Giulia Sambataro

giulia.sambataro@enpc.fr | +33 77 44 47 11 8
52, Avenue Emile Cossonneau, 93160, Noisy Le Grand (France)
Nationality: italian, | 31 years

Research interests

Numerical methods for partial differential equations (especially model reduction)

Data-based/simulation-based methods, machine learning techniques

Multiphysics coupled systems, variational inequalities (contact mechanics)

Optimization

Education

2019 - 2022 **Doctor of Philosophy**
Applied Mathematics and Scientific Computing
Institut des Mathématiques de Bordeaux, University of Bordeaux, France

2016-2019 **Master of Science**,
Mathematical Engineering
Politecnico di Milano, Milan, Italy
Final grade: 106/110

2012 - 2015 **Bachelor of Science**,
Computer science and automation engineering
Università Politecnica delle Marche, Ancona, Italy
Final grade: 110/110 with honors

Teaching experience

Course: Analysis for partial differential equations.
École des Ponts Paristech September 2023-January 2024
Full course (theoretical and exercise lessons)

Appointments and research experience

École des Ponts Paristech — February 2023-February 2025
Cermics laboratory, MATHERIALS team (Inria) — Post-doctoral associate
Adviser: V. Ehrlacher

INRIA Bordeaux South-West — October 2019-December 2022
MEMPHIS team, Institut des Mathématiques de Bordeaux — PhD student
Advisers: A. Iollo, T. Taddei

Politecnico di Milano — April 2018-April 2019
Laboratory for Modeling and Scientific Computing (MOX) — Internship student
Adviser: C. Vergara

Publications

Gigante, G. et al. (2020). "Optimized Schwarz methods for spherical interfaces with application to fluid-structure interaction". In: *SIAM Journal on Scientific Computing* 42.2, A751–A770.

Iollo, A. et al. (2022). "An adaptive projection-based model reduction method for nonlinear mechanics with internal variables: Application to thermo-hydro-mechanical systems". In: *International Journal for Numerical Methods in Engineering*.

Sambataro, G. (2022). "Réduction de modèle basée sur des composants élémentaires pour des systèmes Thermo-Hydro-Mécaniques." PhD thesis. Université de Bordeaux.

Iollo, A. et al. (2023a). "A one-shot overlapping Schwarz method for component-based model reduction: application to nonlinear elasticity". In: *Computer Methods in Applied Mechanics and Engineering* 404, p. 115786.

– (2023b). "An optimization-based model order reduction approach for coupled problems: application to thermo-hydro-mechanical systems". In: URL: https://api.semanticscholar.org/CorpusID:265356225.

PhD Thesis

https://theses.hal.science/tel-04006932/document

In preparation

V. Ehrlacher, G. Sambataro, "A nonlinear reduced basis approximation of discrete contact problems in crowd motion".

Selected invited conference presentations

June 2023, Chania (Greece)	Coupled 2023 X International Conference on Computational Methods for Coupled problems in Science and Engineering Chair: Dr. Irina Tezaur
February 2024, Trieste (Italy)	SIAM UQ24 X SIAM Conference on Uncertainty Quantification Chair: Dr. D. Lombardi, F. Nobile
June 2024, Lisbon (Portugal)	ECCOMAS 2024 9^{th} European Congress on Computational Methods in Applied Sciences and Engineering Chair: M. Manucci, J. Nicodemus, B.Unger
July 2024, Vancouver (Canada)	WCCM-PANACM 16^{th} World Congress on Computational Mechanics Chair: N. Akkari, C. Farhat et al.

Skills

Matlab, Python, LaTeX, FreeFem++, Scilab, C++, Paraview

Languages

- Italian: mothertongue
- English: C1 CEFR level
- French: B2 CEFR level

Research overview

PhD thesis project

Motivation

The application motivating my Phd thesis is the disposal and storage of high-level radioactive waste materials in geological media. I collaborated with Andra, — the French National Agency for Radioactive Waste Management[1] — for radioactive waste management. To protect the environment from the radioactive emission, the radioactive waste is disposed in packages that are located horizontally deep underground (at approximately 300 to 500 meters) and are monitored until their radioactivity has decayed to an acceptable level. Figure 1 is a schematic representation of waste disposal in the repositories. Due to the large temperature of the radioactive waste, a thermal flux is generated inside the alveoli: the thermal flux then drives the mechanical and hydraulic response of the geological medium over the course of several years. This phenomenon requires a careful assessment of the long-term effects on neighboring areas.

