Galerkin Neural Networks to accelerate numerical simulations of poromechanics in heterogeneous media

1 Scientific description of the project

Context and motivation: Poromechanical simulations occur in several engineering contexts and, in particular, in fields of geosciences such as geothermy or the storage of CO_2 in the underground. For these last two applications, numerical simulations aim to prevent, for example, some risks like induced seismicity or the loss of integrity of a storage site. As a prototypical example, for this PhD work, we consider a poroelastic medium where a network of cracks or fractures already exists and which is saturated by a compressible fluid. The fluid flow through the porous medium and the cracks, as well as the medium deformations induced by the pore-pressure variations, are modelled by means of a system of partial differential equations coupling the conservation of the fluid volume and the mechanical equilibrium. The discretization of such a model (see [3] for instance) by means of coupled finite-volume and finite-element methods often leads to large computing times since grids should be refined around fractures to model the singularities of the solutions accurately. In the following, the solution of such discretizations is referred to as the *high-fidelity* (HF) solution.

Objective: Our aim is to develop **new reduced-order modeling techniques in order to quickly compute accurate approximations** of the HF solutions for many values of the input parameters **with certified accuracy**. In particular, we wish to make vary, in a first step, the **flow properties** of the porous medium (porosities, permeabilities...) and the fractures (apertures), and, in a second step, **the geometry of the fracture network** (locations, fractures' length...) since all these parameters are not precisely known in practice.

Notation: To explain the methodology we wish to investigate, we first introduce some mathematical notations. Let $\mathcal{P}$ denote the set of possible values of the model's parameters, and, for all $\mu \in \mathcal{P}$, let us denote by u_μ the corresponding high-fidelity solution. If $N \in \mathbb{N}^*$ denotes the number of degrees of freedom of the discrete scheme mentioned above, then N is typically very large and $u_\mu \in \mathbb{R}^N$.

State-of-the-art: Most state-of-the-art reduced-order modeling (ROM) approaches suffer from severe drawbacks on this type of problems. The latter fall into two main families of methods. On the one hand, the **classical linear approaches** like the Reduced Basis method [7,9] for instance, consist in finding a small-dimensional parameter-independent reduced linear subspace $V \subset \mathbb{R}^N$ in order to make the worst-case error

$$\sup_{\mu\in\mathcal{P}} \inf_{v\in V} \|u_\mu - v\|$$

as small as possible. For all $\mu \in \mathcal{P}$, the solution of the reduced-order model is then typically given as an element u_μ^{red} of the reduced linear subspace V, obtained via Galerkin-type approximations. An important advantage of such approaches is that it is possible to design certified a posteriori error estimates which enables to quantify the error between the high-fidelity solution and the solution of the reduced-order model. However, for the types of problems we wish to consider in this PhD, i.e. parametrized poromechanical problems in fractured media, **there is no small-dimensional parameter-independent subspace** which yields accurate approximations of the parametrized HF solutions. On the other hand, **machine learning** approaches consist in *learning* an approximation of the map $\mathcal{P} \ni \mu \mapsto u_\mu$, using for instance neural networks. Such deep-learning techniques have been investigated and proposed for instance in [5,6]. In these works, a Deep-Learning Reduced Order Model (DL-ROM) is built from two main components: a Deep Feedforward Neural Network to describe the dynamics of the reduced system and a convolutional autoencoder neural network that models the reduced nonlinear trial manifold through its decoder function. Compared to traditional projection-based ROM methods, DL-ROM is non-intrusive and avoids, in particular, the use of hyperreduction techniques. It also enables to obtain approximations of the solution at any time without having to reconstruct the whole dynamics of the system before that time. The main disadvantage of these approaches is that certified a posteriori error estimates cannot be constructed. Hence, **it is not possible to guarantee or estimate the accuracy** of the approximation given by the reduced-order model.

