_\mu) \, \nabla \Phi_\mu^{-1} \nabla \Phi_\mu^{-T} \nabla u \cdot \nabla v \, dx.$

DtM: $r_\mu^k(u, v) = \int_{\Phi_\mu(\mathtt{D}_k)} \nabla u \cdot \nabla v \, dx.$

DtM allows to reuse element-wise assembling routines for residual evaluation $\Rightarrow$ easier to implement.

Refs (DtM): Washabaugh et al. 2016; Dal Santo, Manzoni 2019.

Projection scheme: LSPG+EQ

Introduce reduced-order bases $\mathbf{Z} \in \mathbb{R}^{N,n}$, $\mathbf{Y} \in \mathbb{R}^{N,j_{\mathrm{es}}}$.

Define the weighted residual $R_\mu^{\mathrm{eq}}(u,v) = \sum_{k=1}^{N_{\mathrm{e}}} \rho_k^{\mathrm{eq}} r_\mu^k(u,v)$.

EQ LSPG ROM: find $\widehat{\mathbf{U}}_\mu \in \arg \min_{\zeta \in \mathrm{col}(\mathbf{Z})} \sup_{\eta \in \mathrm{col}(\mathbf{Y})} \dfrac{R_\mu^{\mathrm{eq}}(\boldsymbol{\zeta}, \boldsymbol{\eta})}{\|\boldsymbol{\eta}\|_{\mathcal{Y}}}$.

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Implementation requires to address several points.

- Choice of trial ROB $\mathbf{Z}$.
- Choice of test ROB $\mathbf{Y}$ and the norm $\|\cdot\|_{\mathcal{Y}}$.
- Choice of the EQ weights $\boldsymbol{\rho}^{\rm eq}$.

Taddei, Zhang, *A discretize-then-map approach for the treatment of parameterized geometries in model order reduction*, Arxiv, 2020.

Multifidelity training: offline-online decomposition

Registration-based MOR: preliminary considerations

Registration

- addresses mesh adaptation and data compression;
- highly nonlinear;
- relies on regression for generalization

  $\Rightarrow$ needs extensive parameter explorations, $n_{\mathrm{train}} \gg 1$

Projection-based MOR (EQ LSPG)

- robust for small training sets;
- relies on linear approximations;

  $\Rightarrow$ inadequate for advection-dominated pbs;
- does not address mesh issues.

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Proposal: use "low-fidelity" snapshots for registration and "high-fidelity" snapshots for ROM generation.

Offline stage

1. Generate coarse snapshots $\{U_{\mu^k}\}_k$.
2. Generate a refined FE grid $\mathcal{T}_{\mathrm{hf}}$.
3. $\Phi = \mathrm{registration}\left(\{U_{\mu^k}\}_k, \mathcal{T}_{\mathrm{hf}}\right)$.
4. Linear MOR: build the reduced basis $\mathbf{Z}$ and the ROM for $\mu \mapsto \widehat{\boldsymbol{\alpha}}_\mu$. Greedy sampling.

Online stage (for any $\mu \in \mathcal{P}$)

5. Find $\widehat{\boldsymbol{\alpha}}_\mu$ using ROM, return $\left(\Phi_\mu(\mathcal{T}_{\mathrm{hf}}),\ \widehat{\mathbf{U}}_\mu = \mathbf{Z}\widehat{\boldsymbol{\alpha}}_\mu\right)$.

Numerical results

- Euler equations (with A Ferrero)
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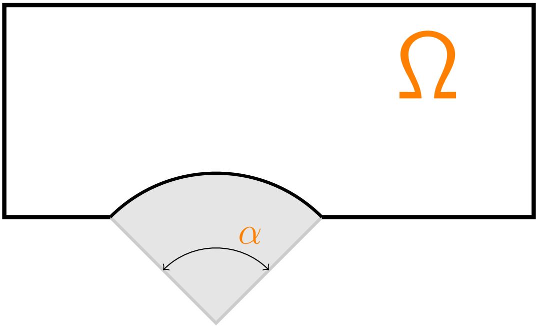
Compressible inviscid supersonic flow past a bump

Consider $\mu = [\alpha, \mathrm{Ma}_\infty] \in \mathcal{P} = [0.75, 0.8] \times [1.7, 1.8]$.



