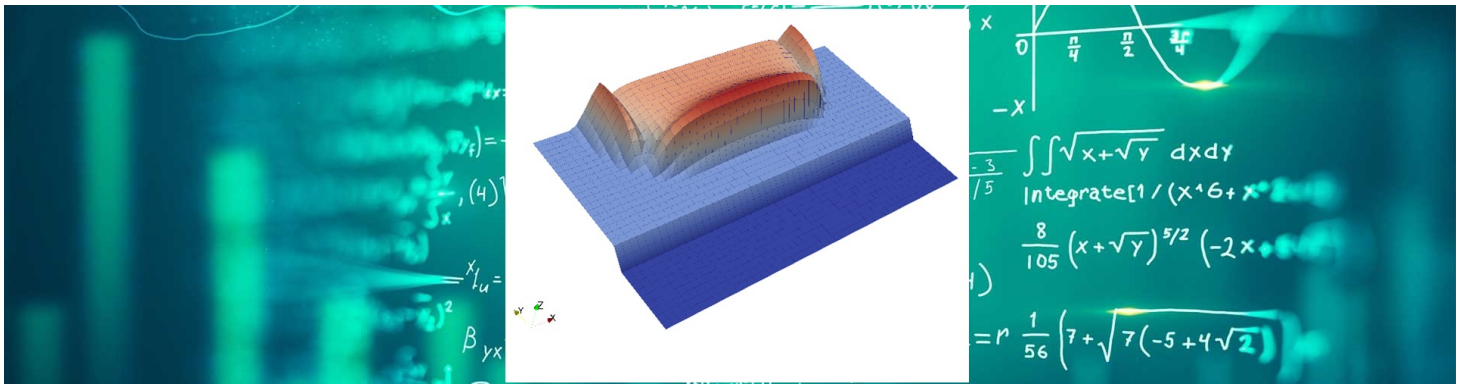


Written on 07 October 2022 10 minutes of reading

News

Fundamental Research

Transfer and transport physics | Fluid mechanics | Numerical methods and optimization

Whether for the development of products, processes or services, **mathematics is essential to the technological innovation led by IFPEN**. In particular, it plays a vital role in the field of numerical simulation, in order to incorporate increasingly complex phenomena and facilitate the design and development of new technological solutions.

Drawn from research projects conducted at IFPEN, **the three examples described here illustrate the essential contribution of numerical methods to the description of fluids for problems related to the underground environment**. They have been used to overcome three recurrent difficulties posed by **the considerable non-linearities of speed, pressure and mixture laws characterizing flows in porous media**. Overcoming these obstacles helps improve the performance of simulators used in the field of geosciences.

Beyond the advances made, these examples perfectly reflect the philosophy of fundamental research at IFPEN, with **high-quality scientific partnerships** involving international PhD students.

LES BRÈVES

The Richards equation is used to simulate water flows in partially saturated soils. Its resolution is difficult in highly heterogeneous porous media where capillary pressure can strongly vary in space. A new methodology has been developed to improve the robustness and the accuracy of the calculations in these media.

Solving the Richards equation: what numerical challenges?

The Richards equation is a simplified flow model, **frequently used in hydrogeology to simulate water flows in partially saturated soils**. It is traditionally solved using a two-point finite-volume method. However, for some cases, **the resulting system of non-linear equations turns out to be difficult to solve** and **the accuracy of the obtained solutions can be deteriorated when the capillary pressure law changes in space**.
During the PhD work [1], researchers from IFPEN and Inria have proposed **a new version of this discretization method**, which is **more robust and more precise with respect to the non-linearities**. They have also established **the existence and uniqueness of the discrete solution**, as well as **its convergence towards a solution of the variational problem**.

Strong non-linearity and spatial discontinuity of capillary pressure

Capillary pressure is defined as the pressure difference existing at the interface between two phases, one considered to be wetting with respect to the porous rock and the other not. In the Richards formulation, these two phases correspond to water and air respectively. Assuming that the air pressure is constant, water pressure directly deduces from the capillary pressure, a measurement generally defined in the form of **a non-linear function of the water saturation and also dependent on the type of the local rock** (Figure 1). This latter dependency can also lead to **water-saturation discontinuities** and hence to water accumulations or suctions on the interfaces between two rock types (Figure 2). The accurate modeling of these phenomena is therefore important.