Methodology: Very recently, a very promising approach, coined as Galerkin Neural Networks methods, has been proposed in [1]. The principle of this approach is the following: a sequence of finite-dimensional subspaces whose basis functions are realizations of a sequence of neural networks are adpatively constructed. The parameter-dependent finite-dimensional subspaces can then be used to define a standard Galerkin approximation of the equation at hand, which makes possible the use of standard certified a posteriori error.

So far, only Lax-Milgram type problems have been considered in [1] with this type of approach. However, the problems we wish to tackle in this PhD involve constraints due to the possible mechanical contacts of both sides of the fractures. As a consequence, the parametrized problems we wish to solve in our framework are parametrized variational inequalities. As such, one then needs to build reduced bases for both the primal and dual variables, the latter being the Lagrange multiplier associated to the constraints in the problem. The methodology proposed in [1] needs to be carefully adapted in this context in the sense that two reduced spaces have to be built in a joint manner: one for the primal variable, and one for the dual variable. Building such reduced spaces independently may lead to reduced-order models which are not stable in practice. In [8], reduced-order models with guaranteed stability have been constructed so as to ensure the stability of reduced-order models for parametrized variational inequalities in a reduced basis framework. One of the issue is also to build a reduced-order model which guarantees the fact that the reduced Lagrange multiplier is non-negative like its HF counterpart. In this PhD, we wish to build on the theoretical developments of [8] and the Galerkin Neural Network approach of [1] to build guaranteed certified and accurate Galerkin Neural Network reduced-order models for parametrized variational inequalities, such as those appearing in the study of fluid flows in fractured porous media.

The hope of this approach is to build **parameter-dependent reduced subspaces** for parametrized variational inequalities, in order to build **accurate reduced-order models** for which **certified a posteriori error estimates** can be computed. The efficiency of the reduced-order model will be evaluated by estimating the gains in computational simulation times as a function of the accuracy between the reduced and HF solutions of the model. These gains will be compared with those obtained by state-of-the-art reduced-order modeling techniques, using either Reduced Bases techniques or standard deep-learning techniques. We would like to stress on the fact that **the approach proposed here is quite generic and could also yield very interesting results for many types of applications beyond the simulations of fractured porous media** targeted in the present project.

Let us mention here other types of applications which would benefit from the development of this PhD, for which reduced-order models for parametrized variational inequalities would be extremely beneficial to significantly decrease the computing times of parametric studies: crowd motion, granular media, mechanical contact, option pricing... Variational inequalities naturally arise in the mathematical models used to describe the evolution of such systems

Work program: State-of-the-art reduced-order modeling techniques using the Reduced Bases method or classical Deep Learning approaches will first be implemented for comparisons' sakes with the approach we wish to investigate here. Then, we consider the following work program, the aim of which is to design Galerkin Neural Network reduced-order models for problems with increasing complexity:

- Darcy flow without fracture and mechanics (parametrized elliptic problem);
- Darcy flow coupled to Poiseuille's flow in a fractures' network (no mechanics);
- Linear elasticity problem without flow;
- Linear mechanical contact without flow (linear variational inequality of the first kind);
- Coupled Darcy and Poiseuille's flows with contact mechanics applied to a reduced number of fractures.

The theoretical and methodological questions will first be investigated on "toy" two-dimensional test cases. We indeed intend to apply the methodology developed here in order to significantly reduce the computing times of test cases, such as the ones proposed, for instance, in [4], by changing parameters like the permeability contrast between the porous medium and the fractures and/or the fracture apertures.