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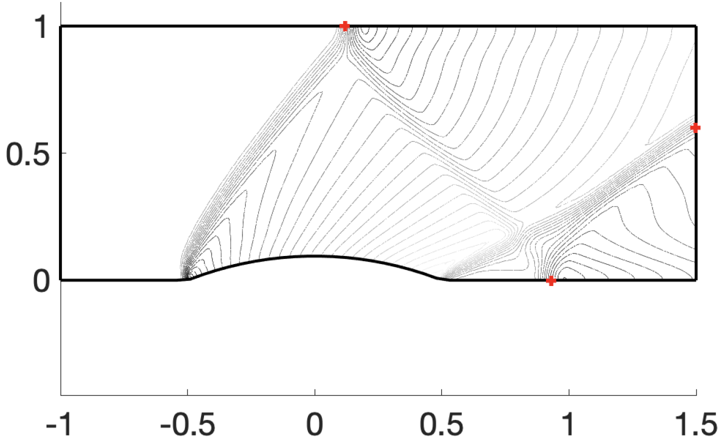
Behavior of Mach number $\mathrm{Ma} = \frac{\|u\|_2}{c}$ for $\mu = [0.75, 1.7]$.



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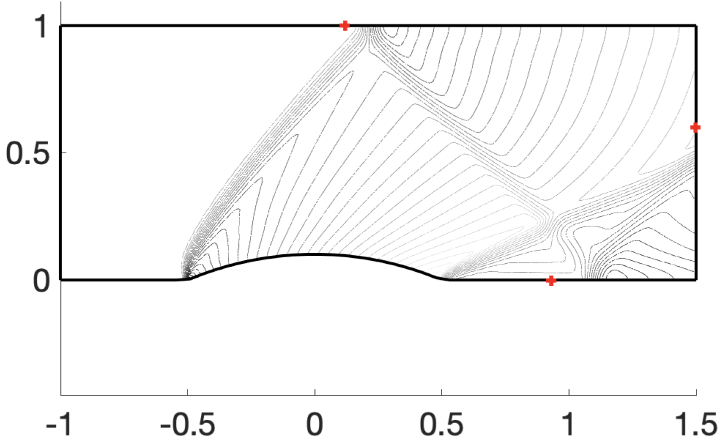


Test 1: one-fidelity training

Consider $n_{\mathrm{train}} = 11^2$ snapshots for training and $n_{\mathrm{test}} = 10$ snapshots for testing.

We measure performance using

$$E_{\mathrm{avg}} := \frac{1}{n_{\mathrm{test}}} \sum_{\mu \in \mathcal{P}_{\mathrm{test}}} \frac{\| U_\mu^{\mathrm{hf}} - \widehat{U}_\mu^{\mathrm{hf}} \|_{L^2(\Omega_\mu)}}{\| U_\mu^{\mathrm{hf}} \|_{L^2(\Omega\Omega_\mu)}}.$$

We rely on a P2 DG discretization with $N_{\mathrm{e}} = 8204$, $N = 197,856$ dofs.

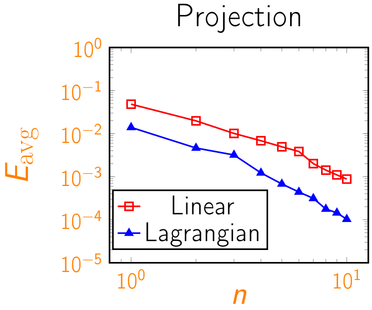
We consider a dilation-based artificial viscosity.

