Localized model reduction for nonlinear elliptic PDEs

Tommaso Taddei Inria, Team MEMPHIS

Inria-CERMICS Seminar Paris, October 14th 2021

Joint work with Kathrin Smetana (Stevens Inst. of Technology) Acknowledgements: A Iollo, G Sambataro





Institut de Mathématiques de Bordeaux

Objective

The goal of parameterized model order reduction (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.

The goal of parameterized model order reduction (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.

- **Pb:** find $u_{\mu} \in \mathcal{X}$: $\mathcal{G}_{\mu}(u_{\mu}, v) = 0 \quad \forall v \in \mathcal{Y}$.
- $\mathcal{G}_{\mu}: \mathcal{X} \to \mathcal{Y}'$ variational (non)linear operator;
- $\mu = [\mu_1, \dots, \mu_P] \in \mathcal{P} \subset \mathbb{R}^P$ vector of parameters; material properties, geometric features,....
- $\mathcal{M} := \{ u_{\mu} : \mu \in \mathcal{P} \}$ solution manifold.

Monolithic projection-based pMOR: general recipe

Pb: find $u_{\mu} \in \mathcal{X}$: $\mathcal{G}_{\mu}(u_{\mu}, v) = 0 \quad \forall v \in \mathcal{Y}, \ \mu \in \mathcal{P}$ **Approx:** $\hat{u}_{\mu} = Z \, \hat{\alpha}_{\mu}, \qquad \hat{\alpha} : \mathcal{P} \to \mathbb{R}^{n}, \ Z : \mathbb{R}^{n} \to \mathcal{X}$



Monolithic projection-based pMOR: general recipe

- **Pb:** find $u_{\mu} \in \mathcal{X}$: $\mathcal{G}_{\mu}(u_{\mu}, v) = 0 \quad \forall v \in \mathcal{Y}, \ \mu \in \mathcal{P}$ **Approx:** $\hat{u}_{\mu} = Z \, \hat{\alpha}_{\mu}, \qquad \hat{\alpha} : \mathcal{P} \to \mathbb{R}^{n}, \ Z : \mathbb{R}^{n} \to \mathcal{X}$
- **Offline (learning) stage:** (performed once) compute $u_{\mu^1}, \ldots, u_{\mu^{n_{\text{train}}}}$ using a FE (or FV...) solver; construct $Z = [\zeta_1, \ldots, \zeta_n]$ and define $\mathcal{Z} = \text{span}\{\zeta_i\}_{i=1}^n$; define a reduced-order model (ROM) for $\widehat{\alpha} : \mathcal{P} \to \mathbb{R}^n$.
- Online (prediction) stage: (performed for new μ') estimate the solution coefficients $\widehat{\alpha}_{\mu'} \in \mathbb{R}^n$. estimate $\|\widehat{u}_{\mu'} - u_{\mu'}\|$.

 $n \ll N =$ dofs of the full-order model (FOM)

=FE....

Limitation of monolithic approaches

Monolithic approaches rely on two assumptions:

- the solution is defined over a parameter-independent domain or over a family of diffeomorphic domains; no topology changes
- it is possible to solve the FOM for several parameters.
- These conditions might not be fulfilled for several problems of interest.
- Example of topology change:



Offline stage

- Define a set of archetype components.
- Build local ROMs for each component.

Online stage

- Define the system as instantiation of components.
- Solve the global problem by gluing together the local ROMs.



Component-based model reduction: research questions

- 1. **Data compression:** how can we build "good" approximation spaces for each archetype component?
- 2. **Reduced formulation:** how can we glue together local ROMs to estimate the global solution?
- non-overlapping conforming methods; scRBE
- non-overlapping non-conforming methods; RBE, LRBMS
- overlapping methods. zonal POD

RBE: Maday, Rønquist, 2002. scRBE: Huynh, Knezevic, Patera, 2013. LRBMS: Kaulmann et al., 2012; Ohlberger, Schindler, 2015. zonal POD: Bergmann et al., 2018.

Define effective local approximation spaces for component-based MOR.

- Linear problems: optimal approximations, randomized methods.
- Randomized methods for nonlinear problems: theoretical and numerical considerations.

Bibliography: (for linear PDEs)

Babuska, Lipton, Multiscale Model. Simul., 2011. Smetana, Patera, SISC, 2016. Buhr, Smetana, SISC, 2018.

