Advances in Geo-Energy Research⁻

Perspective

From digital rock to digital wellbore: Multiscale reconstruction and simulation

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Keywords:

Digital rock digital wellbore multiscale modeling numerical simulation

Cited as:

Chi, P., Sun, J., Yan, W., Cui, L. From digital rock to digital wellbore: Multiscale reconstruction and simulation. Advances in Geo-Energy Research, 2024, 13(1): 1-6. https://doi.org/10.46690/ager.2024.07.01

Abstract:

Subsurface rocks exhibit multiscale heterogeneity characteristics ranging from the microscopic to macroscopic levels. A significant challenge in geophysical exploration research is how to accurately analyze the cross-scale characterization of rock component structures and physical responses. The advancement of rock imaging equipment and computational resources has led to the emergence of digital rock physics technology as a crucial tool for addressing these challenges. This paper explores common methods and issues in three dimensional modeling and numerical simulations, spanning from micro-nano scale rocks to meter-scale wellbores, and presents relevant research insights. An initial review of the previous research and evolving trends in multiscale rock modeling and physical property simulation is firstly carried out. Subsequently, the primary methods and application range of multiscale simulation are summarized, followed by an outline of the modeling approaches and application directions for digital wellbores. The progression from digital rocks to digital wellbores signifies the successful cross-scale application of digital rock physics technology from the microscopic to macroscopic levels.

1. Introduction

Digital rock and digital wellbore technologies have become effective means for studying the physical response mechanisms of subsurface rocks. Digital rock technology focuses on analyzing the characteristics of rock physical responses with nanometer to micrometer precision, enabling the direct assessment of how pore structure and mineral composition influence physical properties. Utilizing digital rock technology facilitates the intuitive and visual examination of response mechanisms and features of physical parameters such as rock electricity, elasticity, permeability, and nuclear magnetic resonance at the microscale (Andrä et al., 2013; Lucas-Oliveira et al., 2020; Sadeghnejad et al., 2021). Currently, the research scale of digital rock technology can reach the size of a full-diameter core, but this is still microscale for meter-scale wellbores or formations, with limitations in scale and data discreteness. A digital wellbore can be viewed as a continuous, large-scale digital rock, created by integrating core and logging data to provide richer formation information and analyze how macroscopic factors like bedding and fractures influence rock physical properties. From digital rock to digital wellbore, it represents a crossing of scales in digital rock physics technology. This paper will address challenges and solutions encountered in multiscale modeling and simulation of digital rock and digital wellbore.

Yandy Scientific Press

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2207-9963 © The Author(s) 2024.
Received March 29, 2024; revised April 15, 2024; accepted April 22, 2024; available online April 25, 2024.

2. Multiscale digital rock technology

The pore structure of underground rocks generally exhibits multiscale characteristics. Achieving multiscale digital rock modeling and physical property simulation is crucial for bridging the gap between methodological research and field application. Currently, digital rock multiscale modeling mainly comprises two methods: the fusion modeling method based on the volume of digital rock data and the integration method based on the pore network. The former method allows for a three dimensional (3D) representation of rock pores and minerals, enabling numerical simulations of multiple physical fields, albeit with a large overall data volume. On the other hand, the integration method based on the pore network primarily captures the multiscale pore structure, offering a smaller data volume and higher simulation efficiency, but with limitations in mineral description and calculable physical properties. Given the comprehensive study of rock physical properties, this paper mainly focuses on the discussion of multiscale modeling and simulation methods based on 3D digital rock data volume.

The 3D digital rock modeling methods can be categorized into physical experimental methods and numerical reconstruction methods. Physical experimental techniques mainly include X-ray computed tomography (Saxena et al., 2019) and focused ion beam scanning electron microscopy (Zakrzewski et al., 2019). Numerical reconstruction methods mainly utilize experimental information or two dimensional images for 3D reconstruction. Common methods include process-based method (Coelho et al., 1997), simulated annealing method (Hazlett, 1997), sequential indicator simulation (Keehm et al., 2004), multiple point statistics (MPS) (Okabe and Blunt, 2004), and Markov chain Monte Carlo method (Wu et al., 2006). Additionally, deep learning techniques have found application in digital rock modeling, employing methods like generative adversarial networks (GAN), variational autoencoders, and diffusion models to enhance the efficiency of 3D digital rock generation tasks (Wang et al., 2021; Luo et al., 2024).

Models generated through different methods vary in scale, making multiscale modeling of 3D digital rocks dependent on a combination of physical experimentation and numerical reconstruction. Common approaches to multiscale modeling currently include superposition, template matching, and deep learning. Superposition, as the earliest multiscale fusion method, aligns digital rocks of varying sizes constructed via different methods to a consistent resolution, superimposing them into a multiscale data volume (Tahmasebi et al., 2015). Template matching, involves comparing whether information from two scales matches by using fine-scale details to pinpoint the most relevant region on coarse-scale data for refinement purposes (Lin et al., 2019). Deep learning methods for multiscale modeling mainly involve the fusion of super-resolution models with various GAN models, such as combinations with CycleGAN, CinCGAN, AttentionGAN, converting low-resolution rock images to high-resolution ones (Chen et al., 2020; Niu et al., 2020; Chi et al., 2024). Another direction involves refining coarse-scale pore structures while adding fine-scale information. The advantage of deep learning methods lies in the efficient fusion of data once the model is trained, and the fully convolutional neural network can be applied to rock images of any size.

In general, different multiscale modeling methods have their own advantages and limitations. The superposition method offers high computational efficiency but is susceptible to information overlap across scales. Conversely, the template matching method is more in line with the statistical characteristics of rocks but has lower modeling efficiency. Deep learning is more suitable for processing large amounts of data, with long training time but high efficiency in data fusion in later stages. The current issue is that existing multiscale modeling work is all completed under the condition of not much difference in resolution, typically a resolution difference of 2-20 times. Due to the above data fusion is based on the processing of rock images, which inherently contain limited information, it lacks the capability to seamlessly integrate data across significantly disparate scales. Multiscale digital rock modeling is generally suitable for rock types with relatively small pore size spans such as sandstone, conglomerate, and pore-type carbonate rocks. In contrast, for rocks featuring multiscale information spanning from nanometers to micrometers, such as shale, coal, and fractured carbonate rocks, where scale differences can exceed thousands of times, a single data set proves inadequate in capturing the full structural characteristics. Current methods often add the information of pores into models through equivalent substitution, failing to achieve the purpose of intuitive display.

Compared to multiscale digital rock modeling, numerical simulation faces greater challenges. The primary issue stems from the higher computational performance requirements in numerical simulations. Failure to strike a balance between data size and computational performance would render the construction of the aforementioned multiscale models futile. For instance, simulating the absolute permeability of a digital rock of 1,000³ size via the lattice Boltzmann method demands over 60 GB of runtime memory for smooth computation, with computation time spanning from tens to hundreds of hours. Furthermore, employing the finite element method to determine the electrical and elastic properties of a model necessitates even greater memory and computational power. Hence, the capability to achieve efficient numerical simulation directly influences the potential extension of multiscale modeling methods into field applications. To effectively serve the scientific research or field application requirements, multiscale digital rocks typically need exceed a size of 1,000³ voxels, or even larger, to prevent multiscale integration efforts from losing their practical significance. In practical applications, small-sized data volumes can be directly obtained using a physical imaging method or numerical reconstruction method, without the need for cross-scale data integration. Therefore, the feasibility of conducting numerical simulations on largescale digital rock volumes fundamentally dictates the meaningfulness of multiscale modeling.



Fig. 1. Example of direct simulation process of multiscale digital rock. Divide a multiscale integrated large size digital rock into 64 regions for simulation respectively, and then use the obtained rock physical parameters for upscaling simulation to obtain the results of the entire model.

3. Recommended approaches for multiscale numerical simulation

In response to the above issues, two multiscale digital rock simulation methods have been summarized: direct simulation method and indirect simulation method. The direct simulation method entails conducting simulation calculations directly on the multiscale digital rock to determine rock physical properties, such as elasticity, electricity, and permeability. If the model size is too large, it can be partitioned into multiple subregions for sequential simulation, with subsequent aggregation of results to derive the overall physical parameters through subregion numerical simulation or homogenization methods (Dehghan Khalili et al., 2013). Utilizing the deep learning technology, varying resolution information can be consolidated to construct a large-scale, high-precision digital rock. However, the data volume is too large to directly perform numerical simulations. The process of multiscale digital rock simulation for a sandstone, as depicted in Fig. 1, involves dividing the constructed large-scale multiscale integrated digital rock into multiple subregions. Each subregion simulates the physical parameters, which are then integrated into the corresponding positions to conduct further simulations for the physical properties of the entire model. Furthermore, employing layered homogenization methods with data-driven surrogate models can enhance computational efficiency in predicting physical properties (Ahmad et al., 2023; Elmorsy et al., 2023; Jiang et al., 2023; Liu et al., 2023).

Multiscale digital rock modeling is essentially the processing of 3D images, which requires that the resolution gap between the datasets used for fusion is manageable to prevent excessive model data volume that could overwhelm computer computation capabilities. For rock structures with significant scale differences like shale, coal, and vuggy carbonate rocks, direct simulation may not be applicable, prompting the use of an indirect simulation method. The indirect simulation method is an equivalent alternative method that does not use multiscale digital rocks but integrates the physical properties of

rocks expressed by different scale data to calculate the overall properties of the samples (Miarelli and Della, 2021; Najafi et al., 2021). Fig. 2 shows a multiscale simulation process of shale, with the selected sample pores mainly consisting of nanoscale pores and fractures, and occasionally micrometerscale pores. The thickness of the laminations ranges from micrometers to millimeters, exhibiting clear multiscale characteristics. Various techniques like CT, Modular Automated Processing System (MAPS), and Quantitative Evaluation of Materials by Scanning Electron Microscopy (QEMSCAN) are utilized to capture diverse scale features. CT data with a 2 μ m resolution forms a coarse-scale framework; each voxel represents a basic unit for simulation, comprising minerals and pores. OEMSCAN identifies mineral distribution, while MAPS, with a 4 nm resolution, extracts and reconstructs nanoscale pores of different minerals. The 3D reconstruction result depicts developed pores in each basic unit, creating highprecision digital rocks. Initial nano-scale simulations on each basic unit determine their physical properties in the coarsescale data, establishing the fundamental characteristics of each type of mineral. At this point, the coarse-scale data can be further used for simulation to obtain the overall upscaled physical properties. In cases where high-precision data is lacking, theoretical formulas can deduce the basic physical properties of minerals for input into coarse-scale data, enabling sample property simulations (Liu et al., 2021; Wang et al., 2022). Both simulation methods, direct and indirect, can be synergistically employed based on specific requirements to enhance parameter calculation accuracy and efficiency.

Furthermore, there remain numerous promising avenues to investigate within the realm of multiscale digital rock technology. These include the integration of multiscale information through both direct and indirect methods, the characterization and fusion of samples at multiple levels, and the development of lightweight multiscale grids to achieve a comprehensive depiction of rock properties.



Fig. 2. Example of indirect simulation process of multiscale digital rock. Coarse-scale data serves as the overall framework, with each voxel representing the basic unit of numerical simulation. The 3D reconstruction fine-scale samples are used to determine the physical properties of each basic unit, and upscaling simulation can obtain the physical properties of the entire sample.

4. Exploration of digital wellbore modeling and simulation methods

The development of digital wellbore technology is based on the multiscale digital rock. A digital wellbore is a data volume at the scale of a wellbore, similar to a digital rock, generally representing a depth range from a few meters to hundreds of meters. Three-dimensional digital wellbore modeling is also a multiscale modeling process. In contrast to digital rock, the grid data of the wellbore model is generally continuous, rather than having clearly defined boundaries with singlemineral composition. Well logging curves and images are used as coarse-scale data, and digital rock as fine-scale data for matching, aiming to reconstruct complete wellbore formation images (Zhang, 2015). The specific modeling process involves dividing the well section into distinct layers based on lithofacies, under the assumption that each layer exhibits similar internal structural characteristics. Subsequently, well logging data and images are utilized to construct a complete 3D cylindrical image of wellbore porosity. Digital rock images serve as the training images, with wellbore porosity image serving as hard data and porosity curve as soft data for the hierarchical construction of a digital wellbore porosity model. Ultimately, the mineral composition of each grid point is finetuned using elemental logging data. This results in multicomponent digital wellbore models, which can then be used to conduct numerical simulations of rock physical properties.

The research on simulating rock physical properties using digital wellbores can be categorized into direct simulation of formation physical properties and forward simulation of logging instrument detection characteristics in wellbores. Fig. 3 shows the two approaches for digital wellbore modeling and simulation. Before the forward simulation, determining the physical parameters of the formation is essential, and these steps are interrelated. Similar to multiscale digital rock

simulation, direct simulation of formation physical properties is also a multiscale process. In the fine-scale digital rock shown in Fig. 2, each grid point represents a single composition, facilitating the acquisition of physical properties. Conversely, in the coarse-scale digital rock, each grid point contains both minerals and pores, necessitating reliance on the fine-scale model to determine physical properties. Notably, at the digital wellbore scale, each grid point contains more information, including pores and various minerals. Hence, rock samples in different formations, despite having similar mineral compositions, may exhibit distinct physical properties. Therefore, it is difficult to directly determine physical properties based solely on mineral composition proportions. Similarly, the physical properties of the digital wellbore can be inferred through an upscaling process utilizing finite element or effective medium theory. This involves assigning fine-scale physical parameters to wellbore grid points to deduce the wellbore's physical parameters. Subsequent to determining the formation parameters, further simulations can be conducted on the logging instrument in the digital wellbore, setting parameters like formation temperature, pressure, and drilling fluid invasion to establish a realistic formation environment. By adjusting mineral and fluid proportions, researchers can effectively explore the instrument's detection characteristics under varying factors. The digital wellbore simulation involves complex processes like multiscale data fusion modeling and equivalent substitution simulation, leading to significant computational demands in field application. To balance computational efficiency and accuracy, it is possible to bypass the multiscale fusion modeling step in digital rock simulations and occasionally skip the digital wellbore modeling process for wellbore parameter simulations. In recent years, deep learning has been applied at a deeper level in digital rock modeling, such as conditional generative adversarial network, conditional variational auto-encoder generative adversarial network, multi-



Fig. 3. Two approaches for digital wellbore modeling and simulation. One is to use well logging data and multiscale digital rocks to construct large-scale models of the wellbore and surrounding formations for simulating logging responses. The other is to batch construct continuous-depth digital rocks for simulating at the core scale.

condition denoising diffusion probabilistic model, leading the digital rock technology based on deep neural networks from research to field application (Chi et al., 2023; Luo et al., 2024). By applying the above methods, it is possible to construct digital rock samples with different pore structures based on predefined conditional information. For instance, porosity and pore size distribution can be used as constraints to control digital rock modeling. Introducing well logging data as control conditions during training and generation phases allows for the batch generation of continuous-depth digital rock samples along the entire wellbore, enabling the exploration of various factors affecting rock physical parameters and solving the issue of inadequate continuity in rock samples.

5. Conclusions

This paper provides an overview of the common methods, key challenges, and research directions related to digital rock and digital wellbore in multiscale modeling and numerical simulation. For rocks with small-scale structural variations, the integration of multi-resolution data offers a viable approach to develop a model containing multiscale information for simulation purposes. However, for rocks with significant structural variations, direct fusion of multi-resolution data becomes impractical. It is recommended to develop models of varying resolutions and progressively analyze their physical properties from small to large scales. Of course, these methods can also be combined to improve computational accuracy and efficiency. The thought for multiscale modeling and simulation can transition from the core scale to the wellbore scale. Through the integration of logging and core data, macroscale digital wellbore and surrounding formation models can be established for investigating the response characteristics of downhole logging instruments. Additionally, creating continuous-depth digital rocks with diverse pore structures in batches can address discontinuity issues in core data. The transition from digital rock to digital wellbore establishes a link between microstructure and macro response. In future work, a combination of direct and indirect fusion techniques, multilevel representation and fusion of multiscale data, as well as the development of lightweight multiscale grids, is essential for the complete expression of rock information. Ultimately, constructing a full-scale 3D digital model centered around the wellbore will accurately describe formation parameters at micro and macro levels, leading to enhanced reservoir transparency and robust support for geological resource exploration and development.

Acknowledgements

This work was supported by a grant from the National Natural Science Foundation of China (No. 42174143) and Technology Innovation Leading Program of Shaanxi (No. 2024ZC-YYDP-27).

Conflict of interest

The authors declare that they have no conflict of interest.

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