A nonlinear Model Order Reduction procedure for hyperbolic problems

Angelo Iollo, Tommaso Taddei

INRIA, MEMPHIS Team

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inventeurs du monde numérique

Institut de Mathématiques de Bordeaux

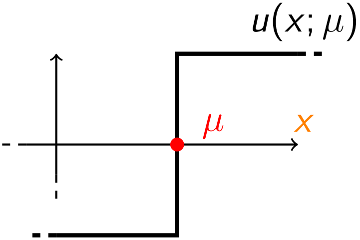
Objective

Develop a Model Order Reduction (MOR) procedure for

hyperbolic stationary equations

in the presence of parameter-dependent shocks.

Example



$$u(x,\mu) = \operatorname{sign}(x-\mu),$$
$$x \in \Omega := (0,1)$$
$$\mu \in \mathcal{P} = \left[\tfrac{1}{3}, \tfrac{2}{3}\right]$$

Failure of linear MOR strategies

Linear Reduced Order Models (ROMs) rely on N-term linear expansions to approximate u:

$$u(x,\mu) \approx \widehat{u}_N(x,\mu) = Z_N(x)\boldsymbol{\alpha}(\mu), \qquad Z_N = [\zeta_1, \dots, \zeta_N]$$

If $u(x,\mu) = \mathrm{sign}(x-\mu)$,

$$\sup_{\mu \in \mathcal{P}} \inf_{(Z_N, \boldsymbol{\alpha})} \| u(\cdot;\mu) - Z_N(\cdot)\boldsymbol{\alpha} \|_{L^2(\Omega)} = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

for Lagrangian spaces (i.e., $Z_N = \left[u(\mu^1), \dots, u(\mu^N)\right]$).

Linear ROMs are ill-suited for travelling fronts.

Taddei, Perotto, Quarteroni, 2015.

Eulerian approaches to nonlinear MOR

Recipe: given $\mu \in \mathcal{P}$,

1. define the reduced operator $Z_{N,\mu} : \mathbb{R}^N \to L^2(\Omega)$;
2. determine the approximation $\widehat{u}_N(\mu) = Z_{N,\mu}(\boldsymbol{\alpha}(\mu))$ using a projection method.

Selected references:

Manifold learning

Amsallem, Farhat, 2008; Lee, Carlberg, 2018[1].

"Transported/transformed snapshot" methods

Nair, Balajewicz, 2017; Welper, 2017.

hp-in-parameter adaptive refinement

Eftang et al., 2010; Peherstorfer, Willcox, 2015.

[1] Here, the authors consider $\widehat{u}_N(x,\mu) = g(x;\boldsymbol{\alpha}(\mu))$

Lagrangian approaches to nonlinear MOR

Recipe: given $\mu \in \mathcal{P}$,

1. define a bijective mapping $\Phi_\mu : \Omega \to \Omega$;
2. determine the approximation $\widetilde{u}_N(\cdot;\mu) = \widetilde{Z}_N \boldsymbol{\alpha}(\mu)$ of $\widetilde{u}(\mu) := u(\mu) \circ \Phi_\mu$ using a projection method.

Selected references:

Iollo, Lombardi, 2014; Ohlberger, Rave, 2015; Cagniart et al., 2017; Mojgani, Balajewicz, 2017.

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Example $u(x,\mu) = \mathrm{sign}\,(x-\mu)\,,\; x \in \Omega = (0,1)$.

If we choose $\Phi_\mu(X) = \begin{cases} 2\mu X & X < \frac{1}{2} \\ \mu + (1-\mu)(2X-1) & X \geq \frac{1}{2} \end{cases}$,

the mapped field is μ-independent.

$$\widetilde{u}(X,\mu) = \mathrm{sign}(2X-1).$$

Lagrangian approaches: offline/online decomposition[2]

Offline stage: (performed once)

1. compute $u(\mu^1), \ldots, u(\mu^{n_{\mathrm{train}}})$ using a FE/FV solver;
2. define the mapping Φ_μ for all $\mu \in \mathcal{P}$;
3. define the ROM for $\tilde{u} = u \circ \Phi$.