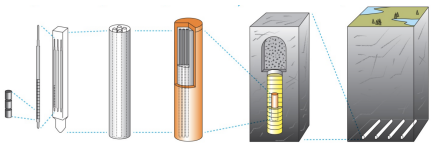


Figure 1: Multi-barrier disposal concept

The THM problem

From a mathematical viewpoint, the system behaviour is described by time-dependent large scale coupled systems of partial differential equations (PDEs) called Thermo-Hydro-Mechanical (THM) systems: they model the behaviour of temperature, pore water pressure and solid displacement in

[1] Andra website: https://www.andra.fr

the neighborhood of geological repositories. To introduce the mathematical formulation, we consider the spatial variable x in the Lipschitz domain $\Omega \subset \mathbb{R}^d$ with dimension $d = 2$, and the time variable t in the time internal $(0, T_\mathrm{f}] \subset \mathbb{R}$, where T_f is the final time. We further define the vector of parameters μ in the compact parameter region $\mathcal{P} \subset \mathbb{R}^P$. Given a parameter $\mu \in \mathcal{P}$, we introduce the state (or primary) variables $\underline{U}_\mu : \Omega \times (0, T_\mathrm{f}] \to \mathbb{R}^D$, like the solid displacement, water pressure and temperature. Internal variables $\underline{W}_\mu : \Omega \times (0, T_\mathrm{f}] \to \mathbb{R}^{D_\mathrm{cl}}$ can be thought of as local physical variables that contribute to well characterise the physical dynamics of the system: they are not associated with conservation laws but with constitutive laws.

The system can be written in the following abstract form:

$$\begin{cases} \mathcal{G}_\mu(\underline{U}_\mu, \partial_t \underline{U}_\mu, \underline{W}_\mu) = 0, & \text{in } \Omega \times (0, T_\mathrm{f}], \\ \dot{\underline{W}}_\mu = \mathcal{F}_\mu(\underline{U}_\mu, \underline{W}_\mu), & \text{in } \Omega \times (0, T_\mathrm{f}], \end{cases} \tag{1}$$

with suitable initial and boundary conditions. Here, $\mathcal{G}_\mu$ is a nonlinear second-order in space, first-order in time differential operator that is associated with the equilibrium equations.

Methodology overview

We consider a finite dimensional approximation of problem (1): indeed, we take a finite dimensional subspace $\mathcal{X}^\mathrm{hf} \subset \mathcal{X}$ (of dimension N^hf) of a suitable Hilbert space $\mathcal{X}$ defined in Ω. We refer to this approximation as *high-fidelity* (HF) discretization; to solve the discretized PDE problem we employ the finite-element (FE) method.

Parametric model order reduction (pMOR) techniques are applied to problems of form (1) to construct a model of low dimension requiring short simulation times and low data storage, but still keeping the approximation error between the *reduced-order* solution and the so called *full-order* one (computed from a high-fidelity discretization of the parametrized PDE) under control. Reduced basis (RB) methods represent a particular instance of reduced order models: the RB solution is obtained through a *projection* of the high-fidelity problem onto a small subspace. This latter is made by a small number of global basis functions, constructed for the specific problem at hand, rather than by a much larger number of basis functions.
The essential constituent of a RB method is the *offline/online* procedure. The solution to the full-order model is needed for a few instances of the parameters during a computationally demanding *offline* stage (also called *training* stage), in order to construct a reduced space of basis solutions and to build the reduced order model (ROM); the reduced order model enables rapid prediction of the solution field for new instances of the parameters during the *online* (or *prediction*) stage. At the training stage, standard pMOR techniques rely on high-fidelity (HF) solves, which might be unaffordable for very large-scale problems or in the case where very fine meshes are needed to reach a good level of accuracy. Furthermore, standard pMOR techniques rely on the assumption that the solution field is defined over a parameter-independent domain or over a family of diffeomorphic domains. In fact, for systems with many geometric parameters, dealing with changes in domain topology requires major changes to the offline/online paradigm of MOR. To provide a concrete example, let us consider a PDE problem as in form (1) to be solved in a domain as the one in figure 2, in which the red boundaries model the presence of radioactive waste repositories and are associated with a certain type of boundary condition in problem (1). Despite its simplicity, if the position