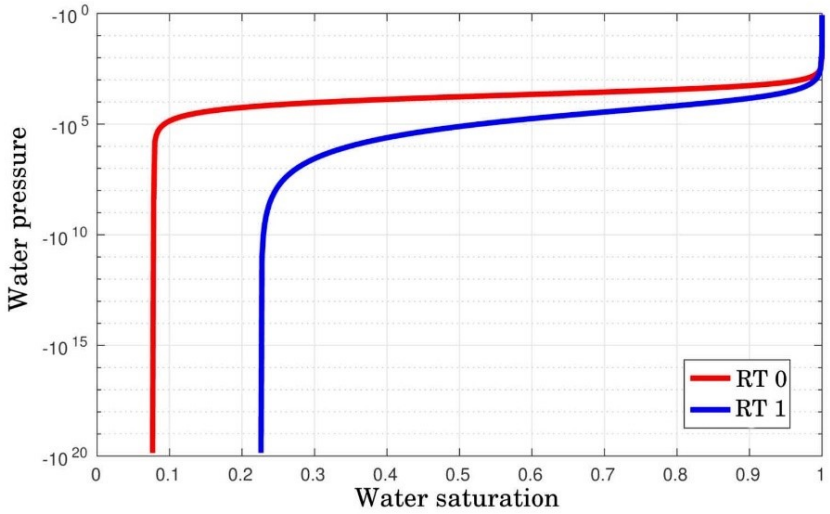


Figure 1 : An example of pressure as a function of water saturation obtained with a Van Genuchten-Mualem-type model for two types of rock Position: RT0 and RT1.

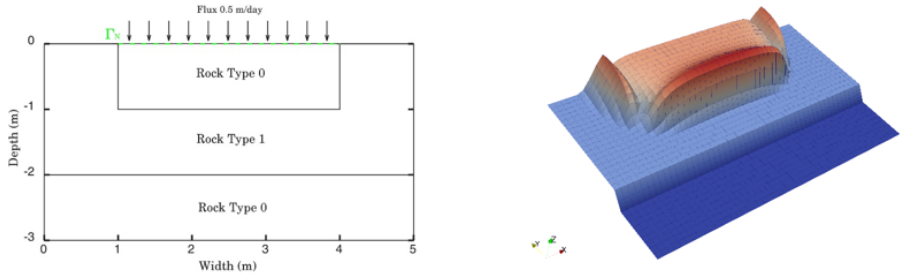


Figure 2 : Example of an imbibition simulation in a heterogeneous medium and saturation profile obtained with the proposed process and a Van Genuchten Mualem model

A parametrization technique to improve the convergence of Newton's algorithm

Because of the non-linearity of the law describing capillary pressure, Newton's algorithm, which is used to solve the discrete system, can barely converge, or not at all. This pitfall can be avoided thanks to an appropriate and regular change of the variable during the iterations. That is the principle of the parametrization technique proposed in [2]. This previous work used the Kirchhoff transformation as a possible variable to be used in Newton's algorithm. In practice this variable cannot always be calculated. The work done during this study has led to propose **parametrizations that are directly based on water saturation and capillary pressure. These new parametrizations ensure a good convergence of the calculations with highly non-linear laws** [3].

A simplified refinement for an increased accuracy on rock-change interfaces

The "two-point" finite-volume discretization is widely used in simulation softwares. But this resolution scheme is known to suffer from a lack of precision on interfaces presenting a change in the capillary-pressure law. A classical solution to improve its precision consists in adding unknowns on the faces between two rock types [4]. The research, conducted here, has also shown that **the simple addition of two fine cells on each side of the rock interface makes it possible to numerically improve the convergence order of this scheme**. In practice, this solution requires no change to an existing code. This solution has also been compared with other ones in a second study [5] and was shown to be the most appropriate one in the majority of the test cases.

A methodology with future applications

The proposed methodology can easily be extended to more general two-phase or three-phase flow models in porous media. This result will thus benefit **other applications**, such as **the simulation of the underground storage of CO_2**. In particular, **its use is planned within the ArcGeoSim computation platform which is developed by IFPEN in partnership with the CEA** [6, 7].