ROM: $\mu \mapsto \tilde{u}_N(\mu) = \widetilde{Z}_N \boldsymbol{\alpha}(\mu)$

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

1. query the ROM to compute $\tilde{u}_N(\bar{\mu})$;
2. (if needed) compute $\widehat{u}_N(\bar{\mu}) = \widetilde{u}_N(\bar{\mu}) \circ \Phi_{\bar{\mu}}^{-1}$.

[2] Mojgani, Balajewicz have proposed to simultaneously learn the mapping and the coefficients during the online stage.

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Refined goal: develop a *general* registration algorithm for the construction of Φ_μ for Lagrangian approaches.

Agenda of the talk:

1. Registration algorithm.
2. Application to a linear advection-reaction problem.
3. Conclusions and perspectives.

General = independent of the underlying PDE model.

Registration algorithm

Well-posedness

Projection is performed in the mapped configuration.
Therefore, for all $\mu \in \mathcal{P}$, the map Φ_μ should satisfy

$$\Phi_\mu(\Omega) = \Omega,\ \mathfrak{J}_\mu(X) = \left|\nabla\Phi_\mu(X)\right| > 0,\ \ X \in \Omega.$$

Efficiency

The map Φ_μ should be designed such that the manifold

$$\widetilde{\mathcal{M}} = \{\widetilde{u}(\mu) = u(\mu) \circ \Phi_\mu :\ \mu \in \mathcal{P}\}$$

is "more favorable" than[3] $\mathcal{M} = \{u(\mu) :\ \mu \in \mathcal{P}\}$
for linear approximation methods.

[3] This notion should be formalized by means of the introduction of a Kolmogorov N-width.

Overall strategy

Inputs: snapshots $\{u^k = u(\mu^k)\}_{k=1}^{n_{\mathrm{train}}}$, reference[4] $\bar{u}$.

Output: mapping $\Phi_\mu : \Omega \to \Omega$ for all $\mu \in \mathcal{P}$.

1. Determine a family of mappings $\{\Psi(\cdot; \mathbf{a})\}_{\mathbf{a} \in \mathbb{R}^M}$ for the domain Ω;
2. choose $\Psi(\cdot; \mathbf{a}^k)$ using u^k and $\bar{u}$;

   $\to \{\mu^k, \mathbf{a}^k\}_{k=1}^{n_{\mathrm{train}}}$
3. learn $\mathbf{a} : \mathcal{P} \to \mathbb{R}^M$ based on $\{\mu^k, \mathbf{a}^k\}_{k=1}^{n_{\mathrm{train}}}$;

   regression problem
4. set $\Phi_\mu = \Psi(\cdot; \mathbf{a}(\mu))$.

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[4] Here, $\bar{u}$ is set equal to $u(\bar{\mu})$, where $\bar{\mu} = \frac{1}{n_{\mathrm{train}}} \sum_k \mu^k$.

Family of mappings $\{\Psi(\cdot;\mathbf{a})\}_{\mathbf{a}}$: a theoretical result[5]

Let Ω be diffeomorphic to $\widehat{\Omega} = \{x \in \mathbb{R}^d : f(x) < 0\}$ where f is convex.

Let $\Phi : \Omega' \to \mathbb{R}^d$, $\Omega \subset\subset \Omega'$, satisfy

(i) $\Phi \in C^1(\Omega'; \mathbb{R}^d)$;

(ii) $\inf_{X\in\Omega} \mathfrak{J}(X) = |\nabla\Phi(X)| > 0$;

(iii) $\mathrm{dist}\,(\Phi(X), \partial\Omega) = 0$ for all $X \in \partial\Omega$.

i.e. $\Phi(\partial\Omega) \subset \partial\Omega$

Then, Φ is a bijection from Ω into itself.

Examples: $\widehat{\Omega} = (0,1)^d$, $\widehat{\Omega} = \mathcal{B}_1(0), \ldots$

[5] We thank Pierre Mounoud (University of Bordeaux) for fruitful discussions.