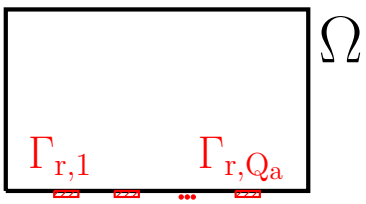


Figure 2: Domain Ω and boundaries $\Gamma_{\mathrm{r},1}, \ldots, \Gamma_{\mathrm{r},\mathrm{Q_a}}$ that can vary in number and position.

and/or the number of the repositories — which we denote as Q_{a} — change, the solution to problem (1) becomes prohibitive for the standard ROMs introduced so far: if the number of repositories is sufficiently large, we would indeed end up with a very high-dimensional parametrization, which would require several full-order solves. Furthermore, solutions for different numbers of repositories are defined over different meshes and satisfy different sets of boundary conditions: therefore, they cannot be considered into a single reduced space. To adress these issues, several authors have proposed component-based (CB) pMOR procedures, which combine domain decomposition (DD) techniques with model order reduction. CB-pMOR procedures aim to construct local (in space and/or in time) reduced spaces that have support on a portion of the domain and compute a global approximation by suitable coupling of the local spaces. We refer to the standard pMOR methods in a single domain as the *monolithic* approach and we distinguish it from the CB-pMOR approach in which the decomposition of the original domain into a partition of subdomains comes into play.

CB-pMOR strategies consist of two distinct building blocks: (i) a rapid and reliable DD strategy for online global predictions, and (ii) a localized training strategy exclusively based on local solves for the construction of the local reduced bases. I developed, during my PhD thesis, a general component-based pMOR procedure for both steady and unsteady nonlinear problems. The domain decomposition is based on *overlapping* subdomains: overlapping domain decomposition methods feature a simplified imposition of the continuity conditions of solutions at the interface boundaries among subdomains. Therefore, it is desirable in the case of non-linear problems requiring demanding implementations.

The adoption of a component-based reduction method requires a suitable adaptation of the offline/online decomposition introduced so far, since the MOR methodology has to be extended to a component-based framework. The key point of the CB-pMOR approach we use in this work is the concept of *archetype* and *instantiated* domains. Archetype components are reference components which are built for a certain user-defined fixed value of geometric parameters. The instantiated components are the actual components which are created for each parameter of interest; they are connected through predefined interface boundaries (or faces) named *ports* to form a global synthesized system. In figure 3 the global domain Ω is decomposed into an overlapping partition $\{\Omega_i\}_{i=1}^{N_{\mathrm{dd}}}$ for

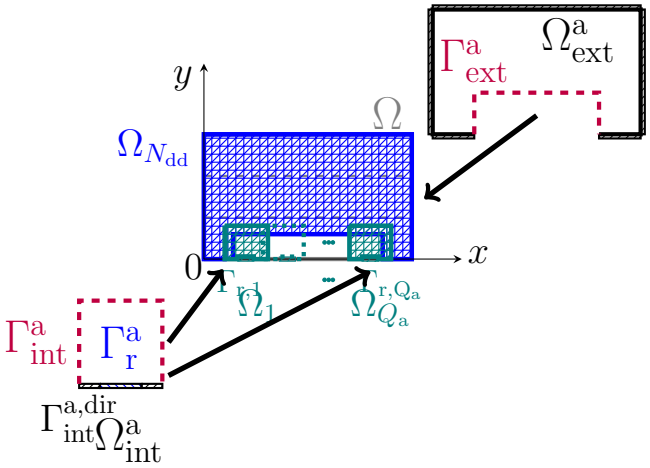


Figure 3: Instantiated components $\{\Omega_i\}_{i=1}^{N_{\mathrm{dd}}}$ for a given value of geometric parameter Q_{a}.

a given value of the geometric parameter Q_{a}; next to the instantiated subdomains, the corresponding "internal" and the "external" archetype components are depicted.