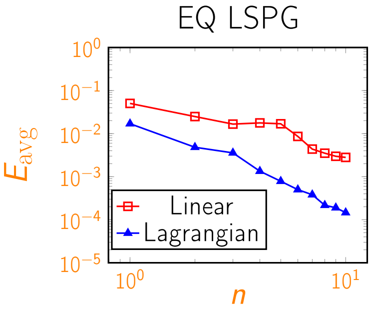
cf. Nicoud, Ducros, 1999; Ye, Hesthaven, 2020.

Test 1: projection and LSPG errors (POD)

	Linear	Lagrangian
Projection error ($n = 10$)	$0.9 \cdot 10^{-3}$	$0.10 \cdot 10^{-3}$
LSPG error ($n = 10$)	$2.8 \cdot 10^{-3}$	$0.14 \cdot 10^{-3}$

Construction of $\mathbf{Z}$ based on POD, $n_{\text{train}} = 121$.

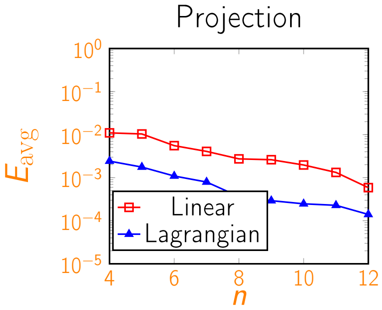


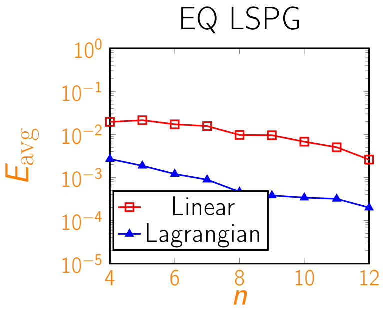


Test 1: projection and LSPG errors (Greedy)

	Linear	Lagrangian
Projection error ($n = 10$)	$2.0 \cdot 10^{-3}$	$0.25 \cdot 10^{-3}$
LSPG error ($n = 10$)	$6.8 \cdot 10^{-3}$	$0.34 \cdot 10^{-3}$

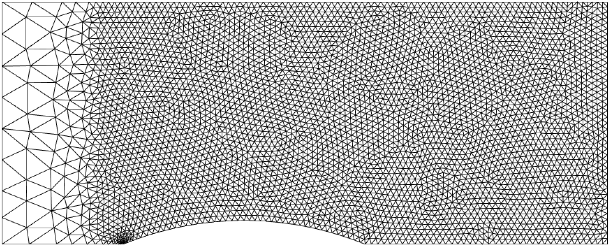
Construction of $\mathbf{Z}$ based on weak Greedy.

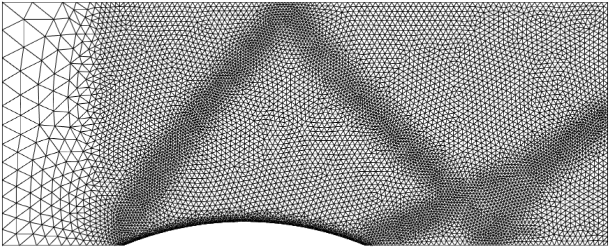




Coarse: $N_{\mathrm{e}} = 8204$, $N = 197856$.

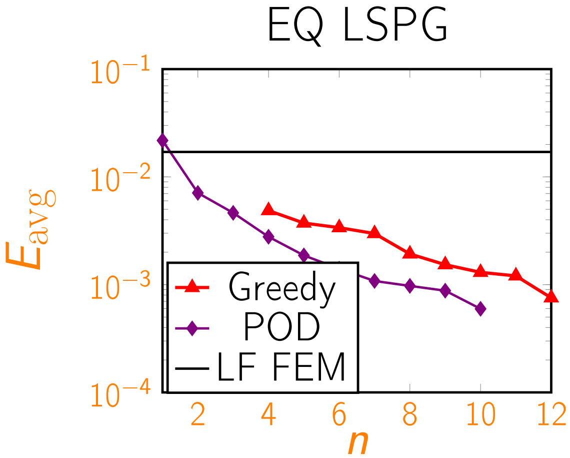
Fine: $N_{\mathrm{e}} = 16752$, $N = 402048$ based on $U_{\bar{\mu}}$