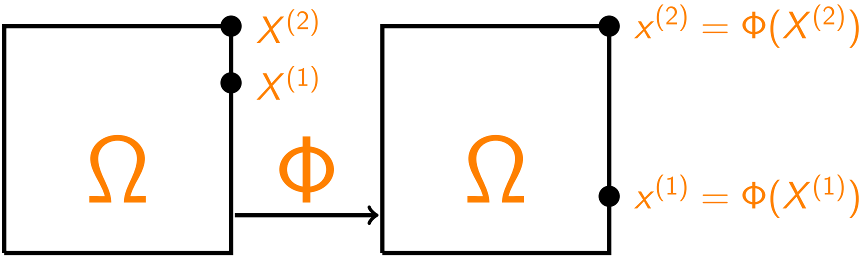
Family of mappings $\{\Psi(\cdot;\mathbf{a})\}_{\mathbf{a}}$: implications for $\Omega = (0,1)^2$

Consider $\Psi(X;\mathbf{a}) = X + \sum_{m=1}^{M} a_m \varphi_m(X)$, with

$$\varphi_m(X)\cdot\mathbf{e}_1 = 0 \ \text{ on } \{X_1 = 0, 1\},\ m = 1, \dots, M;$$

$$\varphi_m(X)\cdot\mathbf{e}_2 = 0 \ \text{ on } \{X_2 = 0, 1\},\ m = 1, \dots, M.$$

(ii) holds for $\mathbf{a} = \bar{\mathbf{a}} \Rightarrow \Psi(\cdot;\bar{\mathbf{a}})$ is bijective + $\Psi(\Omega;\bar{\mathbf{a}}) = \Omega$.



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In our implementation, we resort to a tensorized polynomial expansion.

$$\varphi_1(X) = \ell_0(X_1)\ell_0(X_2)X_1(1-X_1)\begin{bmatrix}1\\0\end{bmatrix}, \ldots$$

$$\varphi_M(X) = \ell_p(X_1)\ell_p(X_2)X_2(1-X_2)\begin{bmatrix}0\\1\end{bmatrix}.$$

ℓ_i = Legendre polynomial of degree i

Registration algorithm for $(u^k, \bar{u}) \to \mathbf{a}^k$

Find $\mathbf{a}^k$ to minimize

$$\min_{\mathbf{a}} \int_\Omega \|u^k(\Psi(X;\mathbf{a})) - \bar{u}(X)\|_2^2 dX \; + \xi \left|\Psi(\cdot;\mathbf{a})\right|^2_{H^2(\Omega)}$$

$$\text{s.t.} \int_\Omega \exp\left(\frac{\epsilon - \mathfrak{J}_{\mathbf{a}}(X)}{C_{\exp}}\right) + \exp\left(\frac{\mathfrak{J}_{\mathbf{a}}(X) - 1/\epsilon}{C_{\exp}}\right) dX \; \le \; \delta$$

Non-convex nonlinear optimization problem.

Solver: Matlab 2018b `fmincon` (interior-point).

Initial condition: $\mathbf{a}^1 = \mathbf{0}$, $\mathbf{a}^k = \mathbf{a}^{k-1}$.

We reorder $\mu^1, \ldots, \mu^{n_{\text{train}}}$ so that
$\mu^{k+1} = \arg\min_{\mu \in \{\mu^{k'}\}_{k'=k+1}^{n_{\text{train}}}} \|\mu^k - \mu^{k'}\|_2$.

Registration algorithm for $(u^k, \bar{u}) \to \mathbf{a}^k$: interpretation

$\int_\Omega \| u^k(\Psi(X; \mathbf{a})) - \bar{u}(X) \|_2^2 dX$ measures the "distance" between u^k and $\bar{u}$ in the mapped configuration;

$\xi \left| \Psi(\cdot; \mathbf{a}) \right|_{H^2(\Omega)}^2$ is a regularization term to bound gradient and Hessian of $\Psi(\cdot; \mathbf{a})$;

the constraint

$$\int_\Omega \exp\left(\frac{\epsilon - \mathfrak{J}_{\mathbf{a}}(X)}{C_{\exp}} \right) + \exp\left(\frac{\mathfrak{J}_{\mathbf{a}}(X) - 1/\epsilon}{C_{\exp}} \right) dX \le \delta$$

imposes weakly that $\mathfrak{J}_{\mathbf{a}}(X) \in [\epsilon, 1/\epsilon]$ for all $X \in \Omega$.

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The statement depends on $\xi, \epsilon, C_{\exp}, \delta$:

Here, we set $\xi = 10^{-3}, \epsilon = 0.1, C_{\exp} = 0.005, \delta = 1$.