The offline/online MOR subdivision introduced in the case of monolithic ROM is substantially adapted as follows.

1. During the offline stage, a library of archetype components is defined and local reduced-order bases (ROBs) and local ROMs are built; this stage requires HF solves and may thus be relatively expensive, but it is carried out only once as a library preprocessing step.

2. During the online stage, local components are instantiated to form the global system and the global solution is estimated by coupling local ROMs. In this stage, the user may instantiate any of the archetype components and assign to each component instantiation the desired parameter values; this phase is supposed to be much less expensive.

In my thesis I worked on a novel component-based formulation which relies on a constrained optimization formulation that penalizes solutions jumps at the ports, subject to the approximate satisfaction of the PDE of interest in each instantiated component Ω_i, for $i = 1, \dots, N_{\text{dd}}$. We present here the formulation in the case of a steady PDE. Given the set of parameters $\mu = (\mu_1, \dots, \mu_{N_{\text{dd}}}) \in \mathcal{P} = \bigotimes_{i=1}^{N_{\text{dd}}} \mathcal{P}_{\text{L}_i}$, we propose the CB full-order model: find $\underline{U}^{\text{hf}} = (\underline{U}_1^{\text{hf}}, \dots, \underline{U}_{N_{\text{dd}}}^{\text{hf}}) \in \mathcal{X} := \bigotimes_{i=1}^{N_{\text{dd}}} \mathcal{X}_i$ to minimize

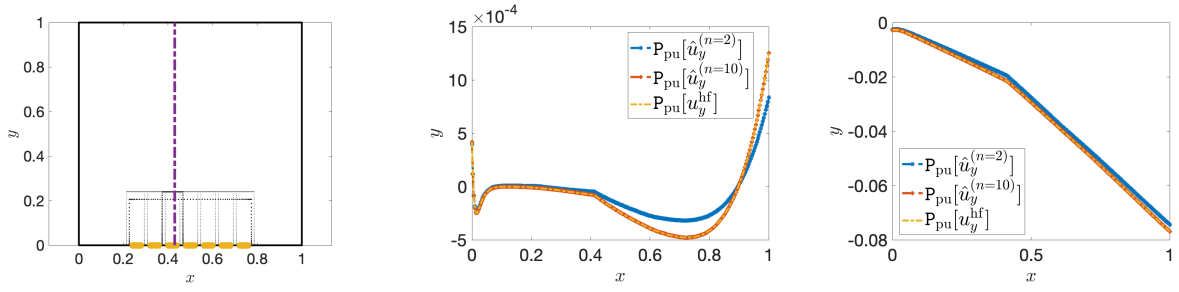
$$\min_{\underline{U} \in \mathcal{X}} \frac{1}{2} \sum_{i=1}^{N_{\text{dd}}} \sum_{j \in \text{Neigh}_i} \|\underline{U}_i - \underline{U}_j\|^2_{L^2(\Gamma_{i,j})} \quad \text{s.t.} \;\; \mathcal{G}_i(\underline{U}_i, \underline{V}_i) = 0 \;\; \forall \underline{V}_i \in \mathcal{X}_{i,0}, \; i = 1, \dots, N_{\text{dd}}, \tag{2}$$

where $\text{Neigh}_\text{i} := \{j : \Omega_i \cap \Omega_j \neq \emptyset, j \neq i\}$ and the interface boundaries are defined as $\Gamma_{ij} = \Gamma_i \cap \Omega_j$ for $j \in \text{Neigh}_\text{i}$. The formulation (2) is proved to be the limit of Overlapping Schwarz iterations: we thus refer to our approach as the one-shot (OS) overlapping Schwarz (OS) method and use the acronym OS2.

By the exploitation of the underlying principle of static condensation, the constrained problem is recast into an unconstrained minimization problem, which has the form of a nonlinear least-squares problem and which is then solved by Gauss-Newton method. The extension of classical pMOR techniques to the DD framework is driven by the definition of local reduced bases (rather than a global reduced basis), which are associated with the archetype components.

