Advances in Geo-Energy Research

Vol. 15, No. 2, p. 95-98, 2025

Perspective

Experimental and numerical challenges in multiscale study on geomechanical and hydrological systems

Zhenqi Guo[1], Lele Liu[2], Zhichao Liu[3], Xianda Shen[4], Liang Lei[1]*

[1]*School of Engineering, Westlake University, Hangzhou 310030, P. R. China*

[2]*Shandong Engineering Research Center of Marine Exploration and Conservation, Ocean University of China, Qingdao 266100, P. R. China*

[3]*Faculty of Engineering, China University of Geosciences, Wuhan 430074, P. R. China*

[4]*Department of Geotechnical Engineering, College of Civil Engineering, Tongji University, Shanghai 200092, P. R. China*

Keywords:
Multiscale challenges
geo-materials
multiphysics

Cited as:
Guo, Z., Liu, L., Liu, Z., Shen, X., Lei, L. Experimental and numerical challenges in multiscale study on geomechanical and hydrological systems. Advances in Geo-Energy Research, 2025, 15(2): 95-98.
https://doi.org/10.46690/ager.2025.02.02

Abstract:
Cross-scale studies in geomechanical and hydrological systems employ a variety of approaches, either experimental, simulation or theoretical, each characterized by corresponding scale-specific methodologies. This perspective identifies and discusses challenges encountered at various scales, ranging from molecular to field scale, and examines issues related to integrating these scales. It highlights discrepancies in resolution and data compatibility, emphasizing the necessity for improved scale transition techniques. Insights and recommendations are proposed for future research to enhance multiscale modeling frameworks. These suggestions are crucial for bridging knowledge gaps on geological systems and improving the analyses accuracy for better engineering applications or earth system modelling.

1. Introduction

Geomechanical and hydrological systems explore the critical interactions between geo-materials, such as soil and rock, and various pore fluids, including water, oil, and gas. Due to the pronounced heterogeneity inherent in these systems, physical processes are categorized by distinct characteristic spatial scales: molecular, sub-pore, pore, core, and field. These categories and their implications are illustrated in Fig. 1, which shows how each scale is associated with specific physical processes. Understanding these scales is essential for accurately modeling the overall system dynamics, as each scale provides unique physical insights into the system's behavior.

A big challenge in current research is how to incorporate microscale characteristics into macroscale studies, thereby effectively coupling physical processes across multiple scales to more accurately represent the system's dynamics. Bridging these scales requires robust approaches for integrating data and revealing underlying physical laws in complex systems. This perspective first discusses the research challenges at various scales, then explores the issues of data integration encountered during scale-up processes, and concludes by offering potential suggestions for future research directions. The discussion aims to contribute to ongoing efforts toward more integrated analyses of geomechanical and hydrological systems.

2. Challenges at different scales

The spatial scales are categorized into field, core, pore, sub-pore, and molecular scales. As the scale decreases, the time required to reach equilibrium generally decreases. Gravitational forces, regional stress fields, and fluid dynamics drive long-term changes in geological formations at both the field and core scales, affecting processes such as hydraulic conduction,

Yandy Scientific Press

*Corresponding author.
E-mail address: guozhenqi@westlake.edu.cn (Z. Guo); lele.liu@ouc.edu.cn (L. Liu); liuzhichao@cug.edu.cn (Z. Liu); xshen@tongji.edu.cn (X. Shen); leiliang@westlake.edu.cn (L. Lei).

Received November 7, 2024; revised November 20, 2024; accepted December 2, 2024; available online December 5, 2024.

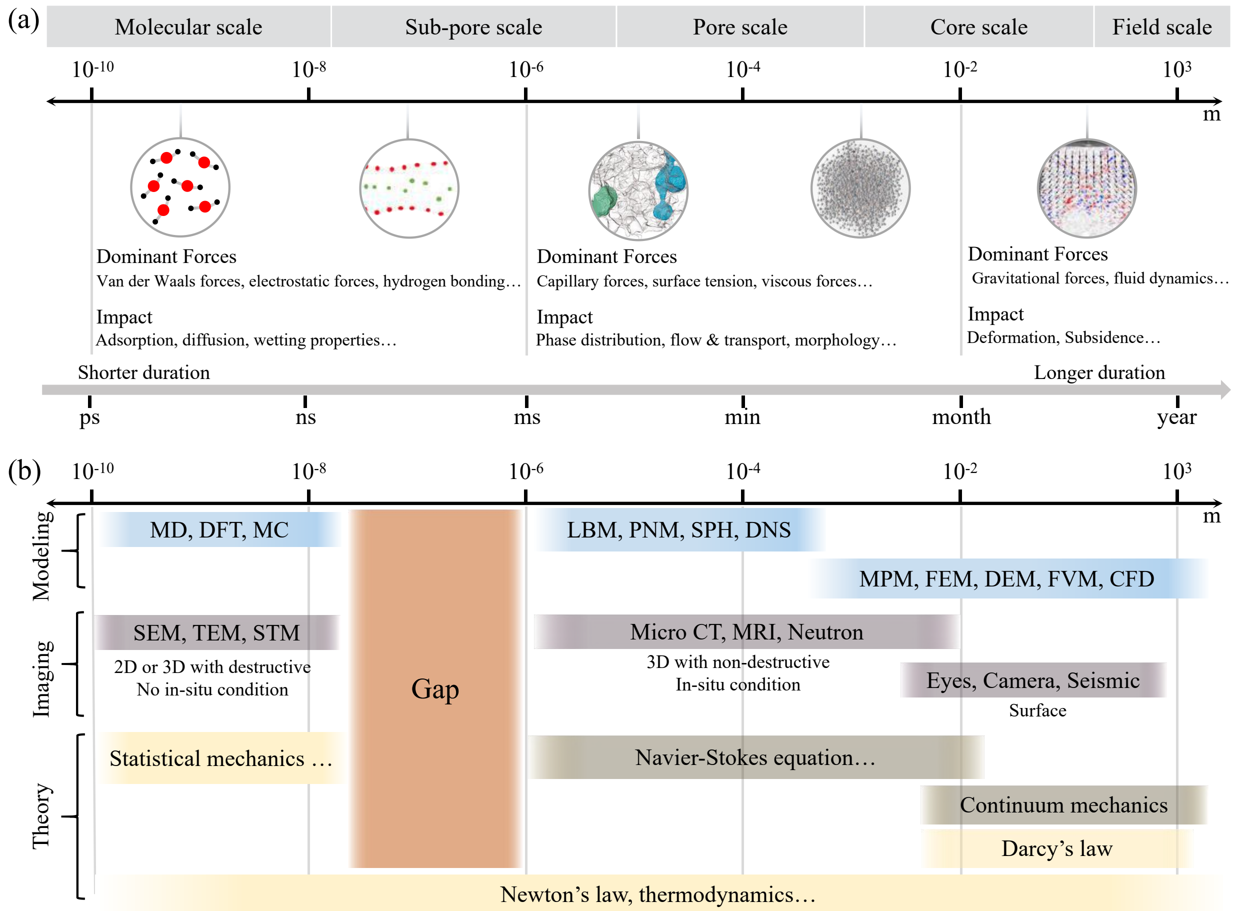

Fig. 1. Overview of scale-specific forces, impacts, and study approaches in geomechanical and hydrological systems. (a) Dominant forces and their impacts across different scales (the general positive correlation between temporal and spatial scales is not strict can vary significantly); (b) study approaches and theoretical frameworks by scale. Abbreviations: MD-molecular dynamics, DFT-density functional theory, MC-Monte Carlo, LBM-lattice Boltzmann method, PNM-pore network modeling, SPH-smoothed particle hydrodynamics, DNS-direct numerical simulation, MPM-material point method, FEM-finite element method, DEM-discrete element method, FVM-finite volume method, CFD-computational fluid dynamics, SEM-scanning electron microscopy, TEM-transmission electron microscopy, STM-scanning tunneling microscopy, CT-computed tomography, NMR-nuclear magnetic resonance.

subsidence, and geological deformation over extended periods. As shifting from the larger core scale to the smaller pore scale, capillary forces, surface tension, and viscosity primarily govern fluid behavior, influencing phenomena such as fluid migration. At the sub-pore scale, molecular forces such as Van der Waals and electrostatic interactions significantly influence adsorption and diffusion processes. These forces, acting across different scales, collectively shape the overall behavior of geomechanical and hydrological systems.

2.1 Field and core scale challenges

More and more advanced experimental setups and simulation models have significantly enhanced our understanding of geomechanical and hydrological systems. Additionally, centrifuge modeling in enhanced gravity fields has offered crucial insights into the behavior of geological materials under extreme conditions, simulating scenarios that are otherwise challenging to replicate (Li et al., 2024). Deep in-situ core sampling and high-fidelity testing further provide direct insights into subsurface environments, offering valuable data on the natural state of geological formations (Xie et al., 2024). However, investigation on field-scale deformation and crustal stress, due to technological and financial limitations, are often short term, post-hoc and under disturbed rather than in-situ conditions. Laboratory experiments using both triaxial and true triaxial testing have enhanced stress-strain analysis, revealing intricate details about rock and soil behavior under applied stresses (Cardona and Santamarina, 2023). On the simulation front, the continuum approach, alongside methods such as the finite element method, computational fluid dynamics, and the finite volume method, has been instrumental in modeling complex interactions within geological formations. These techniques allow for a detailed exploration of dynamic behaviors and fluid flow at various scales, offering a more comprehensive understanding of system dynamics (Gao et al., 2024a; Liu et al., 2024).

The inherent heterogeneity and anisotropy of geological formations pose significant challenges. Variations in properties such as permeability and mechanical strength, which differ significantly across layers, complicate the accuracy of large-scale models. Simplifying these variations into homogeneous fields can obscure critical details like high-permeability zones or areas of mechanical weakness, which can adversely impact predictions of fluid flow paths and mechanical stability. Additionally, imaging techniques such as seismic surveys and well logging, while essential for understanding subsurface conditions, have their limitations. Seismic imaging often struggles with resolution constraints, potentially missing finer structural details, leading to incomplete data interpretation. Similarly, well logging, precise at a local scale, may not adequately capture broader field heterogeneities. The presence of faults, fractures, and layer interfaces further complicates simulations. These geological features, which can act as conduits or barriers for fluid flow, significantly affect the mechanical stability of formations, particularly during operations like hydraulic fracturing or gas injection. While modern tools such as finite volume method and computational fluid dynamics have made strides in incorporating these features, capturing their dynamic behavior-such as the opening or sealing of fractures due to stress changes-remains a significant challenge. This limitation critically affects predictions of induced seismicity, subsurface leakage, or unexpected reservoir performance changes. Overall, the most critical challenge is the insufficient knowledge or information about the geological formations, with which the available numerical approaches can adequately assess or simulate processes in these formations. This insufficiency is limited by both the dilemma between resolution and representativeness in geophysical assessment and the lack of verified underlying rules or patterns, even just statistical.

2.2 Pore, Sub-pore and Molecular Scale Challenges

Advances in both two-dimensional (2D) and three-dimensional (3D) imaging technologies have greatly enhanced our understanding of physicochemical processes. At the pore scale, techniques such as computed tomography, magnetic resonance imaging, and neutron imaging offer insights into 3D structures, allowing for detailed investigations of interfacial processes (Gao et al., 2024b). These imaging tools enable the visualization of phenomena such as phase transitions and fluid displacement, which are critical for understanding fluid behavior in porous media. Theoretically, established laws at this scale, such as the Navier-Stokes equation for fluid flow, capillary action dynamics, and diffusion processes described by Fick's laws, guide our understanding (Cai et al., 2024; Qin et al., 2024). discrete element modeling, grounded in Newton's laws, facilitates the simulation of granular interactions, offering a robust platform for exploring complex dynamics (Shen and Marinelli, 2022; Dou et al., 2024). A broad spectrum of simulation tools, ranging from pore network modeling to lattice boltzmann methods, are instrumental in examining multiphase flow and transport phenomena. Coupling these approaches, such as integrating lattice boltzmann methods with discrete element modeling to simulate fluid-solid interactions, or combining lattice boltzmann methods with material point method for enhanced microscale resolution, is critical for developing comprehensive models that accurately reflect the complex interplay of physical processes across scales.

At the molecular scale, advancements in computational tools like molecular dynamics, density functional theory, and Monte Carlo simulations provide robust approaches for exploring atomic interactions. However, experimentally, the complexity of geo-environments presents substantial challenges. Techniques such as scanning electron microscopy, transmission electron microscopy, and scanning tunneling microscopy are primarily surface-focused or involve destructive 3D analysis, limiting their ability to capture in situ molecular interactions, phases in materials, and intricate boundary conditions (Kiselev et al., 2017). Especially, interfaces pose significant obstacles. While theoretical models from physics are often employed to assist, they are frequently oversimplified for the complex systems encountered in geosciences. As a result, a critical gap remains in fully understanding molecular interactions in geological settings, with limited focus on studying these intricate systems.

At the sub-pore scale, challenges become more pronounced due to the intermediate nature of this scale. Simulation tools like molecular dynamics are often inadequate, as the scale is too large to efficiently simulate molecular interactions, yet too small for techniques like discrete element modeling and lattice boltzmann methods to be applicable. The applicability of established theories, such as capillarity—identified to be effective down to scales as small as 50 nm—remains under reassessment at this scale. Furthermore, there is a significant lack of experimental methods capable of probing these scales under true in-situ conditions, as most techniques are designed for surface or 2D samples, often operating under vacuum rather than realistic environmental settings. Innovations such as Nano-CT could potentially bridge some of these gaps, but their full potential and application scope have yet to be fully realized. This gap highlights a research area filled with unknowns and the lack of established approaches for exploration.

3. Challenges in Scale Integration

A primary challenge in integrating data across scales is ensuring consistency and compatibility. Data collected at the microscale, such as from molecular dynamics simulations or atomic force microscopy, often contain highly detailed, small-scale information. In contrast, field-scale data, from sources like seismic surveys or well logs, capture broader geological phenomena but at a lower resolution. Incorporating these datasets into a coherent model requires addressing a range of challenges:

1) Resolution mismatch: pore-scale models provide detailed insights into fluid dynamics at the microscale but often fail to represent broader, macro-scale phenomena effectively. Such models might accurately predict phenomena within individual pores, yet when these models are applied to larger scales, such as core or field scales, errors can propagate and magnify. This discrepancy arises because microscale properties do not always average

linearly to predict macroscale behaviors, leading to significant deviations and inaccuracies when scaled up.

2) Data compatibility issues: integrating data from different scales presents technical challenges, as datasets often come in diverse formats and are derived from varied methodologies. Standardizing these data for multiscale modeling is fraught with difficulties that can affect the accuracy and relevance of the integrated models. These technical disparities can introduce biases or systematic errors in multiscale models, complicating the interpretation of results and potentially misleading decision-making processes.
3) Lack of effective scale transition techniques: currently, there are insufficient statistically robust methods to effectively transit data across scales. Techniques like upscaling, downscaling, and homogenization are available but must be applied with precision to ensure that they do not distort critical information. The absence of reliable statistical approaches for data transformation across scales remains a significant hurdle, limiting the ability to create models that are both accurate and reflective of complex real-world conditions.

4. Perspectives on future research directions

The identified challenges underscore the urgent need for continued innovation in new experimental approaches, theoretical frameworks, data integration techniques and multiscale modeling frameworks. Our perspective has identified several key areas that are ripe for future research:

Future research could prioritize the development of advanced characterization techniques suitable for in-situ environments, such as fiber optic monitoring technologies. These technologies can provide real-time, multi-data transmission capabilities that are crucial for energy and geotechnical engineering applications in field settings. Furthermore, robust multiscale modeling frameworks to effectively address the integration challenges identified across geomechanical and hydrological scales. Bridging the significant resolution gap between microscale observations and macroscale applications is critical for translating detailed insights into broader, practical solutions. Additionally, the integration of artificial intelligence has the potential to greatly enhance data analysis and improve predictive accuracy across scales. The linkage between field-core scale models has largely been realized, and future efforts could focus on integrating regional geological models with detailed data such as well logging information and pressure maintenance sample testing. This integration would enable a comprehensive geological engineering approach that embeds varied data types into a unified model. Interdisciplinary collaborations will be essential in driving innovative solutions, particularly in overcoming complex challenges and ensuring the reliability and applicability of multiscale models in real-world scenarios.

Acknowledgements

This work is supported by Research Center for Industries of the Future (RCIF), the Natural Science Foundation of Shandong Province (No. ZR2022YQ54), and the Taishan Scholars Program (No. tsqn202306297).

Conflict of interest

The authors declare no competing interest.

References

Cai, J., Qin, X., Xia, X., et al. Numerical modeling of multiphase flow in porous media considering micro- and nanoscale effects: A comprehensive review. Gas Science and Engineering, 2024, 131: 205441.

Cardona, A., Santamarina, J. C. A Convenient device to measure the permeability of intact rock (Heterogeneity and Anisotropy). Geotechnical Testing Journal, 2023, 46: 699-711.

Dou, X., Wu, Q., Liu, Z., et al. 3D DEM investigation on macro-meso mechanical responses of gas hydrate-bearing sediments in process of unloading confining pressure. Gas Science and Engineering, 2024, 130: 205434.

Gao, X., Tian, R., Jiang, Y., et al. Frozen saline sand can be highly permeable. Geophysical Research Letters, 2024a, 51: e2024GL111946.

Gao, Y., Yin, Y., Li, B., et al. Multistate transition and coupled solid-liquid modeling of motion process of long-runout landslide. Journal of Rock Mechanics and Geotechnical Engineering, 2024b, 16: 2694-2714.

Kiselev, A., Bachmann, F., Pedevilla, P., et al. Active sites in heterogeneous ice nucleation—the example of K-rich feldspars. Science, 2017, 355: 367-371.

Li, J., Guan, L., Wang, Y., et al. Centrifuge modelling on seismic failure of MSW landfills with high Xiewater level. Soil Dynamics and Earthquake Engineering, 2024, 182: 108753.

Liu, L., Liu, T., Wu, C., et al. A multi-orientation system for characterizing microstructure changes and mechanical responses of fine-grained gassy sediments associated with gas hydrates. Review of Scientific Instruments, 2024, 95: 073704.

Qin, X., Wang, H., Xia, Y., et al. Micro- and nanoscale flow mechanisms in porous rocks based on pore-scale modeling. Capillarity, 2024, 13: 24-28.

Shen, X., Marinelli, F., Buscarnera, G. Constitutive modeling of structured granular materials with anisotropic grain skeleton and cement bonds. Acta Geotechnica, 2022, 17: 5465-5479.

Xie, H., Gao, M., Zhang, R., et al. Application prospects of deep in-situ condition-preserved coring and testing systems. Advances in Geo-Energy Research, 2024, 14: 12-24.