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A finite volume method for solving the Richards equation in a heterogeneous porous medium

Flow simulation in the underground environment involves complex multiphase mixtures in which phases can appear and disappear over time. To manage this complexity, several approaches were tested (unified formulation, non-parametric interior point method, etc.) within the framework of a PhD thesis. The new method employed is very robust and makes it possible to obtain good convergence of resolution algorithms.

Mixture phase management

In many underground simulators (CO_2 storage, geothermal energy, reservoir), a challenging aspect concerns multiphase mixtures and, more specifically, the incorporation of thermodynamic equilibrium laws relating to the chemical species present. The difficulty resides in the management of the appearance and disappearance of phases for different components. The conventional dynamic approach, known as *variable switching*, consists in only keeping **the unknowns of present phases and the associated equations**. It is nevertheless cumbersome and expensive, to the extent that the action has to be carried out continuously, even from one iteration to another within a numerical resolution procedure, such as the conventional Newton algorithm.

The contribution of the unified formulation

An alternative approach, known as unified formulation and recently proposed by Lauser et al. [1], makes it possible **to maintain a fixed set of unknowns and equations throughout the calculations**. In terms of theory, this represents a significant advance that has since led to numerous research projects in the scientific calculation community. In terms of practice, however, the new formulation involves **complementarity equations that are non-differentiable**. As a result, it is necessary, after discretization, to use the s**emi-smooth Newton-min method**, which **does not guarantee convergence to a single solution**. Hence the difficulty of the problem is transferred to the numerical resolution step but it has not disappeared.

Design of a non-parametric interior point method

To avoid abandoning the unified formulation approach midway through the process and exploit its potential to the full, a team of researchers from IFPEN and the INSA engineering school in Rennes decided to overcome this final obstacle. Within the framework of a jointly supervised thesis [2], they set about developing better adapted resolution algorithms, offering greater calculation convergence. The approach adopted consisted in drawing inspiration from tried and tested methods in the field of optimization under constraints and transposing them to general systems of equations (which do not necessarily come from an optimization problem). As a result, **a non-parametric version[1] of interior point methods[2]**, called **NPIPM**, was proposed for algebraic systems. These methods are recognized for their considerable optimization efficiency [3].

[1] “non-parametric” means that it is not necessary to have the regularization parameter that is used in interior point methods and is often their “weak link” tend to 0 “by hand”.
[2] “interior” means that during the iterations, the unknown vector remains inside a region where the

positivity constraints are strictly satisfied.

Analysis and extension of cubic equations of state

Another major contribution of the thesis [3] was the understanding and partial resolution of an additional obstruction to the efficiency of the unified formulation approach, hitherto not identified in the literature. This concerns **the limitation of the field of definition of the Gibbs functions[3] associated with cubic equations of state[4]** . To deal with the potential non-existence of any system solution, a natural extension of Gibbs functions was recommended. Similarly, a large number of previously unknown theoretical properties of the unified formulation were established [4]. The complementarity of these results with numerical aspects of the NPIPM method was tested as described below.

[3] Gibbs free energy (free enthalpy) function G associated with the second principle of thermodynamics.
[4] equation of state of a fluid that can be written as a third-degree polynomial as a function of volume.

Numerical comparison for several phase equilibrium models

In terms of robustness of convergence, the combination of the new NPIPM method with Gibbs function extension makes it possible to improve on the results obtained using the Newton-min method. For example, the red area on **the left part of figure 1**, in the concentrations space (c1, c2), highlights the states for which **Newton-min diverges**, for a given choice in terms of the calculation start point. **On the right**, with the same start point but with NPIPM, **these problematic states have disappeared** in the various field zones: liquid (green), gas (blue) two-phase (liquid-gas, cyan).