Working problem

Model pb: $-\nabla \cdot (\kappa_{\mu}(u_{\mu})\nabla u_{\mu}) = f_{\mu} \text{ in } \Omega, \ u_{\mu}|_{\partial\Omega} = 0$ $\Omega = (0,1)^2 = \bigcup_{i=1}^{N_{\text{dd}}} \Omega_i, \ \mu = [\mu^{(1)}, \dots, \mu^{(N_{\text{dd}})}, i^*],$ $\kappa_{\mu}(u)|_{\Omega_i} = \frac{36}{\mu_2^{(i)}} \left(\frac{u(1-u)}{u^3 + \frac{12}{\mu_2^{(i)}}(1-u)^3} \right)^2 + \mu_1^{(i)}, \ i = 1, 2, \dots$

 $\mu^{(i)} \in \mathcal{P} = [0.1, 0.2] \times [30, 40], i^* \in \{1, \dots, N_{\mathrm{dd}}\}.$

• Idealized model for subsurface flows; challenging problem for monolithic MOR — $2N_{dd} + 1$ parameters.

Working problem

Model pb: $-\nabla \cdot (\kappa_{\mu}(u_{\mu})\nabla u_{\mu}) = f_{\mu} \text{ in } \Omega, \ u_{\mu}\big|_{\partial\Omega} = 0$ $\Omega = (0,1)^2 = \bigcup_{i=1}^{N_{\text{dd}}} \Omega_i, \ \mu = \big[\mu^{(1)}, \dots, \mu^{(N_{\text{dd}})}, i^{\star}\big],$

$$f_{\mu}(x) = 100e^{\left(-100\frac{\|x-x_{c,i^{\star}}\|_{2}^{2}}{2}\right)} \mathbb{1}_{\Omega_{i}^{\star}}(x), \ x_{c,i^{\star}} := \frac{1}{\Omega_{i}^{\star}} \int_{\Omega_{i}^{\star}} x \, dx.$$

 $\mu^{(i)} \in \mathcal{P} = [0.1, 0.2] \times [30, 40], i^* \in \{1, \dots, N_{\mathrm{dd}}\}.$

• Idealized model for subsurface flows; challenging problem for monolithic MOR — $2N_{dd} + 1$ parameters.

Working problem

Model pb: $-\nabla \cdot (\kappa_{\mu}(u_{\mu})\nabla u_{\mu}) = f_{\mu} \text{ in } \Omega, |u_{\mu}|_{\partial\Omega} = 0$









Target application (PhD thesis of G Sambataro)

Goal: assess long-term behavior of radioactive waste districts. Projet CIGEO

Mathematical model: THM equations — nonlinear unsteady parabolic equations with internal variables.



Monolithic pMOR: Iollo, Sambataro, Taddei, Arxiv, 2021.

Localized training

- Oversampling
- Linear problems
- Randomization
- Numerical results

Localized training

• Oversampling

- Linear problems
- Randomization
- Numerical results

Archetype components

Three archetype components: corner (co), edge (ed) and internal (int).

- $\widehat{\Omega} = (0, h)^2$ reference domain;
- $\Phi_i : \widehat{\Omega} \to \Omega_i$ *i*-th deformation map;
- $I \in {co, ed, int}^{N_{dd}}$ instantiated components' labels.



Oversampling (I): basic idea

Task: find low-dimensional spaces Z^{co}, Z^{ed}, Z^{int} s.t. $\min_{\zeta \in Z^{l_i}} \|u_{\mu}\|_{\Omega_i} \circ \Phi_i - \zeta \|_{H^1(\widehat{\Omega})} \ll 1 \text{ for } i = 1, \dots, N_{dd}$

Idea:

- Define the patch $U \supset \widehat{\Omega}$ with input boundary $\Gamma_{in} \subset \partial U$.
- Define the transfer operator T s.t., given $g \in G \subset H^{1/2}(\Gamma_{\text{in}})$ and $\mu \in \mathcal{P}$, $T_{\mu}(g) = w|_{\widehat{\Omega}}$ with
- $abla \cdot (\kappa_{\mu}(w) \nabla w) = f_{\mu} ext{ in } U, ext{ } w|_{\Gamma_{\mathrm{in}}} = g, ext{ } w|_{\partial U \setminus \Gamma_{\mathrm{in}}} = 0.$
- Determine a low-dimensional approximation space for the manifold $\widehat{\mathcal{M}} = \{ T_{\mu}(g) : g \in G, \mu \in \mathcal{P} \}.$

scRBE: Eftang, Patera 2013; Smetana, Patera, 2016. multiscale FE: Henning, Peterseim, 2013.

Oversampling (II): role of U, G

Input boundary $\Gamma_{\rm in}$ should be well-separated from $\widehat{\Omega}$ to ensure decay of high-frequency modes, **but** $|U| \ll |\Omega|$ to ensure computational speed-ups.