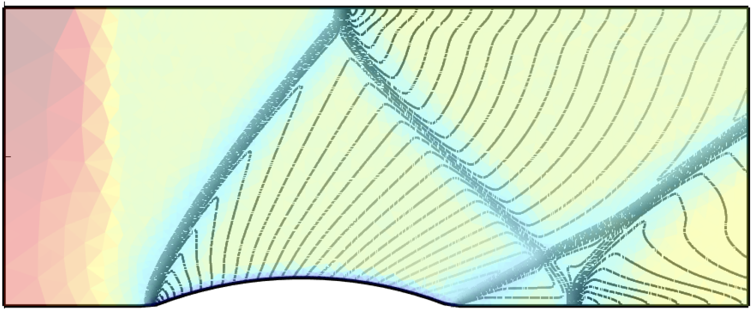
Test 2: LSPG error

Registration based on coarse simulations leads to accurate ROMs for small *n*.



Test 2: mesh adaptation

Plot: Mesh density $h(x) = \sum_k \sqrt{|\mathtt{D}_{k,\Phi}|}\mathbb{1}_{\mathtt{D}_{k,\Phi}}$ vs Mach contour lines.



Registration + mesh refinement lead to accurate meshes for all parameters r+h adaptivity.

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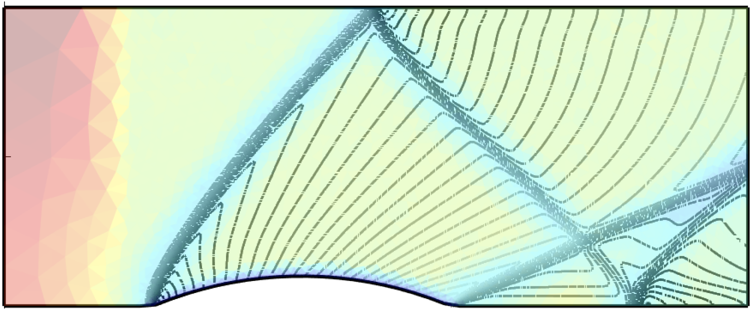

Registration + mesh refinement lead to accurate meshes for all parameters $r+h$ adaptivity.

Numerical results

- Euler equations (with A Ferrero)
- Shallow water equations (with C Goeury, A Ponçot)

Problem statement

Consider the problem: find $U = [h, q]^T$ such that

$$\begin{cases} \partial_t U + \partial_x f(U) = -gh\partial_x b e_2, & (x,t) \in \Omega \\ q(0,t) = q_{\mathrm{in},\mu}(t), \quad h(L,t) = 2, \quad U(x,0) = U_0(x), \end{cases}$$

with $f(U) = [q, \frac{q^2}{h} + \frac{g}{2}h^2]^T$, $b(x) = -0.2 + e^{-0.125(x-10)^4}$, $\Omega = (0, L) \times (0, T)$, and

$$q_{\mathrm{in},\mu}(t) \ = \ q_0 \ \left(1 + \mu_1 \, t \, e^{-\frac{1}{2\mu_2^2}(t-0.05)^2}\right), \quad q_0 = 4.4,$$

U_0 is the steady-state solution obtained for $q_{\mathrm{in},\mu} \equiv q_0$.