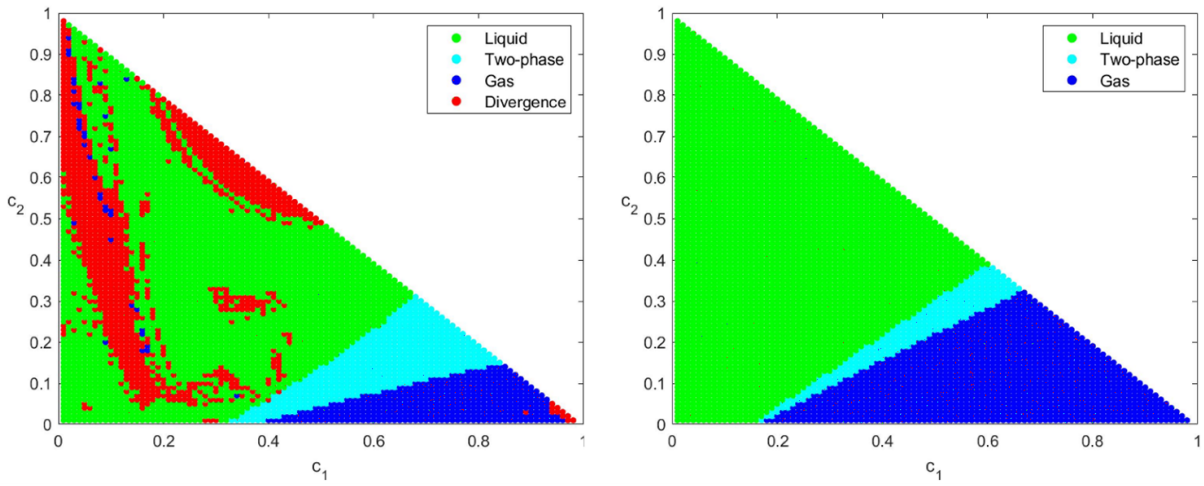


Figure 1: Convergence of Newton-min (left) and NPIMP (right) with the extended Peng-Robinson equation of state and the same start point

Figure 2 illustrates the advantage of the the new method in another way: it indicates **the number of situations (start point) for which each of the two algorithms converges**. It can be seen that NPIMP (right) obtains a score of 100% for all cases considered unlike Newton-min (left). For these numerical tests, we considered the Peng-Robinson cubic equation of state with extended Gibbs functions [5].

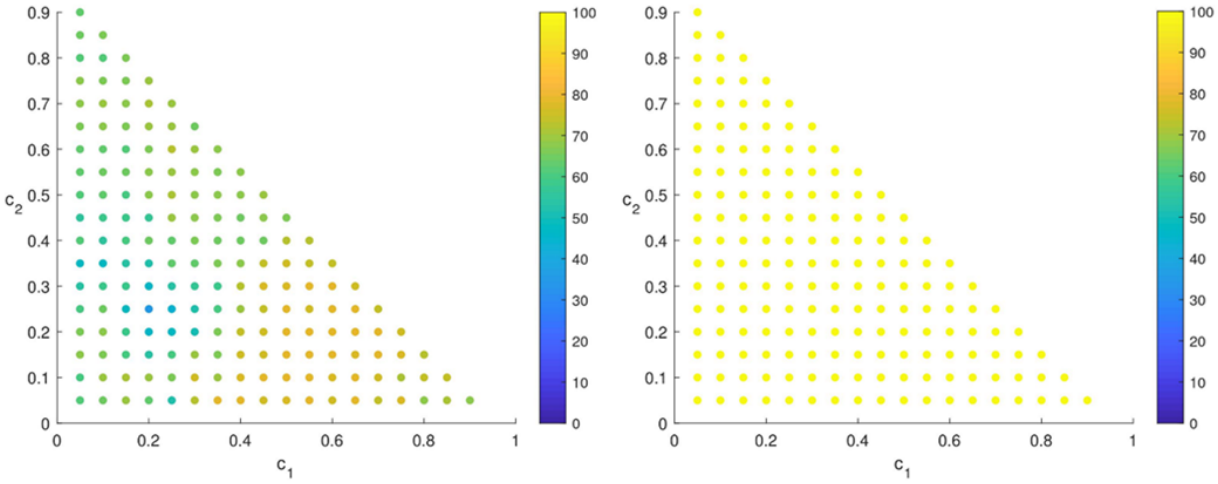


Figure 2 : Percentage od convergence of Newton-min (left) and NPIMP (right) for several start points with the extended Peng-Robinson equation of state

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A new numerical resolution method for simulating the thermodynamics of multiphase mixtures

The calculation of water and gas flows in complex and heterogeneous media is central to technological solutions aimed at tackling current climate and energy challenges, such as the underground storage of CO_2 or heat.

For calculations of this type, an adaptive model was developed by researchers at IFPEN and PoliMi[1] in order to better incorporate the highly discontinuous nature of the underground environment. Collaboration between the two institutes is continuing with a view to improving the performance of these numerical simulations.