Set *G* should be representative of the behavior of $u_{\mu}|_{\Gamma_{\text{in}}}$: \Rightarrow in absence of prior information, *G* is high-dimensional; **Question:** why should the localized manifold $\widehat{\mathcal{M}} = \{T_{\mu}(g): g \in G, \mu \in \mathcal{P}\}$ be reducible?

Motivating example: semi-infinite wave-guides (I)

Consider the problem for $g(x_2) = \sum c_n \cos(n\pi x_2)$ n=1 $-\Delta u_g - \mu^2 u_g = 0 \text{ in } U$ $\partial_{x_2} u_g = 0 \text{ on } \mathbb{R}_+ \times \{0, 1\}$ $u_g = g \text{ on } \{0\} \times (0, 1)$ Define $\widehat{\Omega} = (L, \infty) \times (0, 1)$, $C, \overline{\mu} \in \mathbb{R}_+$ and the extracted manifold $\mathcal{M}_{L} = \{ u_{g} |_{\widehat{\Omega}} : \|g\|_{H^{1/2}} \leq C, \ \mu = \overline{\mu} \}.$

 $G = \{g : ||g||_{H^{1/2}} \le C\}$ is infinite-dimensional and is irreducible.

Motivating example: semi-infinite wave-guides (II)



The differential operator acts as a **low-pass filter**.

- Effect of evanescent modes is negligible far from $\Gamma_{\rm in}$.
- Manifold \mathcal{M}_L can be well-approximated by an *n*-dimensional space if $e^{-\alpha_{n+1}L} \ll 1$.

Filtering properties depend on the value of $\overline{\mu}$.

Localized training

- Oversampling
- Linear problems
- Randomization
- Numerical results

Transfer operator

Define the transfer operator $T : \mathcal{U} \times \mathcal{P} \to \mathcal{Y}$. For second-order elliptic PDEs, $G \subset \mathcal{U} \subset H^{1/2}(\Gamma_{\text{in}})$, $\mathcal{Y} \subset H^1(\widehat{\Omega})$; $(\mathcal{U}, \| \cdot \|_{\mathcal{U}})$, $(\mathcal{Y}, \| \cdot \|_{\mathcal{Y}})$ Hilbert spaces. We assume that $\mathcal{P} = {\overline{\mu}}$ and that T is **compact**.

Transfer operator

Define the transfer operator $T : \mathcal{U} \times \mathcal{P} \to \mathcal{Y}$. For second-order elliptic PDEs, $G \subset \mathcal{U} \subset H^{1/2}(\Gamma_{\text{in}})$, $\mathcal{Y} \subset H^1(\widehat{\Omega})$; $(\mathcal{U}, \| \cdot \|_{\mathcal{U}})$, $(\mathcal{Y}, \| \cdot \|_{\mathcal{Y}})$ Hilbert spaces. We assume that $\mathcal{P} = {\overline{\mu}}$ and that T is **compact**.

Proposition: Sufficient conditions for compactness of T: • dist $(\widehat{\Omega}, \Gamma_{in}) > 0$;

• $\|T(g)\|_{H^1(U')} \leq C(U, U') \|T(g)\|_{L^2(U)}$ for $U' \subseteq U$. Caccioppoli's ineq.

Caccioppoli's inequality is satisfied by a broad class of elliptic problems (Helmholtz, advection-diffusion, Stokes).

Babuska, Lipton, 2011. Taddei, Patera, 2018.

Transfer eigenproblem (TE)

Introduce the transfer eigenproblem:

 $(\varphi_i, \lambda_i) \in \mathcal{U} \times \mathbb{R}_+ \ (T(\varphi_i), \ T(g))_{\mathcal{Y}} = \lambda_i (\varphi_i, g)_{\mathcal{U}} \ \forall g \in \mathcal{U}$

with $i = 1, 2, \ldots, \lambda_1 \ge \lambda_2 \ge \ldots$

Define the transfer eigenspace $\mathcal{Z}_n^{\text{te}} = \text{span}\{T(\varphi_i)\}_{i=1}^n$.

Transfer eigenproblem (TE): properties (I)

Introduce the transfer eigenproblem:

 $(\varphi_i, \lambda_i) \in \mathcal{U} \times \mathbb{R}_+ \ (T(\varphi_i), \ T(g))_{\mathcal{Y}} = \lambda_i (\varphi_i, g)_{\mathcal{U}} \ \forall g \in \mathcal{U}$ with $i = 1, 2, ..., \ \lambda_1 > \lambda_2 > ...$

Define the **transfer eigenspace** $\mathcal{Z}_n^{\text{te}} = \text{span}\{T(\varphi_i)\}_{i=1}^n$.