Main results

The OS2 method is developed for two classes of problems: a two-dimensional (plane stress) nonlinear neo-Hookean elasticity problem; a THM system with internal variables briefly described in section 8. The results on the former application are summerized below; for the results on the latter application I refer to Sambataro 2022. We achieved a speedup factor of the order of 20 compared to a standard monolithic FE model, with less than 0.1% prediction error. Figure 4 shows the behavior of the solution over a vertical slice of the domain for a test configuration with $Q_\text{a} = 7$. The points of the slice belong to either the instantiated component Ω_3 or Ω_8 (or both). We apply the partition of unity operator `Pu` to generate globally-defined solutions. We compute therefore approximate solutions $\texttt{P}_{\text{pu}}[\hat{u}_\star^{(n=2)}]$ $\texttt{P}_{\text{pu}}[\hat{u}_\star^{(n=10)}]$ corresponding to two choices of the reduced order bases (ROB) port and bubble size $n = m = 2$ and $n = m = 10$ and for subscript $\star$ corresponding to x and y components; we also compare the reduced solutions with the HF globally defined solutions $\texttt{P}_{\text{pu}}[u_\star^{\text{hf}}]$. We observe that the choice $n = m = 2$ enables qualitatively accurate approximations of the vertical displacement (cf. 4(c)), but extremely inaccurate approximations of the horizontal displacement (cf. Figure 4(b)), while the choice $n = m = 10$ leads to accurate predictions for both horizontal and vertical displacements.



(a) geometry configuration and slice (b) horizontal displacement (c) vertical displacement

Figure 4: visualization of the horizontal and vertical displacement components for a vertical slice.

In figure 6 we study the performance of the multiplicative Overlapping Schwarz (OS) method and the proposed OS2 method with respect to the overlap size δ, as depicted in figure 5. The results obtained for the proposed method are promising: OS2 and OS show comparable average values of the objective function for increasing dimensions of the reduced spaces; the average computational costs show a high dependence on the size of the overlap in the case of OS unlike the case of OS2.

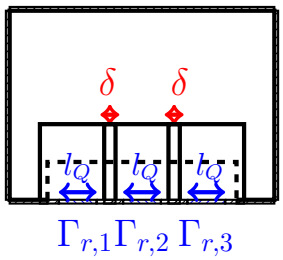
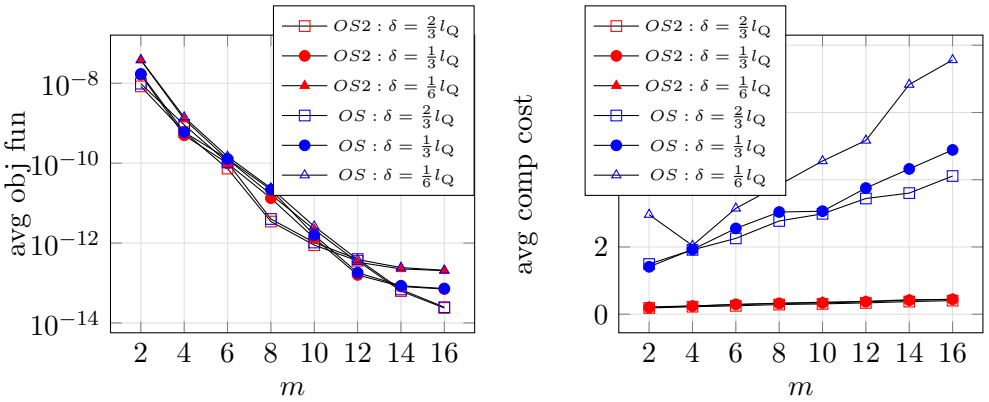


Figure 5: Example of geometric overlapping instantiated configuration for $Q_a = 3$.



(a) average objective function

(b) average computational cost

Figure 6: Out-of-sample test: (a) average values of the objective function, (b) average computational cost of OS2 and OS for $\delta = \frac{2}{3} l_Q$, $\delta = \frac{1}{3} l_Q$ and $\delta = \frac{1}{6} l_Q$.

