**Digital Rock Applications Review (10 pages)**

Digital rock technologies are the set of methods that help engineers simulate rock features at the pore scale, in order to predict their behavior before or during well exploration and completion strategies. The basic understanding for digital rock physics (DRP) methods consist of an image-and-compute framework, where a depiction of a rock sample is then represented in a three-dimensional model, which is used to simulate physical processes without the need of excessive exploration or drilling (Sudakov et al., 2019). Over the years, these methods have been enhanced to allow the use of artificial intelligence and learning algorithms.

In the next few pages, we will review the latest advances on the applications of these methods in the oil and gas sector, focusing mainly on hybrid models that combine algorithms with learning models aided by artificial intelligence, on applications that use the lattice Boltzmann framework for estimating fluid flow, and on molecular dynamics that rely on nanofluidics and the study of finite elements. As a few examples, we encounter artificial neural networks (ANN) used in combination with algorithms to predict permeability, three-dimensional printing of simulated rocks with varying permeability estimations, lattice Boltzmann used as an image processing tool, and molecular dynamics used to understand flow regimes at the microscopic level.

In the midst of this exploration, a series of trade-offs are identified, as well as the strengths and shortcomings of some models over others. While most of these techniques help decrease drilling and exploration costs significantly, due to their ability to perform more early work in laboratory settings, the more common challenges of these methods appear to be related to computational strains that invite researchers to look at alternatives. With that said, there are plenty of avenues for future research that have been opened wide and are ready to be explored in the next few years.

**Physics-based simulations/methods**

The experimental analysis of reservoir rocks is key to develop and stimulate oil and gas fields, due to their potential for improving reservoir characterization and saving costs in exploration and unnecessary manipulation. In this sense, experiments are inseparable from the in-field work (Huang et al., 2021). Most of the current DRP technologies rely on the strength of data to develop robust simulations for rock features like porosity and permeability, as well as elastic and electrical properties (Al-Marzouqi, 2018). However, the use of physics-based contrasting tools has gained more traction in the past few years, with the objective of grounding sometimes abstract results to physical principles affecting reservoirs, limiting their outcomes to realistic real-world scenarios.

* **Machine Learning Hybrid Models**

There have been several works dealing with the combination of data-driven and physics-based methods, that we will now review. First, the work of Saad et al. (2018) highlights the hybrid nature of this combination, where the use of machine learning (ML) technologies is added to help predict the mechanical properties of rocks, known as Young’s modulus predictions, where parameters like mineralogy, density, and porosity are analyzed. Aided by support vector regression (SVR) methods, a supervised learning model for regression analysis, the authors enhance their DRP model with ML methods to obtain an improved estimation of rock properties.

Similarly, Karimpouli and Tahmasebi (2019) study images from the Berea sandstone to improve image segmentation, occurring when rock representations are processed to be understood as a set of distinct minerals that a learning method ought to recognize and differentiate as such. Using convolutional neural networks (CNN) as their ML counterpart, a deep learning method that classifies and recognizes image patterns and augments data, the authors run algorithms to produce reliable outputs with a higher categorical accuracy than conventional models.

Meanwhile, Fokin et al. (2022) provide a hybrid approach for automatic segmentation of tomographic data, aided by an optimized 3D U-net neural network and a statistical clustering technique that is based on the Gaussian mixture model used to separate pore-space phases. Problems at this stage can occur when sand grains have a weak gray-level contrast that does not allow a learning method to separate the sand grains being analyzed. Here, the new challenge posed to engineers is related to the possibility of generating hundreds of times more data from gas-hydrate formations to be analyzed, while lacking the ability to streamline adequate segmentation procedures.

In turn, Matinkia et al. (2022) combine a multilayer perception (MLP) neural network with the social ski-driver (SSD) algorithm to create a hybrid technique that helps predict rock permeability. This model is contrasted with two other hybrid methods, genetic algorithm plus MLP, and particle swarm optimization plus MLP, with the featured model providing the highest degree of accuracy in permeability prediction. With that said, the other two models have their own promising degrees of estimation while also providing some advantages in convergence, making them less computationally expensive.

An important note on the use of these methods is related to the trade-offs that are found when investigating their various features. For instance, there are methods that provide a fast analysis while relying on a large amount of data, with the caveat of possessing an excessive degree of abstraction that is not grounded in the physical properties of the rock. Therefore, physics-based considerations are added, which may also add computational constraints that make models slower. Due to these encounters, researchers have developed other models that incorporate techniques like finite elements analysis and electrical properties, which we review below.

* **Lattice Boltzmann**

A popular technique to simulate flow of liquids and gases, the lattice Boltzmann method (LBM) has been used in conjunction with DRP to improve the understanding of unconventional reservoirs. For instance, Yang et al. (2018) study artificially induced fractures in the Berea sandstone shale site located in Ohio, United States, using LBM to calculate their permeability and a partial least square (PLS) regression framework to observe the marginal effects of each independent variable added to the model in explaining that degree of permeability.

Furthermore, in their own exploration of tight sandstone sites, Cao et al. (2020) use a two-phase D3Q27 LBM model to simulate flow behavior, and a U-net deep learning model to improve pore boundary qualities, something pivotal for the estimation of tight sandstone properties. LBM models are described as , with being the number of dimensions while being the number of particle velocities. In the case of three-dimensional lattice models, there are fifteen-velocity , nineteen-velocity , and twenty-seven-velocity frameworks (Arumuga Perumal and Dass, 2015).

The collaboration between ML and LBM can be better understood when we highlight the contributions of each method to arrive at more accurate estimations. First, lattice Boltzmann is used as a single-phase direct simulation for the permeability of a rock sample, obtained from images, data, or both. Then, researchers can use the wide range of artificial intelligence-based techniques to train algorithms on image-based features, which ground results to physical rock features and constrain ML techniques, so that more accurate and generalizable predictions are obtained (Rizk et al., 2021).

An important reason for the increase in the use of LBM techniques in the past few years is the simplification that these models offer in the simulation of flow, while also providing an accurate representative elementary volume (REV), a measurement at which the simulations do not vary significantly after a change in rock volume, making it insensitive to the choice of boundary conditions (Saxena et al., 2018). REV serves as an important obstacle to the optimal representation of some rock types, thus a tool that allows for an accurate representation of their features, while remaining cost-effective, is a step forward for the discipline (Mehmani et al., 2020).

The development of these simulation techniques has expanded the laboratory examination of rock features, a move that decreases field trips and lowers costs in drilling and site exploration. In this sense, quite a significant portion of new reservoir characterization strategies can be done through estimations and simulations that are proving increasingly more accurate. The current improvement of DRP workflows includes strategies that involve nascent technologies, such as the use of 3D printing to validate the simulations done *in silico*. Ibrahim et al. (2021) take advantage of this and generate synthetic surfaces that expand from images, confirming the reliability of the simulation methods.

* **Molecular Dynamics**

Methods that utilize molecular dynamics (MD) consist of an exploration at the pore level that moves away from the Navier-Stokes continuum equations, which assume lower uncertainty. According to Berezovsky et al. (2018), molecular dynamics is concerned with the macroscopic properties of porous media and the three-dimensional reconstruction of the microstructure of the rock. In order to obtain rock property estimations that account for transport mechanisms and flow dynamics, nanometer-scale, micrometer-scale, and centimeter-scale simulations can be run, which will have varying degrees of accuracy (Ning et al., 2019).

Some examples of the use of molecular dynamics in the digital rock framework use similar workflows as the other techniques we have reviewed, starting from the creation of three-dimensional models of rocks with a series of parameters like pressure and temperature, which are complemented with a simulation technique to estimate features like permeability. Such is the case with the work of Zhang et al. (2020), who combine first-principles MD with lattice Boltzmann flow simulations to predict shale matrix permeability, with the goal of improving its overall estimation.

Then, Feng and Akkutlu (2018) develop a molecular kerogen pore-network model that is interested in studying the transport of small hydrocarbon molecules inside organic nanopores. With the goal of uncovering this flow transport question, the authors populated the skeleton of a kerogen pore-network that is capable of transporting hydrocarbon, through 3D digital segments from high-resolution TEM tomographs. Monte Carlo simulation was performed in order to charge the simulated porous networks with simple reservoir fluids, while non-equilibrium MD simulation was done to account for the fluid properties that are assumed no longer to be homogenous.

Moreover, exploring 3D model replica of Type II kerogen rocks from original sources being located in Delaware and Midland basins in the United States, Bui et al. (2018) use MD techniques to improve the enhance oil production estimations through an improved understanding of hydrocarbon transport in kerogen. By modifying the existing molecular forces in the pore networks in kerogen molecules so that they can use targeted chemistry technologies, the authors can alter the degrees of maturation of three-dimensional kerogen models. In these examples, MD methods helped shift pore size distribution to larger sizes, with the goal of enhancing pore connectivity.

* **Electrical/Elastic Properties of Rock**

Moreover, novel techniques have been developed to study and predict the electrical properties of rocks, such as resistivity, or their strength in resisting electric currents. For instance, the work of Wu et al. (2020) examines shale formations and the prediction of physical properties through the creation of hybrid models. The authors develop a stochastic modeling algorithm that integrates the discrete element method (DEM) technique with the quartet structure generation set algorithm (QSGSA), and they find that both electrical resistivity and elastic moduli decrease when organic matter or clay minerals increase.

In a similar framework, Dong et al. (2018) analyze CT scanning images of hydrate reservoir rocks from permafrost and advance a diffusion limited aggregation (DLA) model to develop three-dimensional images, while the finite elements method (FEM) was used to simulate their electrical features. This was done in order to assess the influence of parameters like hydrate saturation, formation of water salinity, and different hydrate distribution types on electrical properties. Some results show that resistivity decreases with the increase of salinity in the water formation, provided there exists the same hydrate saturation condition.

Then, Yan et al. (2018) explore low-resistivity sandstones to estimate the electrical properties of rocks, so that water saturation in oil and gas reservoirs can be calculated. After generating a series of 3D digital rock models based on tomography technology, the resistivity of each of the components of these representations was assigned, and rock resistivities were calculated through FEM. The list of relevant parameters affecting rock resistivity were found to be, among others, porosity, clay content, temperature, water salinity, and wettability. As we can see, enhanced DRP methods can help in determining rock features with increasing accuracy, with finite element method being an integral part of these more novel workflows.

Lastly, the elastic properties of rocks were assessed by Sawayama et al. (2020), who employed experiments and digital fracture simulation. They found that a parameter like permeability can be formulated as a function of velocity or resistivity, independent of the sizes of the fractures. Likewise, changes in permeability and resistivity are controlled by the disconnection of flow paths, while changes in velocity are dependent on the roughness dependency of porosity.

* **Finite Element Method/Modeling (FEM)**

This method is used to numerically solve differential equations in mathematical modeling, dividing a large system into smaller parts, called finite elements, making it easier to be analyzed in a simpler manner. In the case of fluid flow simulations, FEM can help discretize the geometrically complex flow domain of rocks. Working on the Berea sandstone, Yang et al. (2020) use FEM to study the effects of viscosity and thickness of adsorption boundary layers (ABL) in pore throats at the microscopic level, helping in achieving a more complete understanding of fluid flow.

Meanwhile, Fan et al. (2020) study clay-bearing sandstones and apply a FEM framework to calculate the effect of factors like the conductivity of pore water, the volume fraction of clay, and the clay minerals, on rock conductivity. The authors find that clay volume had significant effects on the saturation exponent, while the conductivity of clay minerals varies with the pore-water conductivity. Furthermore, additional elements like rock elasticity can also be obtained with FEM and under the umbrella of DRP methods. In this sense, Andhumoudine et al. (2021) find that elastic features like bulk and shear moduli decrease with rising porosity, while the compressional and shear wave velocities decline.

Studying Berea sandstone samples once more, Fakhimi et al. (2018) inquired about rock fractures and the induced displacement patterns that generate once a fracture is initiated and propagated. FEM methods were used as part of a three-point test for physical fracture bending, simulating deformation patterns, and the mechanical behavior of the entire process. However, when comparing it to the output of a bonded-particle model, where rocks are represented by spherical particles that are bonded together at their contact points, FEM is actually less accurate.

With that said, FEM has shown promising results when estimating the elastic properties of rocks. Wei et al. (2018) use a workflow that combines an advanced Markov Chain Monte Carlo (MCMC) method with FEM to evaluate reservoir properties in shale reservoirs. MCMC was utilized to reconstruct three-dimensional digital cores of these types of rocks, while FEM assisted to estimate the equivalent static elastic moduli from those 3D digital cores. Results show that linear relationships confirm a strong anisotropy, or the capacity to change and assume different properties in different directions, of shale.

**Open-source datasets**

* **Image segmentation**

To lower the significant number of hours that researchers spend processing data and images, a series of deep learning techniques has appeared to identify rock properties from high-resolution pictures obtained from sedimentological studies. The work of Guo et al. (2022) explores the image segmentation of blasted rocks, normally more noisy than conventional rock images. Using the Phansalkar method for image thresholding, which relies on an algorithm that calculates different thresholds to binarize an image into only black and white pixels, and a watershed algorithm that considers the contour properties of segmented rock blocks, limiting the noise from the blasted rocks.

In this area, we have witnessed a sustained growth of software tools and algorithms developed to improve image segmentation. For instance, Malik et al. (2022) apply two distinct segmentation models, U-Net and LinkNet, to identify and segment images by class, separating them into sandstone, mudstone, and background types. Using machine learning methods like pre-trained networks to assist with image segmentation shows promising results. In this case, the authors work with *Resnet34*, *Inceptionv3*, *VGG16*, and *Efficientnetb7* as backbone for the two models, something that forecasts a greater use of these techniques in the sector in the next few years.

Similarly, a growing set of open databases and software programs have appeared, with some examples being Tensorflow, which offers the use of a deep convolutional neural network for image segmentation of rock fractures. Predominately using Python, the user needs to download a repository found on *github.com/Montherapy/Rock-fracture-segmentation-with-Tensorflow*, which allows for processing and segmentation. Also, Split Desktop is a program developed for the analysis of digital images of blasted rock, that provides manual and automatic segmentation tools (Tavakol Elahi and Hosseini, 2017).

* **Physical simulations**

With regards to the availability of rock images with which to perform simulations, and the development of open-source platforms to perform physical simulations, we can cite a few examples. For example, Santos et al. (2022) present a dataset of over seventy 3D binary images of complex media, available for free access at *digitalrocksportal.org/projects*. Moreover, a valuable tool developed in the past few years is DigitalROCK, a software program that uses the latest Lattice-Boltzmann physics, powered by their Simulia platform, to simulate two-phase flow of oil and water with promising results. This paid product can be found at 3ds.com/products-services/simulia/products/digitalrock.

Additionally, the toolbox OpenFOAM has been used to simulate fluid dynamics and reconstruct 3D segmented rock images through rock physics methods driven by Generalized Network Modeling (GNM). This software is written in C++ language and was developed by Imperial College London, along with the platform GNextract that is used to reconstruct upscaled versions of rock images in the form of pore elements. In their work, Regaieg et al. (2021) combine these elements while also using the pore-scale network simulator DynaPNM, and running all codes in TOTAL’s supercomputer PANGEA, they have managed to improve the precision of the simulation methods greatly.

Meanwhile, Particula is a simulator tool that allows users to estimate the rock features of granular media, by generating series of spherical and non-spherical shapes that bond together and are subject to gravitational forces. Granular dynamics help researchers uncover details about the contact-scale physics of loose sediments (Al Ibrahim et al., 2019). To help in a similar manner, a 3D image processing software called Simpleware was developed by Synopsis. This program helps the user visualize, segment, and quantify various types of scan data, as well as facilitating the analysis of porous media and mesh creation in order to describe and deploy 3D digital rock images.

Lastly, PorePy is an open-source simulation tool that provides a semi-automatic gridding framework to construct a discrete-fracture-matrix model that allows for subsequent simulations. Following the path of software packages like TOUGH2, OpenGeoSys, and CSMP, PorePy seeks to incorporate flow-ruled dynamics in fractured rocks. Implemented in Python, this software is fully open, and can help researchers in developing and reproducing their simulations with a community of like-minded people who are looking to enhance these methods (Keilegavlen et al., 2017).

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