If
$$\mathcal{U} = \operatorname{span}\{\phi_k\}_{k=1}^{N_{\operatorname{in}}}$$
, then $\varphi_i = \sum_{k=1}^{N_{\operatorname{in}}} (\varphi_i)_k \phi_k$, $\mathsf{A}\varphi_i = \lambda_i \mathsf{B}\varphi_i$

with $\mathbf{A}_{k,k'} = (T(\phi_k), T(\phi_{k'}))_{\mathcal{Y}}, \mathbf{B}_{k,k'} = (\phi_k, \phi_{k'})_{\mathcal{U}}.$

- Solution to TE requires computation of $\{T(\phi_k)\}_k$.
- If $\{\phi_k\}_k$ is orthonormal, then $\mathcal{Z}_n^{\text{te}}$ is the POD space associated with the snapshots $\{T(\phi_k)\}_k$.

Transfer eigenproblem: properties (II)



• The transfer eigenspace is optimal in the sense of Kolmogorov.

Error analysis: (Taddei, Patera, 2018) $\frac{\|\Pi_{(\mathcal{Z}_{n}^{\text{te}})^{\perp}}^{\mathcal{Y}} T(g)\|_{\mathcal{Y}}}{\|g\|_{\mathcal{U}}} \leq \|T\|_{\mathcal{L}(\mathcal{U}^{\perp};\mathcal{Y})} \frac{\|\Pi_{\mathcal{U}^{\perp}}^{\mathcal{U}}g\|_{\mathcal{U}}}{\|g\|_{\mathcal{U}}} + \sqrt{\lambda_{n+1}}$

for any $g \in H^{1/2}(\Gamma_{\rm in})$.

• If $g \notin \mathcal{U}$, performance of $\mathcal{Z}_n^{\text{te}}$ depends on the product $\|\mathcal{T}\|_{\mathcal{L}(\mathcal{U}^{\perp};\mathcal{Y})} \|\Pi_{\mathcal{U}^{\perp}}^{\mathcal{U}}g\|_{\mathcal{U}}$.

Extension to the parametric case

 $\begin{aligned} \mathsf{TE} + \mathsf{POD: given } \mathcal{U} &= \operatorname{span}\{\phi_i\}_{i=1}^{N_{\mathrm{in}}}, \{\mu^k\}_{k=1}^{n_{\mathrm{train}}}, n \in \mathbb{N} \\ \text{For } k &= 1, \dots, n_{\mathrm{train}} \\ \text{Compute } \mathcal{Z}_{n,k}^{\mathrm{te}} &:= \operatorname{span}\{T_{\mu^k}\varphi_i^k\}_{i=1}^n \text{ s.t. } (\varphi_i^k, \varphi_j^k)_{\mathcal{U}} = \delta_{i,j}. \\ \text{EndFor} \end{aligned}$

Return $\mathcal{Z}_n := \text{POD}\left(\{T_{\mu^k}\varphi_i^k\}_{i,k}, n\right).$ $i = 1, \dots, n, k = 1, \dots, n_{\text{train}}$

Taddei, Patera, SISC, 2018.

Extension to the parametric case

 $\begin{aligned} \mathsf{TE} + \mathsf{POD:} \text{ given } \mathcal{U} &= \operatorname{span}\{\phi_i\}_{i=1}^{N_{\mathrm{in}}}, \{\mu^k\}_{k=1}^{n_{\mathrm{train}}}, n \in \mathbb{N} \\ \text{For } k &= 1, \dots, n_{\mathrm{train}} \\ \text{Compute } \mathcal{Z}_{n,k}^{\mathrm{te}} &:= \operatorname{span}\{T_{\mu^k}\varphi_i^k\}_{i=1}^n \text{ s.t. } (\varphi_i^k, \varphi_j^k)_{\mathcal{U}} = \delta_{i,j}. \\ \text{EndFor} \end{aligned}$

Return $\mathcal{Z}_n := \text{POD}\left(\{T_{\mu^k}\varphi_i^k\}_{i,k}, n\right).$ $i = 1, \dots, n, k = 1, \dots, n_{\text{train}}$

- Equivalent to hierarchical approximate POD. Himpe, Leibner, Rave, 2018.
- Alternative approach: TE + strong Greedy in parameter. Smetana, Patera 2016.

Taddei, Patera, SISC, 2018.

Localized training

- Oversampling
- Linear problems
- Randomization
- Numerical results

Motivation

TE + POD requires $N_{in} \cdot n_{train}$ PDE solves. **Possible fix:** Krylov subspace methods for the TE.

Randomized methods offer an alternative strategy to tackle the problem.

Mahoney 2016: randomness is an algorithmic resource creating efficient, unbiased approximations of nonrandom operations.

Key features of randomized algorithms:

- Incremental (iterative) approach.
- Probabilistic error estimation.