$$\mu = [\mu_1, \mu_2] \in \mathcal{P} = [2, 8] \times [0.1, 0.2].$$

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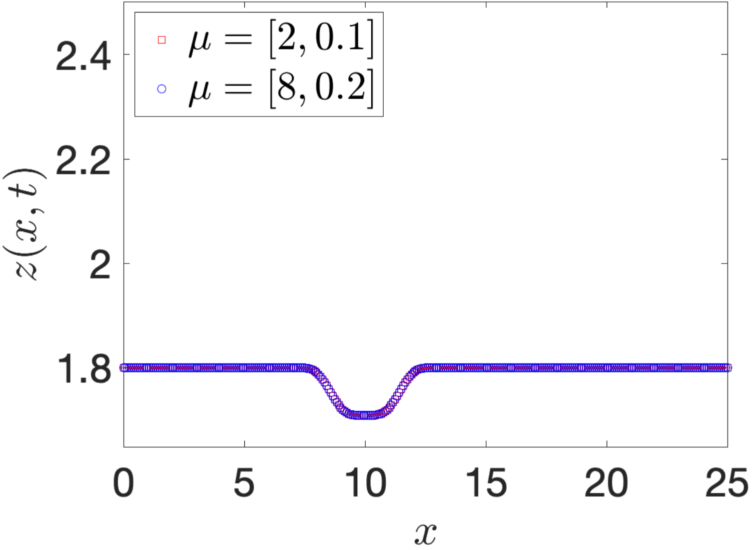
The problem shares relevant features with **dam-break studies** with non-constant bathymetry.



$\mu = [2, 0.1]$
$\mu = [8, 0.2]$
2.4
2.2
2
1.8
$z(x,t)$
0
5
10
15
20
25
x

Space-time formulation

We consider a **space-time** variational formulation:

$$\nabla \cdot F(U) = S(U) \text{ in } \Omega$$

where $\nabla = [\partial_x, \partial_t]$, $F(U) = [f(U), U]$.

Schwab, Stevenson, 2009; Urban, Patera, 2012.

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where $\nabla = [\partial_x, \partial_t]$, $F(U) = [f(U), U]$.

Space-time formulation is motivated by **approximation considerations**:

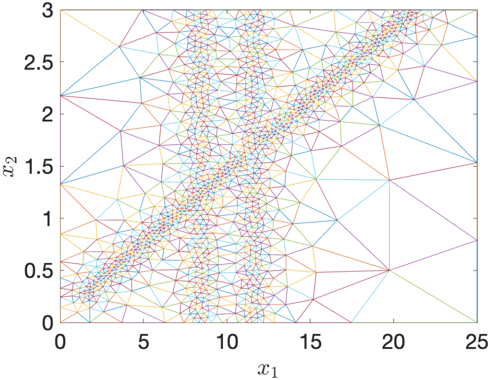
space-only registration does not deal effectively with shock interactions. cf. Taddei, Zhang, M2AN, 2021.

Space-time formulation also shows superior stability and allows sharper error bounds.

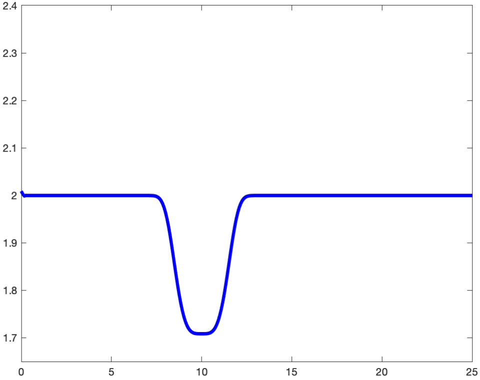
Schwab, Stevenson, 2009; Urban, Patera, 2012.

We build the sensors $\{s_k\}_k$ for registration using a **time-marching RKDG** solver.

We consider an adapted space-time mesh with $N_{\mathrm{e}} = 2314$.

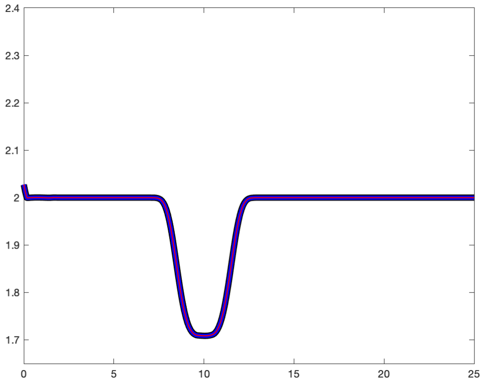


Linear method (projection $N = 5$)



Details: $n_{\mathrm{train}} = 100$, POD data compression.