[1] Polytechnic University of Milan

Irregular spatial distributions of porosity and permeability

Numerically simulating water and gas flow in a heterogeneous porous medium is very important for some new applications associated with climate/energy challenges, such as the underground storage of CO2 or of heat. The **heterogeneities of the medium** in question stem both from the **diverse nature of the rocks** and the presence of **complex geological structures**, such as **channels** and **macropores**: they are reflected in irregular spatial porosity and permeability distributions, as illustrated by the examples shown in figure 1.

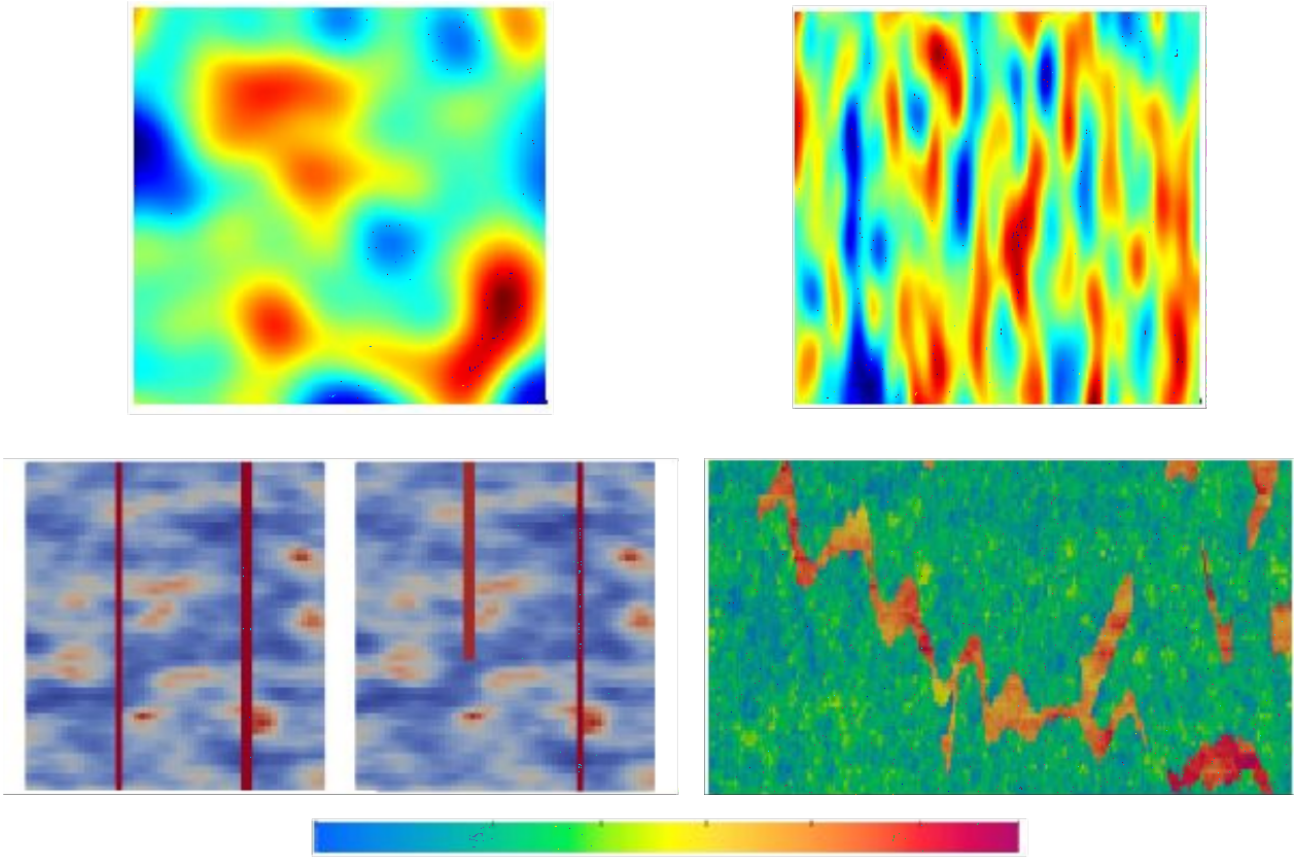


Figure 1: Simulated and real permeability profiles (low values in blue, high values in red)
Top left: generated by an isotropic Gaussian distribution [3]
Top right: generated by an anisotropic Gaussian distribution [3]