Randomized SVD: Mahoney, Martinsson, Tropp... Randomized model reduction: Buhr & Smetana; Smetana, Zahm, Patera.

Adaptive randomized algorithm

Inputs: maxit, r_{train} , $n \in \mathbb{N}$, pdfs p_{μ} , p_{G} (sampling); **Output:** $Z_n = \operatorname{span}\{\zeta_i\}_{i=1}^n$ reduced space. $(\zeta_i, \zeta_i) = \delta_{i,i}$ Set $\mathcal{Z}_n = \emptyset$, $\lambda_1 = \ldots = \lambda_n = 0$. For $i = 1, \ldots, \text{maxit}$ Generate $\mu^{(k)} \stackrel{\text{iid}}{\sim} p_{\mu}$, $g^{(k)} \stackrel{\text{iid}}{\sim} p_{G}$, $k = 1, \ldots, r_{\text{train}}$. Compute $u^{k,i} = T_{\mu^{(k)}}g^{(k)}$ for $k = 1, \ldots, r_{\text{train}}$. Compute $\widehat{E} = \frac{1}{r_{\text{train}}} \sum_{k=1}^{r_{\text{train}}} \|\Pi_{\mathcal{Z}_n^{\perp}} u^{k,i}\|_{\mathcal{Y}} / \|u^{k,i}\|_{\mathcal{Y}}.$ if $\widehat{E} \leq tol$, BREAK else $[\mathcal{Z}_n, \{\lambda_j\}_j] = \text{POD}\left(\left\{\zeta_j \sqrt{\lambda_j}\right\}_{j=1}^n \cup \left\{u^{k,j}\right\}_{k=1}^{r_{\text{train}}}, n\right)$ EndFor

Adaptive randomized algorithm: comments

Interpretation: incremental randomized POD in parameter and boundary data. Yu, Chakravorty, 2015

- Snapshots $\{u^{k,i}\}_{k,i}$ are used for testing and then to update the reduced space.
- $[\mathcal{Z}_n, \{\lambda_j\}_j] = \operatorname{POD}\left(\left\{\zeta_j \sqrt{\lambda_j}\right\}_{j=1}^n \cup \left\{u^{k,j}\right\}_{k=1}^{r_{\operatorname{train}}}, n\right)$

• Snapshots from previous iterations are not stored.

- Factors $\{\sqrt{\lambda_i}\}_i$ serve to properly fuse information from different iterations. Himpe, Leibner, Rave 2018
- \widehat{E} is a MC estimate of $\mathbb{E}_{\mu \sim p_{\mu}, g \in p_{G}} \left[\frac{\|\Pi_{\mathcal{Z}_{n}^{\perp}} T_{\mu}(g)\|_{\mathcal{Y}}}{\|T_{\mu}(g)\|_{\mathcal{V}}} \right]$

For linear problems, see also Buhr, Smetana, 2018.

Randomized Greedy: Cohen et al, M2AN, 2020.

Idea: since we expect solution to be smooth, we control the smoothness of the samples.

$$\begin{array}{l} \text{Consider } g_{\text{co}}(s; \mathbf{c}^{\text{re}}, \mathbf{c}^{\text{im}}) = \sum_{k=0}^{N_{\text{f}}-1} \frac{c_k^{\text{re}} + \mathrm{i} \, c_k^{\text{im}}}{\sqrt{1 + (2\pi k)^{2\alpha}}} \, e^{2\pi k s \mathrm{i}},\\ \text{with } c_k^{\text{re}}, c_k^{\text{im}} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1). \text{ Then, if } \alpha \in \mathbb{N}\\ \|g_{\text{co}}(\cdot; \mathbf{c}^{\text{re}}, \mathbf{c}^{\text{im}})\|_{L^2(0, 1)}^2 + \|g_{\text{co}}^{(\alpha)}(\cdot; \mathbf{c}^{\text{re}}, \mathbf{c}^{\text{im}})\|_{L^2(0, 1)}^2 \sim \chi^2(2N_{\text{f}}) \end{array}$$

Idea: since we expect solution to be smooth, we control the smoothness of the samples.