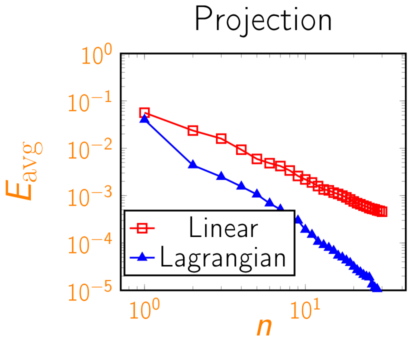
Lagrangian (registration +EQ-LSPG, $N = 5$)

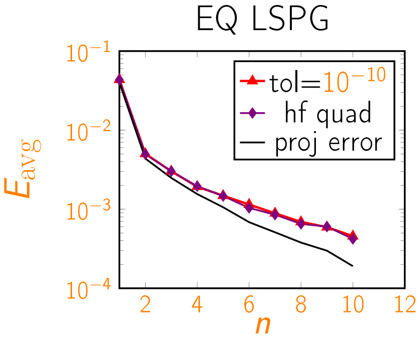


Details: $n_{\text{train}} = 100$, POD data compression.

Registration offers remarkable improvements compared to linear methods.

EQ-LSPG is able to find nearly-optimal coefficients for $n_{\text{test}} = 10$ out-of-sample configurations.





Analysis: expressivity of nonlinear approximations

Nonlinear approaches to model reduction (I)

We can distinguish between four classes of methods.

1. Adaptive partitioning of $\mathcal{P}$.
   Eftang et al., SISC, 2010.
2. Online basis refinement.
   Carlberg, IJNME, 2015; Peherstorfer, SISC, 2020;
3. Reformulation of the problem and/or of the ROB.
   Amsallem, Farhat, AIAA, 2008; Gerbeau, Lombardi, JCP, 2014; Ohlberger, Rave, CR Math., 2013; **this talk.**
4. Fully-nonlinear approximations.
   Lee, Carlberg, JCP, 2020; Kim et al, Arxiv 2020;
   Ehrlacher et al, M2AN, 2020; Mojgani, Balajewicz, AIAA, 2017.

Approaches in 4. do not involve projection of a (modified) problem on a linear subspace.

Nonlinear approaches to model reduction (II)

All MOR approaches introduce an **approximation class** $\mathcal{C}$ where they seek the low-rank operator $\mathtt{Z} : \mathbb{R}^q \to \mathcal{X}$.

Relevant examples: linear $\mathcal{C}_n^{\mathrm{lin}}$; Lagrangian $\mathcal{C}_{n,m}^{\mathrm{lag}}$; convolutional $\mathcal{C}_{n,\ell}^{\mathrm{co}}$.

$$\mathcal{C}_n^{\mathrm{lin}} := \left\{ \mathtt{Z} : \mathtt{Z}\boldsymbol{\alpha} = \sum_{i=1}^{n} (\boldsymbol{\alpha})_i \zeta_i \right\}$$

$$\mathcal{C}_{n,m}^{\mathrm{lag}} := \left\{ \mathtt{Z} : \mathtt{Z}(\boldsymbol{\alpha}, \mathbf{a}) = \sum_{i=1}^{n} (\boldsymbol{\alpha})_i \zeta_i \circ \Phi(\mathbf{a})^{-1} \right\}$$

$$\mathcal{C}_{n,\ell}^{\mathrm{co}} := \{ \mathtt{Z} : \mathtt{Z}(\boldsymbol{\alpha}_1, .., \boldsymbol{\alpha}_\ell) = \mathtt{N}_\ell \left(\mathtt{N}_{\ell-1} \left(\cdot, \boldsymbol{\alpha}_{\ell-1} \right), \boldsymbol{\alpha}_\ell \right) \}$$

Missing: transported/transformed methods (Welper, Reiss,...)