Bottom left: generated by a Matérn distribution [3,4] with transverse macropores [4] represented by vertical red lines
Bottom right: measured on layer 35 of the SPE10 project implementation [5]

Darcy's law and its limits

In terms of modeling, the choice of constitutive law relating the speed of fluid flow to the pressure gradient is crucial. Traditionally, **Darcy's law** is used for the entire domain concerned by the simulation: it is **linear, and therefore numerically inexpensive**, and accurately describes low-speed flows. When **these speeds increase**, for example in highly permeable structures, linearity is no longer respected and **Darcy's law loses its relevance**. Hence it has been demonstrated experimentally that it leads to an overestimation of the high speeds calculated [6,7]. In order to correct this effect, **a quadratic term is commonly added to Darcy's law**, **thus transforming it into Forchheimer's law**. This additional term incorporates **inertia effects** by increasing flow energy. However, due to the non-linearity thus introduced, the resolution of spatially discretized equations proves to be costly in terms of calculation time.*

Adoption of an adaptive model

To overcome this effect while minimizing the impact on the precision of results, researchers at IFPEN and PoliMi proposed **an adaptive model** [1,2] that only uses Forchheimer's law where appropriate. Hence, for numerical resolution across the entire domain, the choice of law applied is made, for each iteration, as a function of a criterion based on **physical measurements** (such as domain permeability and fluid viscosity) relating to **flow speed**: if this exceeds the value of the criterion, Forchheimer's law is used

Regularization of the adaptive problem

A major difficulty with this adaptive model resides in the discontinuities created when suddenly shifting from one law to another in so-called transition zones. **These discontinuities have a significant impact on the mathematical formulation of the model** and make it difficult to work with. To overcome this difficulty, IFPEN and PoliMi proposed a **regularization of the adaptive model** based on an averaging of the speeds in transition zones. The impact of moving between laws is thus smoothed out, thereby eliminating the detrimental discontinuity. In addition to the existence and uniqueness of the solutions for both approaches ("discontinuous" and "regularized" problems), researchers verified that they did indeed converge to the same one [1,2]. Figure 2 shows the domain partitioning for the SPE10 project from figure 1 for the case of the regularized model, for three distinct speed criterion values: **the lower the criterion, the more extensive are the regions for which Forchheimer's equation applies**.

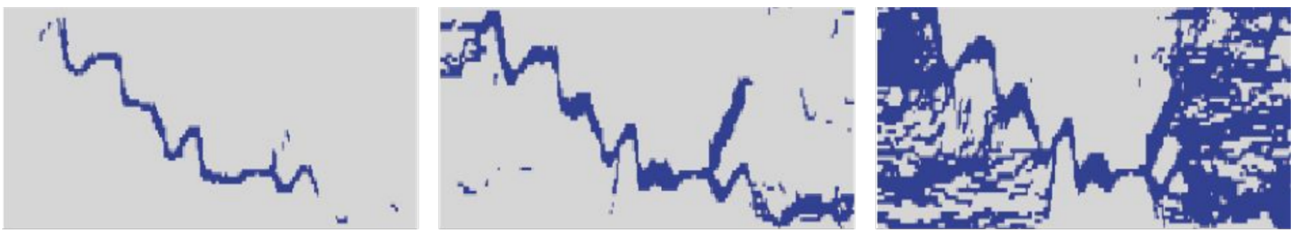


Figure 2: Darcy regions (in gray) and Forchheimer regions (in blue) obtained with the regularized model [2] applied to the SPE10 permeability map in figure 1
From left to right: decreasing speed criterion

Further efforts required to better predict calculation sub-regions

While the regularized model is continuous, it is nonetheless highly non-linear in the transition zones; as a result it can still be numerically costly to use. Partnership research is currently underway to further reduce the calculation time, using the regularized model as a predictor of “Darcy” and “Forchheimer” regions, in such a way as to enable the numerical simulation to be based directly on the law predicted in each region, **without transition zones**. Hence **the discontinuity of the adaptive model and the excess non-linearity of the regularized model will be eliminated**. The prediction step will exploit machine learning techniques, making prior assumptions about the simulation domain: geometry of the constituent regions, boundary conditions on pressure and velocity as the model’s input data.

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Adaptive model for flow simulation in heterogeneous porous media

IFPEN researchers deal with non-linear effects of fluid flow simulations in porous media
07 October 2022

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