Consider
$$g_{co}(s; \mathbf{c}^{re}, \mathbf{c}^{im}) = \sum_{k=0}^{N_{f}-1} \frac{c_{k}^{re} + ic_{k}^{im}}{\sqrt{1 + (2\pi k)^{2\alpha}}} e^{2\pi k s i}$$
,
with $c_{k}^{re}, c_{k}^{im} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$. Then, if $\alpha \in \mathbb{N}$
 $\|g_{co}(\cdot; \mathbf{c}^{re}, \mathbf{c}^{im})\|_{L^{2}(0, 1)}^{2} + \|g_{co}^{(\alpha)}(\cdot; \mathbf{c}^{re}, \mathbf{c}^{im})\|_{L^{2}(0, 1)}^{2} \sim \chi^{2}(2N_{f})$

 $\mathsf{Proposal:} \ g(\cdot; \mathbf{c}^{\mathrm{re}}, \mathbf{c}^{\mathrm{im}}) \ = \ \mathsf{Real} \left[g_{\mathrm{co}}(\cdot; \mathbf{c}^{\mathrm{re}}, \mathbf{c}^{\mathrm{im}}) \right].$

For edge and corner components, we need to enforce Dirichlet boundary conditions. details omitted

Localized training

- Oversampling
- Linear problems
- Randomization
- Numerical results

Linear advection-diffusion-reaction equation

Pb: given $\mu \in \mathcal{P}$, $g \in H^{1/2}(\Gamma_{\text{in}})$, $\kappa(x) = 1 + ||x||_2^2$, $U = [0, 0.3]^2$, $\mathcal{P} = [0.2, 1] \times [-1, 1]^2 \times [0, 1]$, find u_{μ} s.t. $\begin{cases} -\nabla \cdot (\mu_1 \kappa^{-1} \nabla u_{\mu} + [\mu_2, \mu_3] u_{\mu}) + \mu_4 u_{\mu} = 0 \text{ in } U \\ u_{\mu}|_{\partial U = \Gamma_{\text{in}}} = g, \end{cases}$ We consider the extracted domain $\widehat{\Omega} = [0.1, 0.2]^2$.

Linear advection-diffusion-reaction equation

- **Pb:** given $\mu \in \mathcal{P}$, $g \in H^{1/2}(\Gamma_{\text{in}})$, $\kappa(x) = 1 + ||x||_2^2$, $U = [0, 0.3]^2$, $\mathcal{P} = [0.2, 1] \times [-1, 1]^2 \times [0, 1]$, find u_{μ} s.t. $\begin{cases} -\nabla \cdot (\mu_1 \kappa^{-1} \nabla u_{\mu} + [\mu_2, \mu_3] u_{\mu}) + \mu_4 u_{\mu} = 0 \text{ in } U \\ u_{\mu}|_{\partial U = \Gamma_{\text{in}}} = g, \end{cases}$
- We consider the extracted domain $\widehat{\Omega} = [0.1, 0.2]^2$.

Description of the test

• P3 FE with $N_{\rm in} = 360$ dofs on $\Gamma_{\rm in}$.

• TE+POD based on $n_{\text{train}} = 100$.

Linear advection-diffusion-reaction equation

Pb: given $\mu \in \mathcal{P}$, $g \in H^{1/2}(\Gamma_{\text{in}})$, $\kappa(x) = 1 + ||x||_2^2$, $U = [0, 0.3]^2$, $\mathcal{P} = [0.2, 1] \times [-1, 1]^2 \times [0, 1]$, find u_{μ} s.t. $\begin{cases} -\nabla \cdot (\mu_1 \kappa^{-1} \nabla u_{\mu} + [\mu_2, \mu_3] u_{\mu}) + \mu_4 u_{\mu} = 0 \text{ in } U \\ u_{\mu}|_{\partial U = \Gamma_{\text{in}}} = g, \end{cases}$

We consider the extracted domain $\widehat{\Omega} = [0.1, 0.2]^2$.

Description of the test

- Maximum relative projection error $E_{\max, rel}$ based on $n_{\text{test}} = 100 \text{ samples } \{T_{\mu^{(k)}}g^{(k)}\}_k \text{ with } g^{(k)} \stackrel{\text{iid}}{\sim}$ $p_G^{\text{smooth}}(\alpha = 1), \ \mu^{(k)} \stackrel{\text{iid}}{\sim} \text{Uniform}(\mathcal{P}).$
- Randomized training with $r_{\text{train}} = 10$, $g^{(k)} \stackrel{\text{iid}}{\sim} p_G^{\text{smooth}}$, $\mu^{(k)} \stackrel{\text{iid}}{\sim} \text{Uniform}(\mathcal{P})$.

Choice of the boundary distribution: visualization (int)

Samples of the datum on $\Gamma_{\rm in}$ for $\alpha = 1$.



Choice of the boundary distribution: visualization (int)

Samples of the datum on $\Gamma_{\rm in}$ for $\alpha = 2$.



Choice of the boundary distribution: visualization (int)

Samples of the datum on $\Gamma_{\rm in}$ for $\alpha = 3$.