Approximation class $\mathcal{C}$ should be chosen based on

expressivity: measured in terms of the Kolmogorov width

$$\mathfrak{d}(\mathcal{M};\mathcal{C};\|\cdot\|) := \inf_{\mathrm{Z}\in\mathcal{C}} \sup_{w\in\mathcal{M}} \inf_{\boldsymbol{\beta}\in\mathbb{R}^q} \|\mathrm{Z}(\boldsymbol{\beta}) - w\|;$$

learnability: measured in terms of

performance of training algorithms to identify $\mathrm{Z} \in \mathcal{C}$,

performance of ROMs to compute $\widehat{\boldsymbol{\beta}}_\mu$.

Choice of $\mathcal{C}$: expressivity and learnability

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learnability: measured in terms of

- performance of training algorithms to identify $\mathrm{Z} \in \mathcal{C}$,
- performance of ROMs to compute $\widehat{\beta}_\mu$.

Open problems in MOR:

- estimate $\mathfrak{d}(\mathcal{M};\mathcal{C};\|\cdot\|)$;
- estimate performance of learning methods for given $\mathcal{C}$.

Analysis of linear and nonlinear methods

Most analysis is restricted to linear methods.

- Estimates of $\mathfrak{d}(\mathcal{M}; \mathcal{C}_n^{\mathrm{lin}}; \|\cdot\|)$.

  Cohen, DeVore, IMA J. Numer. Anal., 2016.

- Performance of Greedy methods.

  Binev et al., SINUM, 2011.

Several counter-examples show poor performance of linear methods for advection-dominated problems.

Ohlberger, Rave, Arxiv, 2015.

The analysis for nonlinear approximations is extremely limited.

- Estimates for convolutational approximations.

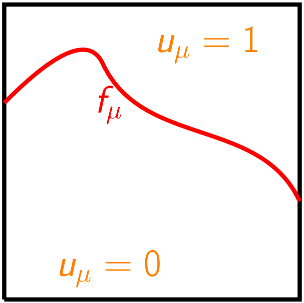
  Rim et al., Arxiv, 2020.

A working example (Taddei, SISC, 2020)

Define $u : (0,1)^2 \times \mathcal{P} \to \{0,1\}$ s.t. $u_\mu(x) = \mathbb{1}_{f_\mu(x_1) < x_2}(x)$.

Assume $f_\mu([0,1]) \subset [\delta, 1-\delta]$ for all $\mu \in \mathcal{P}$. Define

$$\mathcal{C}^{\rm lag}_{n,m} = \Big\{ \mathrm{Z} : \mathrm{Z} = \mathrm{Z}^{\rm lin} \circ \mathbf{\Phi}^{-1}, \ \text{s.t.} \quad \mathrm{Z}^{\rm lin}(\boldsymbol{\alpha}) = \sum_{i=1}^{n} (\boldsymbol{\alpha})_i \zeta_i, \quad \mathbf{\Phi}(\mathbf{a}) = \mathtt{id} + \sum_{i=1}^{m} (\mathbf{a})_i \varphi_i \Big\}$$



$$\Rightarrow \mathfrak{d}\left(\mathcal{M}, \mathcal{C}^{\rm lag}_{n,m}, \|\cdot\|_{L^1(\Omega)}\right) \leq C \, \frac{\mathfrak{d}\left(\mathcal{M}_{\rm f}, \mathcal{C}^{\rm lin}_{m}, \|\cdot\|_{\rm Lip([0,1])}\right)}{\sqrt{n}},$$

Multiplicative effect between n and m convergence.

Conclusions and perspectives

Summary

- We propose a general registration procedure for parameterized PDEs. independent of the PDE model.
- We integrate registration into the offline/online paradigm.
- We apply the approach to two hyperbolic systems of PDEs to show the potential of the method.

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- We apply the approach to two hyperbolic systems of PDEs to show the potential of the method.

Ongoing work

- Adaptive multi-fidelity training.
- Mathematical analysis: when is registration worth?

Thank you for your attention!

For more information, visit the website:

math.u-bordeaux.fr/~ttaddei/ .

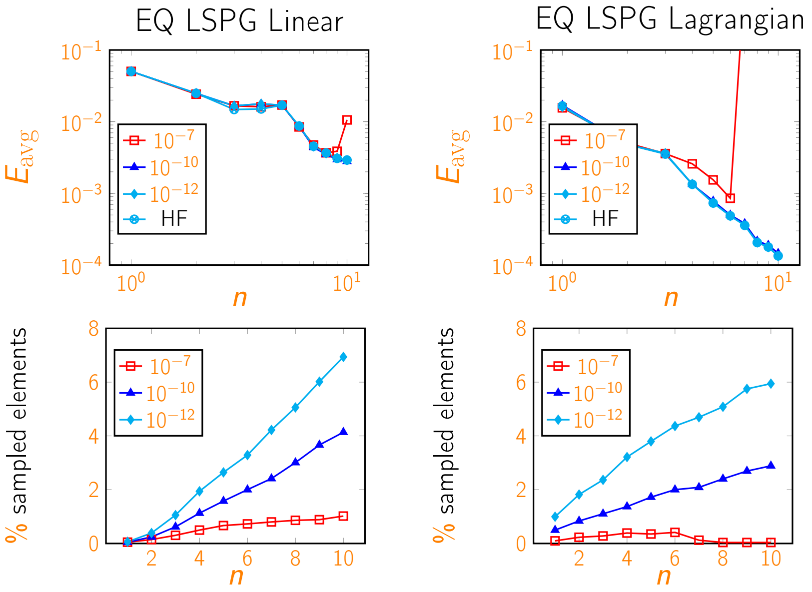
Backup slides

- More results on Euler

Backup slides

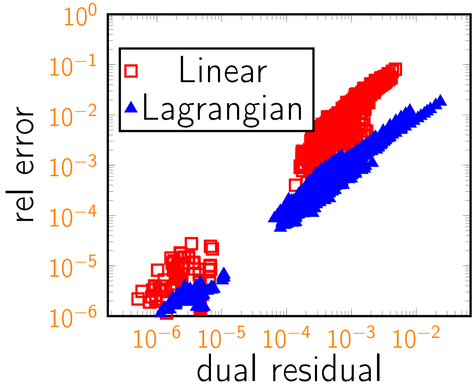
- More results on Euler

Empirical quadrature (test 1; POD training)



We consider $\mathcal{Y} = H^1(\Omega)$. Results are associated with the iterations of the weak-Greedy algorithm on training set.

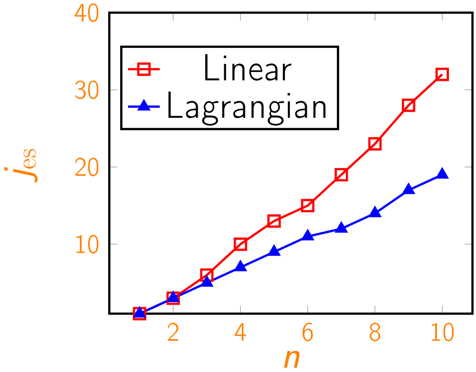
Dual residual evaluation is inexpensive compared to the other steps of the offline stage. $\Rightarrow$ no hyper-reduction.



Construction of the test space

POD-based construction of the empirical test space:

1. Find Riesz elements $(\psi_{k,i}, \mathbf{v})_{\mathcal{Y}} = DR^{\mathrm{hf}}_{\mu^k}[\mathbf{U}^{\mathrm{hf}}_{\mu^k}](\zeta_i, \mathbf{v})$,
$$\forall\, \mathbf{v} \in \mathbb{R}^N,\ i = 1, \ldots, n,\ k = 1, \ldots, n_{\mathrm{train}}$$
2. $\mathbf{Y} = \mathtt{POD}\left(\{\psi_{k,i}\}_{k,i}, tol_{\mathrm{test}}, \|\cdot\|_{\mathcal{Y}}\right)$, $tol_{\mathrm{test}} = 10^{-3}$.



Effect of discretization on hyper-reduction

The empirical quadrature procedure weakly depends on the size of the mesh $\Rightarrow$ larger speedup for large $N_{\rm e}$.