Post-doctoral project

In my current post-doctoral research work I develop new model reduction approaches to predict the solutions of time-dependent parametrized problems. In particular, the application of interest is the crowd motion in the presence of obstacles, described by a discrete contact model (DCM) (cf. Maury and Venel 2011): we consider N_p agents identified to rigid disks of radius r and we define the feasibility region for the positions $\mathcal{Q} = \{\mathbf{q} \in \mathbb{R}^{2N_p} \text{ s.t. } D_{ij}(\mathbf{q}) = |q_i - q_j| - 2r \geq 0, \forall i < j\}$, where D_{ij} is the signed distance between disks i and j.
The DCM problem is formulated as a constrained least-squares optimization statement: the velocity field is seeked as the projection of the spontaneous velocities of each particle $\mathbf{U}_i = \mathbf{U}_i(\mathbf{q})$ into a closed convex cone of admissible velocities:

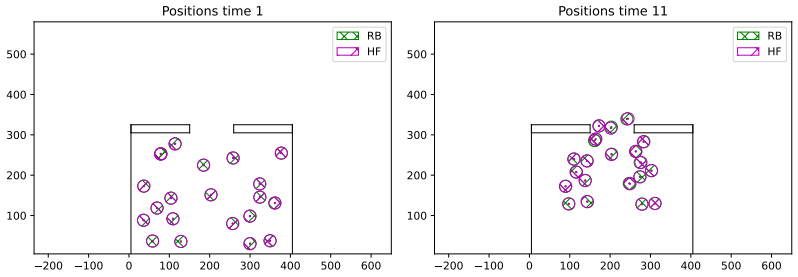
$$\begin{cases} \frac{d\mathbf{q}}{dt} = \mathtt{P}_{\mathcal{C}_\mathbf{q}}(\mathbf{U}(\mathbf{q})), \\ \mathbf{q}(0) = \mathbf{q}_0 \in \mathcal{Q}, \end{cases} \tag{3}$$

where

$$\mathcal{C}_\mathbf{q} = \{\mathbf{v} \in \mathbb{R}^{2N_p}, \forall i < j \text{ s.t. } D_{ij}(\mathbf{q}) = 0 \implies \nabla D_{ij}(\mathbf{q}) \cdot \mathbf{v} \geq 0\}.$$

The parametric variations in the problem are associated to the geometric configuration of the system (for example, the exit width) and to the initial positions of the particles. Parametric variations have

a dramatic impact in the solution, both in terms of the particles positions and in the contact forces, which are represented by the Lagrange multipliers of the underling saddle-point problem.



(a) t^1 (b) t^{21}

(c) t^{21} (d) t^{39}

Figure 7: Agents positions computed by solution of Galerkin ROM: only $n = 20$ modes used at four time steps for an out-of-sample setting $\mu \in \Xi_{\text{valid}}$: comparison between RB and HF solutions.

I investigate new developments of the reduced-basis method and supervised machine-learning techniques to effectively find, in a decorrelated manner, primal and dual reduced spaces. Indeed, for the DCM of interest, linear approximation methods become ineffective, as outlined by the slow decay of the Kolmogorov n-width: the combination of a reduced basis technique with nonlinear methods is promising to achieve a more satisfactory level of accuracy. The reduced basis for the primal variables is found by a Proper Orthogonal Decomposition (POD), and the basis for the dual variables is constructed by a cone-projected greedy algorithm that preserves the non-negativity of the dual basis vectors. In figure 7 the approximation of the agents positions given by the RB method is compared to the HF solution. The computational time required to compute the reduced solutions is approximately 5 times smaller than the cost of finding the HF approximations.
I am currently working on a non-linear reconstruction (e.g. by Random Forest regression) of reduced coordinates from a small number of first coordinates of a linear reduced basis approximation, in order to achieve a even better performance than the linear reconstruction for a big number of agents.

References

Maury, Bertrand and Juliette Venel (2011). “A discrete contact model for crowd motion”. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 45.1, pp. 145–168.

Sambataro, G. (2022). “Réduction de modèle basée sur des composants élémentaires pour des systèmes Thermo-Hydro-Mécaniques.” PhD thesis. Université de Bordeaux.