Out-of-sample performance

Gaussian sampling: $g \sim p_G^{\text{gauss}} \Leftrightarrow g(x) = \sum c_i \phi_i^{\text{fe}}(x)$

 $i \in I_{dir}$



- Randomized training performs similarly to TE+POD after 5 iterations.
- Smooth samping is (slightly) more effective than Gaussian sampling at early iterations.



computed during the iterations of the randomized algorithm with the estimates on the $n_{\text{test}} = 100$ datapoints.



Randomized sampling for nonlinear PDEs

• Numerical results

Objective: extend the localized training procedure to nonlinear PDEs.

- Error estimation and oversampling can be extended as is.
- How should we choose p_G ?
- Theoretical questions
- Compactness of the solution manifold¹.

Caccioppoli's ineq.

• Constructive optimal approximations²

¹Compactness of the transfer operator is key for approximability of the nonlinear set of functions, and ultimately justifies oversampling. ²Generalization of transfer eigenproblems to nonlinear PDEs.

Choice of p_G for the model problem

Model pb:
$$-\nabla \cdot (\kappa_{\mu}(u_{\mu})\nabla u_{\mu}) = f_{\mu} \ln \Omega, \ u_{\mu}|_{\partial\Omega} = 0$$

 $\kappa_{\mu}(u)|_{\Omega_{i}} = \frac{36}{\mu_{2}^{(i)}} \left(\frac{u(1-u)}{u^{3} + \frac{12}{\mu_{2}^{(i)}}(1-u)^{3}} \right)^{2} + \mu_{1}^{(i)}, \ i = 1, 2, \dots$
 $f_{\mu}(x) = 100e^{\left(-100\frac{\|x-x_{c,i}\star\|_{2}^{2}}{2}\right)} \mathbb{1}_{\Omega_{i}^{\star}}(x), \ x_{c,i^{\star}} := \frac{1}{\Omega_{i}^{\star}} \int_{\Omega_{i}^{\star}} x \, dx.$

Obs (I): $u_{\mu} \in [0, 1) \Rightarrow$ we assume that $g(x) \in [0, \overline{u}_{\max}]$ **Obs (II):** $u_{\mu}|_{\Gamma_{in}}$ is expected to be smooth (at least $H^{1/2}$). \Rightarrow smooth sampling. We consider the following sampling algorithm:

- 1. Draw $\mathbf{c}^{\mathrm{re}}, \mathbf{c}^{\mathrm{im}} \in \mathbb{R}^{N_{\mathrm{f}}}$ s.t. $c_k^{\mathrm{re}}, c_k^{\mathrm{im}} \stackrel{\mathrm{iid}}{\sim} \mathcal{N}(0, 1)$.
- 2. Draw $X_1, X_2 \stackrel{\text{iid}}{\sim} \text{Uniform}(0, \overline{u}_{\max})$, set $a = \min\{X_1, X_2\}$, $b = \max\{X_1, X_2\}$.

3. Set
$$g' = \text{Real} \left[g_{\text{co}}(\cdot; \mathbf{c}^{\text{re}}, \mathbf{c}^{\text{im}}) \right]$$
.
4. Set $g = a + \frac{b-a}{\max g' - \min g'} \left(g' - \min g' \right)$.
Memo: $g_{\text{co}}(s; \mathbf{c}^{\text{re}}, \mathbf{c}^{\text{im}}) = \sum_{k=0}^{N_{\text{f}}-1} \frac{c_k^{\text{re}} + ic_k^{\text{im}}}{\sqrt{1 + (2\pi k)^{2\alpha}}} e^{2\pi k s i}$.

Choice of p_G : internal component (visualization)

- p_G encodes the fact that $Im[g] \subset [0, \overline{u}_{\max}]$.
- α encodes prior knowledge on the regularity of g.

Samples of the datum on $\Gamma_{\rm in}$ for $\alpha = 1$ ($\bar{u}_{\rm max} = 0.5$).



Choice of p_G : internal component (visualization)

- p_G encodes the fact that $Im[g] \subset [0, \overline{u}_{\max}]$.
- α encodes prior knowledge on the regularity of g. Samples of the datum on Γ_{in} for $\alpha = 2$ ($\bar{u}_{max} = 0.5$).



Choice of p_G : internal component (visualization)

- p_G encodes the fact that $Im[g] \subset [0, \overline{u}_{\max}]$.
- α encodes prior knowledge on the regularity of g.

Samples of the datum on $\Gamma_{\rm in}$ for $\alpha = 3$ ($\bar{u}_{\rm max} = 0.5$).



Randomized sampling for nonlinear PDEs

• Numerical results

We perform localized training based on $n_{\text{train}} = 10^2$ simulations for each component to build $\mathcal{Z}^{\text{co}}, \mathcal{Z}^{\text{int}}, \mathcal{Z}^{\text{ed}}$.