Generalization: $\{\mu^k, \mathbf{a}^k\}_k \Rightarrow \mathbf{a} : \mathcal{P} \to \mathbb{R}^M$

We proceed as follows.

1. POD reduction: $\mathbf{a} \approx \mathbf{U}_\Phi \mathbf{a}_\mathrm{r}$, $\mathbf{U}_\Phi^T \mathbf{U}_\Phi = \mathbb{1}$, $\mathbf{a}_\mathrm{r} \in \mathbb{R}^{M_\mathrm{r}}$, $M_\mathrm{r} < M$.
2. RBF approximation: $\{\mu^k, \mathbf{a}_\mathrm{r}^k\}_k \Rightarrow \mathbf{a}_\mathrm{r} : \mathcal{P} \to \mathbb{R}^{M_\mathrm{r}}$.

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POD reduction: POD leads to a significant reduction in terms of online costs and reduces the dependence on the preliminary choice of M.

Drawback of RBF regression: there is no guarantee that

$$\min_{X \in \Omega, \mu \in \mathcal{P}} \mathfrak{J}_\mu(X) > 0$$

Current effort focuses on the development of constrained regression procedures.

Application to a linear transport problem

Steady advection-reaction problem

Consider the problem

$$\begin{cases} \sigma_\mu \, u(\mu) + \nabla \cdot (\mathbf{c}_\mu \, u(\mu)) = f_\mu & \text{in } \Omega \\ u(\mu) = u_{\mathrm{D},\mu} & \text{on } \Gamma_{\mathrm{in},\mu} \end{cases}$$

where $\Gamma_{\mathrm{in},\mu} = \{x \in \partial\Omega : \mathbf{c}_\mu \cdot \mathbf{n} < 0\}$, and

$$\mathbf{c}_\mu = [\cos(\mu_1), \sin(\mu_1)], \quad \sigma_\mu = 1 + \mu_2 \, e^{x_1 + x_2},$$

$$f_\mu = 1 + x_1 x_2, \quad u_{\mathrm{D},\mu} = 4 \arctan\left(\mu_3 \left(x_2 - 1/2\right)\right) x_2 (1 - x_2)$$

$$\mu_1 \in \left[-\tfrac{\pi}{10}, \tfrac{\pi}{10}\right], \ \mu_2 \in [0.3, 0.7], \ \mu_3 \in [60, 100].$$

The problem is discretized using a Q2 DG discretization with Local Lax-Friedrichs flux.

65790 dofs.

Mapped configuration; reduced formulation

Offline computations are based on $n_{\mathrm{train}} = 250$ snapshots.

Reduced operator $\widetilde{Z}_N$ built using POD.

Reduced formulation: Galerkin.

Hyper-reduction based on POD with EIM point selection.
[Barrault et al., 2004], [Grepl et al., 2007]

Mapping based on Q6 tensorized polynomials ($M = 72$).

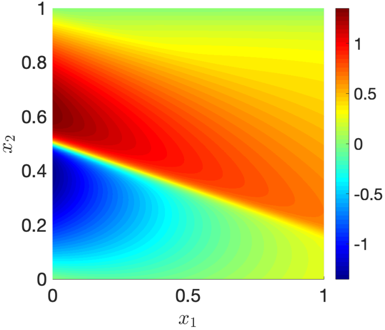
Remark: $\tilde{u}(\mu)$ satisfies an AR problem with

$$\tilde{\sigma}_\mu = \mathfrak{J}_\mu \, \sigma_\mu, \quad \widetilde{\mathbf{c}}_\mu = \mathfrak{J}_\mu \, \nabla \Phi_\mu^{-1} \, \mathbf{c}_\mu, \quad \tilde{f}_\mu = \mathfrak{J}_\mu \, f_\mu, \quad \tilde{u}_{\mathrm{D},\mu} = u_{\mathrm{D},\mu}.$$

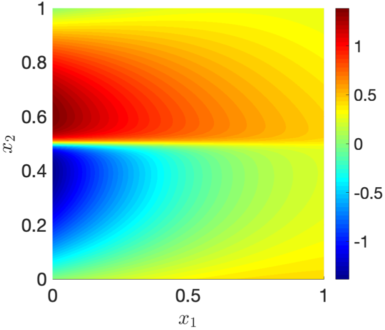
Visualization of the solution field: $\mu = [-\pi/10, 0.3, 60]$

The mapping Φ_μ reduces the sensitivity of the solution to changes in μ_1.

$$\mathbf{c}_\mu = [\cos(\mu_1), \sin(\mu_2)];$$
$$\bar{\mu} = [0, 0.5, 80].$$



(a) $u(\mu)$



(b) $\bar{u}$

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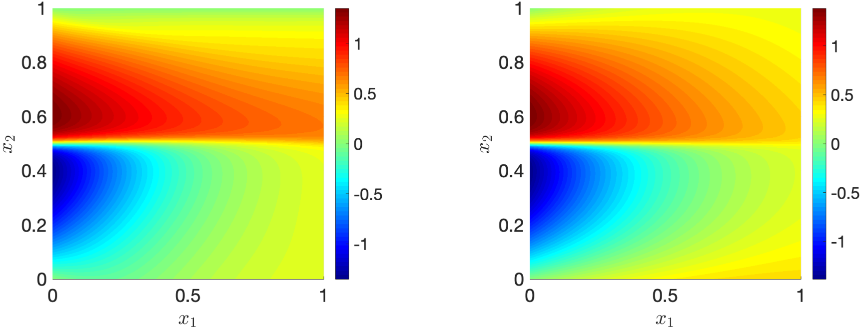
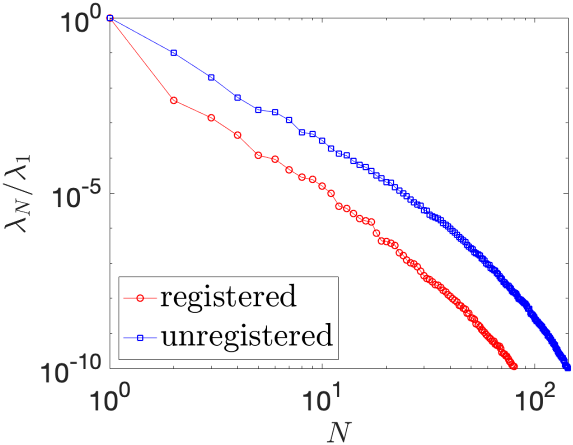


(a) $\tilde{u}(\mu)$ (b) $\bar{u}$

Behavior of the POD eigenvalues

Decay rate is nearly the same for both registered and unregistered configurations, **but**

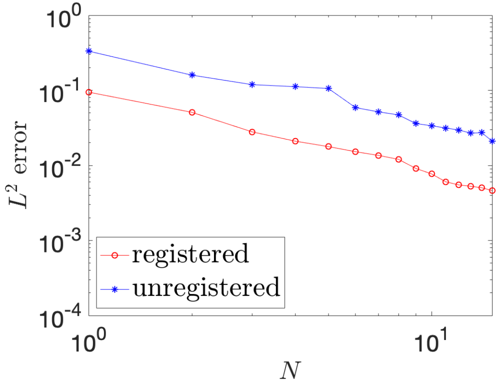
we have $(\lambda_n^{\mathrm{reg}}/\lambda_1^{\mathrm{reg}})/(\lambda_n^{\mathrm{unreg}}/\lambda_1^{\mathrm{unreg}}) = \mathcal{O}(10^2)$.



Performance of the Reduced Basis ROM

Relative error is computed based on $n_{\text{test}} = 20$ parameters, in the physical configuration.

The nonlinear ROM is approximately 4 times more accurate than the linear ROM.



Conclusions and perspectives

Summary

We propose a *general* registration procedure for Lagrangian approaches to nonlinear MOR.

General = independent of the underlying PDE model.

Preliminary results suggest the effectiveness of the approach compared to linear ROMs.

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We propose a *general* registration procedure for Lagrangian approaches to nonlinear MOR.

- General = independent of the underlying PDE model.

Preliminary results suggest the effectiveness of the approach compared to linear ROMs.

Several challenges need to be addressed.

- Definition of the reference field. $\leftrightarrow$ clustering
- Reduction of offline costs $\leftrightarrow$ greedy sampling
  $\leftrightarrow$ hierarchy of models at training stage

Bernard, Iollo, Riffaud, 2018.

Thank you for your attention!