2 General information on the work environment

2.1 Supervision and conduct of the thesis

Academic supervisor. Virginie Ehrlacher (HDR) is a professor at CERMICS, the applied mathematics lab of Ecole des Ponts. She is also a member of the INRIA MATHERIALS team. Her work focuses on the mathematical analysis of high-dimensional and multi-scale problems, in particular model reduction techniques. She co-organized the 2021 CEMRACS summer school on *Data assimilation and reduced-order modeling for high-dimensional problems* and was invited to give plenary talks at the 2020 ICOSAHOM conference and at the 2022 *Model Reduction and Surrogate Modeling* conference, the largest international conference dedicated to reduced-order modeling approaches. She also co-organized an IPAM three-months progamm on "New mathematics for exascale compution: application to materials science". Since 2014, she has (co-)supervised 8 PhD students and defended her habilitation in 2020.
More details: https://team.inria.fr/matherials/team-members/virginie-ehrlacher-galland

IFPEN supervisor. Guillaume Enchéry (PhD) started working at IFPEN in 2006 as a research scientist in the Department of Simulation of Flows and Transfers in Porous Media. In 2013, he joined the Department of Applied Mathematics where he has been in charge of reduced-order models and discretization methods for flows in porous media. From 2007 to date, he has been involved in 8 PhD projects.
More details: https://www.ifpenergiesnouvelles.fr/page/quang-huy-tran

Organization. The PhD student will spend 75% of his/her time at CERMICS and 25% at IFPEN.

2.2 Teams and partnership

IFPEN is a French public-sector research, innovation and training center. Its mission is to develop efficient, clean and sustainable technologies in the fields of energy and transport. IFPEN's *Division of Digital Sciences and Technologies* (DDST) is a research unit affiliated with the ED STIC 580 under a co-accreditation agreement. Through this project IFPEN-DDST seeks to set up a formal collaboration with CERMICS in order to extend a first productive exchange in 2021 at the CEMRACS Summer School [2]. If funded, this PhD thesis would be a first-time collaboration between the two laboratories.

The PhD student will benefit from exchanges with IFPEN-DDST colleagues such as Jana Tarhini (PhD student, 2021–2024) and Isabelle Faille (head of the COORES project on reactive transport), as well as members of the INRIA MATHERIALS team [notably Sébastien Boyaval (LHSV-EDF)] and the INRIA COFFEE team [especially Roland Masson (Université Côte d'Azur) who is currently following Ali Heidar's post-doctoral subject *Discretization on non-coincident mesh of poro-mechanical models with frictional contact at the fault level*, in collaboration with I. Faille and G. Enchéry].

References

[1] M. Ainsworth and J. Dong, SIAM Journal on Scientific Computing, 43 (2021), pp. A2474–A2501.

[2] B. Battisti, T. Blickhan, G. Enchery, V. Ehrlacher, D. Lombardi, and O. Mula, 2022, https://doi.org/10.48550/arXiv.2205.02721.

[3] F. Bonaldi, J. Droniou, and R. Masson, 2022, https://doi.org/10.48550/ARXIV.2201.09646.

[4] B. Flemisch, I. Berre, W. Boon, A. Fumagalli, N. Schwenck, A. Scotti, I. Stefansson, and A. Tatomir, Adv. Water Resour., 111 (2018), pp. 239–258, https://doi.org/10.1016/j.advwatres.2017.10.036.

[5] S. Fresca, L. Dede, and A. Manzoni, J. Sci. Comput., 87 (2021), https://doi.org/10.1007/s10915-021-01462-7. art. num. 61.

[6] S. Fresca and A. Manzoni, Comput. Meth. Appl. Mech. Engrg, 388 (2022), p. 114181, https://doi.org/10.1016/j.cma.2021.114181.

[7] J. S. Hesthaven, G. Rozza, B. Stamm, et al., vol. 590 of Springer Briefs in Mathematics, Springer, 2016, https://doi.org/10.1007/978-3-319-22470-1.

[8] I. Niakh, G. Drouet, V. Ehrlacher, and A. Ern, 2022, https://hal.science/hal-03611982. hal-03611982.

[9] A. Quarteroni, A. Manzoni, and F. Negri, vol. 92 of Unitext, Springer, 2015, https://doi.org/10.1007/978-3-319-15431-2.