Oversampling domains: each subregion is characterized by a value of $\mu \in \mathcal{P}$; source term is activated with probability p = 0.5.



Description of the test: global solves

 x_2^2

We compute n_{test} global solutions for N_{dd} subdomains and we extract solution in each element.

 $n_{
m test} = 15, \; N_{
m dd} = 100, \; \Omega = (0,1)^2$

We use the datasets of local solutions to measure performance of localized training .

 $n_{\text{test}}^{\text{int}} = 960, \; n_{\text{test}}^{\text{co}} = 60, \; n_{\text{test}}^{\text{ed}} = 480$ 0.35 0.3 0.8 0.3 0.8 0.25 0.25 0.6 0.6 0.2 0.2 23 R 0.15 0.4 0.15 0.4 0.1 0.1 0.2 0.2 0.05 0.05 0 0 02 0.8 02 0.8 0406 04 x_1 x_1

Error measures

- Average H^1 relative projection error at component level.
- Average L^2 relative global projection error.

We compare performance of

- smooth sampling for various α ;
- Gaussian sampling with clipping $\max(\min(g, \bar{u}_{\max}), 0)$;
- benchmark: POD space based on test set "opt" ³.

³Not computable for practical applications due to the impossibility to perform global solves.

Results: local errors for non-overlapping domains

- Randomized sampling provides accurate spaces for moderate *n*.
- Gaussian sampling is inaccurate for edge and corner components.
- Performance is nearly independent of α .



Results: local errors for non-overlapping domains

- Randomized sampling provides accurate spaces for moderate *n*.
- Gaussian sampling is inaccurate for edge and corner components.
- Performance is nearly independent of α .



Results: local errors for non-overlapping domains

- Randomized sampling provides accurate spaces for moderate *n*.
- Gaussian sampling is inaccurate for edge and corner components.
- Performance is nearly independent of α .



Results: global errors

Relative error is below 10^{-4} for n = 30.

Total number of degrees of freedom: ROM $n \cdot 100$, FOM 90601.



Conclusions

Component-based model reduction offers the opportunity to address large-scale parameterized problems. topology changes, high-dimensional parameterization

Tasks: localized training and domain decomposition.

Component-based model reduction offers the opportunity to address large-scale parameterized problems. topology changes, high-dimensional parameterization

Tasks: localized training and domain decomposition.

In this talk, we discussed localized training for steady PDEs:

- transfer operator and optimal approximations;
- randomized training based on random samples of BCs;
- probabilistic error estimation.

Extension to nonlinear problems requires major advances to state-of-the-art methods.

Localized training

- Problem-aware sampling distribution of BCs.
- Online basis enrichment. Schlinder, Ohlberger, 2015
 Domain decomposition
- Partition-of-unity overlapping methods.

Melenk, Babuska, 1996

• Hyper-reduction.

Thank you for your attention!

For more information, visit the website:

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

Backup slides

• More plots

Backup slides

• More plots

Choice of the boundary distribution: visualization (corner)

 $g(s; \mathbf{c}^{re}, \mathbf{c}^{im}) = \text{Real} \left[g_{co}(0.7 \cdot s; \mathbf{c}^{re}, \mathbf{c}^{im})\right] s(1-s).$ • g_{co} is not periodic in (0, 1). • $g_{co}(s) = 0$ for $s \in \{0, 1\}$.

Samples of the datum on $\Gamma_{\rm in}$ for $\alpha = 1$.



Choice of the boundary distribution: visualization (corner)

 $g(s; \mathbf{c}^{re}, \mathbf{c}^{im}) = \text{Real} \left[g_{co}(0.7 \cdot s; \mathbf{c}^{re}, \mathbf{c}^{im})\right] s(1-s).$ • g_{co} is not periodic in (0, 1). • $g_{co}(s) = 0$ for $s \in \{0, 1\}$.

Samples of the datum on $\Gamma_{\rm in}$ for $\alpha = 2$.



Choice of the boundary distribution: visualization (corner)

 $g(s; \mathbf{c}^{re}, \mathbf{c}^{im}) = \text{Real} \left[g_{co}(0.7 \cdot s; \mathbf{c}^{re}, \mathbf{c}^{im})\right] s(1-s).$ • g_{co} is not periodic in (0, 1). • $g_{co}(s) = 0$ for $s \in \{0, 1\}$.

Samples of the datum on $\Gamma_{\rm in}$ for $\alpha = 3$.



For $\bar{u}_{max} = 0.5$, Newton solver with line search converges for all training points.

For $\bar{u}_{\rm max} = 0.75$, Newton solver with line search fails to converge 1% of the times for smooth sampling $\alpha = 0.5$ and 30% of the times for Gaussian sampling.

Results for the edge component:

