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Invited review

Multiscale modeling for multiphase flow and reactive mass transport in subsurface energy storage: A review

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Abstract:
Modeling of multiphase flow and reactive mass transport in porous media remains a pivotal challenge in the realm of subsurface energy storage, demanding a nuanced understanding across varying scales. This review paper presents a comprehensive overview of the latest advancements in multiscale modeling techniques that address the inherent complexity of these processes. Three cutting-edge approaches are presented: hybrid multiscale simulation, which leverages both continuum and discrete modeling frameworks to enhance model fidelity; approximated physics, which simplifies complex reactions and interactions to expedite computations without significantly sacrificing accuracy; and machine-learning-assisted multiscale simulation, which integrates predictive analytics to refine simulation outputs. Each method presents distinct advantages and hurdles, collectively advancing the precision and computational efficiency of subsurface modeling. Despite the substantial progress, we recognize the persistent challenges, such as the need for more robust coupling techniques, the balance between model complexity and computational feasibility, and effectively combining machine learning with traditional physical models. Promising directions for future work are discussed to address these challenges, aiming to push the boundaries of current multiscale modeling capabilities.

1. Introduction

Energy transition in the subsurface is crucial for achieving sustainable development and mitigating climate change impacts. It involves the shift from traditional fossil fuel extraction to cleaner and renewable energy sources such as geothermal energy, carbon capture and storage, and subsurface energy storage. This transition helps reduce greenhouse gas emissions, promotes energy security, and supports the global move towards a low-carbon economy (Bauer et al., 2013; Gasanzade et al., 2021). As the demand for energy grows, the development of efficient and scalable subsurface storage solutions becomes paramount. These technologies not only enable the effective integration of intermittent renewable energy sources into the grid but also enhance the resilience of energy systems against environmental and market fluctuations (Krevor et al., 2023). By leveraging the existing geological formations

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and infrastructure, subsurface energy storage presents a viable pathway to stabilize energy supply and foster sustainable energy landscapes worldwide.

Subsurface energy storage in porous media presents a complex challenge due to the heterogeneous nature of geological formations and the intricate interactions between multiple phases of fluids and solids (Bauer et al., 2017; Kabuth et al., 2017). The variability in pore structure and mineral composition across different scales—from the microscopic to the field level—significantly impacts the behavior and efficiency of storage systems. This complexity is further compounded by the reactive transport of chemical species, which can alter the physical properties of the storage medium over time (Tarkowski, 2017; Crotogino et al., 2018; Gasanzade et al., 2021). Additionally, the operational dynamics of injecting and extracting fluids, such as compressed air, hydrogen, or supercritical CO_2, require precise control and understanding to prevent issues like leakage, induced seismicity, and reservoir degradation. These factors make the modeling and optimization of subsurface energy storage systems a critical area of research, necessitating advanced multiscale modeling techniques to accurately predict and enhance system performance.

Given the complexities of multiphase flow and reactive mass transport in heterogeneous porous media, multiscale modeling is indispensable in environmental engineering and geosciences to optimize energy storage technologies (Luo et al., 2009; Golparvar et al., 2018; De Santis et al., 2021; Ramesh Kumar et al., 2021). This approach is crucial as it spans a wide range of spatial and temporal scales—from the microscopic scale of individual pore spaces to the macroscopic scale of entire geological formations (Fig. 1). Multiscale modeling captures key physical and chemical processes occurring at different scales, providing insights into the behavior of energy storage systems (Joekar-Niasar et al., 2012; Sheng and Thompson, 2013). It integrates models from molecular dynamics and pore-scale models to continuum-scale and field-scale models, allowing for a detailed representation of physical and chemical interactions. These interactions among the injected gases, resident fluids, and the porous matrix can lead to complex reactive transport processes, such as dissolution, precipitation, and chemical reactions that alter the porosity and permeability of the medium (Li et al., 2020; Subramaniam, 2020; Heinemann et al., 2021). By accurately simulating these processes, multiscale modeling contributes significantly to optimizing gas injection strategies, assessing storage capacities, predicting the long-term fate of stored gases, and evaluating potential environmental impacts, thereby ensuring the efficiency, safety, and sustainability of energy storage solutions (Tryggvason et al., 2013; Carrillo et al., 2020).

Molecular simulation has emerged as a critical tool in advancing our understanding of gas storage mechanisms at the molecular level, offering insights into the interactions, behaviors, and properties of gas when introduced into various storage mediums (Liu and Wilcox, 2012, 2013; Ma and Ranjith, 2019). Despite its significant contributions, the accuracy of molecular simulations heavily depends on the quality of the mathematical models and the parameters used, which might not always capture the complexity of real-world systems (Zhang et al., 2020). Additionally, computational constraints limit the scale of simulations, making it challenging to directly extrapolate findings to the macroscopic levels relevant for industrial applications (Ma and Ranjith, 2019).

Pore-scale simulation is another way to enhance our understanding and optimization of gas storage within geological formations (Meakin and Tartakovsky, 2009; Wang et al., 2023b; Yang et al., 2023; Xie et al., 2024). By offering detailed insights into the microscopic interactions between gas and the porous rock matrix, these simulations enable us to predict the behavior of gas injection and storage with greater precision (Blunt et al., 2013; Icardi et al., 2014; Molins, 2015; Xie et al., 2023). Such detailed understanding aids in maximizing storage efficiency, ensuring the long-term/periodic security of the stored gas, and mitigating leakage risks. The complexity and heterogeneity of geological formations at the microscopic level introduce significant challenges in accurately modeling the physical processes involved (Liu and Mostaghimi, 2017; Liu et al., 2020; Wang et al., 2023a). The computational resources required for these simulations are substantial, making it difficult to scale up to larger, more practical field scales (Soulaine and Tchelepi, 2016; Chen et al., 2022). These limitations necessitate the development of more advanced computational methods and upscaling techniques to bridge the gap between pore-scale phenomena and field-scale applications.

The application of Darcy-scale simulation in energy storage represents a critical advancement in the field of zero-carbon process (Lyu and Voskov, 2023; Awag et al., 2024). By employing models that operate at the Darcy scale, one can better understand the flow and behavior of gas within subsurface geological formations, thereby enhancing the efficacy and safety of storage operations. These simulations are pivotal for predicting the migration patterns of injected gas, assessing storage capacity, and evaluating potential leakage risks, which are essential for the long-term success of energy-storage projects aimed at mitigating climate change (Pau et al., 2010; Martinez and Hesse, 2016; Vialle et al., 2016; Lyu et al., 2021b). However, the simplifications required for these models may overlook finer-scale geological heterogeneities and fluid interactions, potentially leading to inaccuracies in predictions (Ajayi et al., 2019). Furthermore, the computational demands of these simulations can be substantial, limiting their resolution and the detail they can provide (Pau et al., 2010).

The development of multiscale modeling in subsurface energy storage and multiphase flow has evolved significantly over the past few decades, driven by the need to capture complex fluid behaviors across different spatial and temporal scales. Early approaches primarily relied on continuum-scale models, such as extensions of Darcy's law and capillary pressure formulations, to describe multiphase flow in porous media. As computational resources advanced, pore-scale modeling techniques, including direct numerical simulations and Lattice Boltzmann Methods (LBMs), provided more detailed insights into fluid displacement and reactive transport processes (Blunt et al., 2002; Bijeljic and Blunt, 2007; Balhoff and Wheeler, 2009; Blunt et al., 2013). The emergence of hybrid

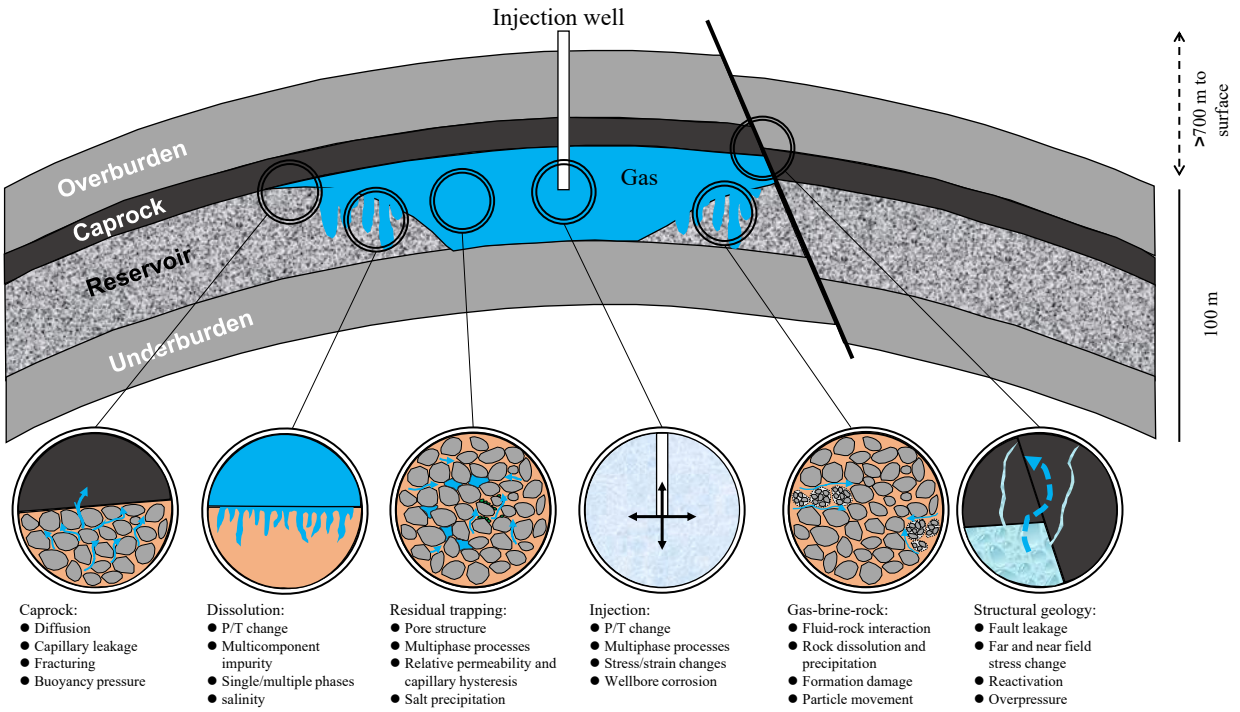

Fig. 1. Gas storage in porous media highlighting all geological uncertainties (modified from Heinemann et al. (2021)).

multiscale frameworks, which integrate molecular dynamics, pore-scale modeling, and continuum-scale formulations, has further refined predictive capabilities for subsurface systems (Balhoff et al., 2007; Tartakovsky et al., 2008; Scheibe et al., 2015).

More recently, approximated physics-based approaches and machine-learning-assisted multiscale simulations have gained traction, offering computationally efficient alternatives to traditional physics-driven methods (Zhu et al., 2022). Machine Learning (ML) techniques, including deep learning, Convolutional Neural Networks (CNNs), and Physics-Informed Neural Networks (PINNs), have been increasingly applied to model complex subsurface processes such as multiphase flow, reactive transport, and reservoir characterization (Wang et al., 2021b; Amini et al., 2022; Zhou et al., 2022; Marcato et al., 2023). These approaches enable rapid surrogate modeling, reducing the computational cost of traditional numerical simulations while preserving key physical constraints. Data assimilation techniques, such as Bayesian inference and ensemble learning, have also been integrated with ML models to enhance uncertainty quantification and parameter estimation in subsurface energy applications (Tang et al., 2021b; Wu et al., 2023a). Furthermore, hybrid artificial-intelligent-physics approaches leverage domain knowledge to ensure physically consistent predictions, bridging the gap between purely data-driven models and conventional physics-based simulations (Karimpouli et al., 2022). As AI-driven methods continue to evolve, their role in subsurface modeling is expanding, offering new opportunities for optimizing energy storage, CO_2 sequestration, and hydrocarbon recovery.

Due to the advantages and limitations of different-scale simulations, the development and refinement of multiscale modeling techniques continue to be of paramount importance. Advances in computational methods, increased understanding of underlying physical and chemical processes, and improved data availability from experimental and field studies are driving progress in this area. This paper concisely outlines the latest developments, pinpoints challenges, and offers insights into the future of subsurface energy storage. Its goal is to significantly advance the adoption of multi-scale numerical coupling simulation technology within this field.

2. Mathematical models in different scales

Understanding the simultaneous flow of multiple phases through porous media in different scales is crucial in various fields, e.g., hydrogeology, petroleum engineering, and energy storage. The multiscale modeling approach integrates information from macroscopic to microscopic scales, capturing the heterogeneity of porous media and providing insights into fluid behavior at both large and small scales (Fig. 2). This holistic perspective enables us to simulate and analyze multiphase flow phenomena accurately, offering valuable insights for optimizing resource recovery and environmental management.

2.1 Molecular dynamic simulation of micro- and nanoscale flow

Molecular dynamics simulation is a computational technique used to study the behavior of molecules and atoms within complex hydrocarbon systems. It involves the simulation of the motion and interactions of individual particles over time, providing insights into the thermodynamic and kinetic properties of the materials. The motions of each particle can be written as follows:

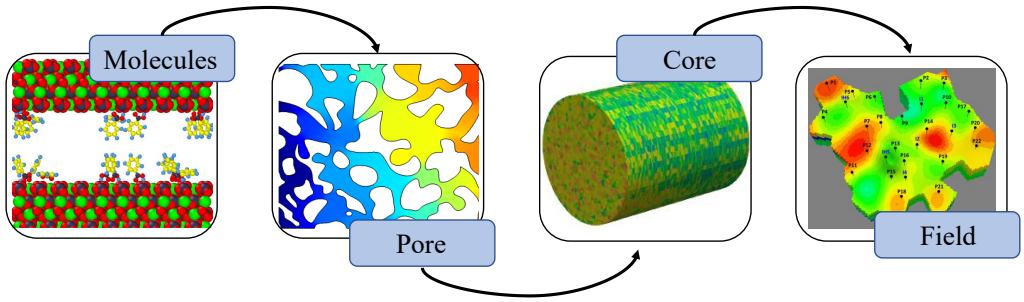

Fig. 2. Schematic representations of porous media with different scales.

$$m\ddot{\mathbf{r}}_\mathbf{i} = f_i = \sum_{k=1,k\neq i}^{N_m} \overrightarrow{F}_{ik} + \sum_{k\neq i,k=1}^{N_w} \overrightarrow{F}_{ikw} + \overrightarrow{F}_{sou}\,\overrightarrow{i} \tag{1}$$

where subscript $i(k)$ denotes particle $i(k)$, $\overrightarrow{i}$ is the unit vector in x-coordinate. m is the particle mass and $\ddot{\mathbf{r}}_\mathbf{i}$ is the position of the particle i. f_i is the total force. N_m is the total number of particles in the simulation system, and N_w is the total number of particles on the solid wall. $\overrightarrow{F}_{ik}$ is the molecular force that particle k exerts on particle i due to Lennard-Jones potential. $\overrightarrow{F}_{ikw}$ represents the molecular force between particle i and all the solid wall particles k. $\overrightarrow{F}_{sou}$ is the external force, which makes the fluid deviate from the equilibrium, e.g., gravity, pressure, or electric force. When a two-body potential model is applied, the interaction force between a pair of molecules comes from the following relation:

$$\overrightarrow{F}_{ik} = -\nabla U(r_{ik}) \tag{2}$$

where $U(r_{ik})$ is the potential energy function, and r_{ik} is the magnitude of the distance between two arbitrary particles.

The Lennard-Jones pair-wise potential energy function can be expressed as:

$$U(r_{ik}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ik}}\right)^{12} - \left(\frac{\sigma}{r_{ik}}\right)^{6}\right] \tag{3}$$

where σ is a molecular length scale, and ε is an interaction strength parameter. The movement of the fluid particles can be predicted by these basic physics laws, with special conditions, e.g., the boundary and initial conditions.

2.2 Pore-scale modeling of multiphase flow in porous media

Pore-scale simulation is one important way to understand the complicated interaction between fluids and pore structures during fluid flow and solute transport. The conventional incompressible Navier-Stokes (NS) equations and the convection-diffusion equation are used to describe the multiphase flow and reactive mass transport in porous media:

$$\nabla\cdot\mathbf{u_j} = 0, \quad j = 1,\cdots,n_p \tag{4}$$

$$\partial_t\mathbf{u_j} + \mathbf{u_j}\cdot\nabla\mathbf{u_j} = -\frac{1}{\rho_j}\nabla p_j + \mu_j\nabla^2\mathbf{u_j}, \quad j = 1,\cdots,n_p \tag{5}$$

$$\partial_t C + \mathbf{u_j}\cdot\nabla C = \mathbf{D}\nabla^2 C + R, \quad j = 1,\cdots,n_p \tag{6}$$

where $\mathbf{u}$, C, and p denote the velocity vector of field, solute concentration, and pressure, respectively. The subscript j and n_p represent the phase index and the number of phases in the system. $\mathbf{D}$ is the molecular diffusion coefficient, which depends on the type of molecules. R is the source term to describe the reaction in the system. The interplay between the fluid and the pore structure is facilitated through the application of appropriate boundary conditions. Typically, pore-scale models exhibit resolutions in the micron range, enabling precise characterization of microscale phenomena that are beyond the scope of Darcy-scale models.

2.3 Darcy-scale simulation of multiphase flow in porous media

The Darcy-scale simulation of multiphase flow in porous media is a complex numerical modeling approach used to understand and predict the behavior of fluids as they move through porous geological formations. This type of simulation is based on Darcy's law, which describes the flow of a fluid through a porous medium. In multiphase flow scenarios, different fluids necessitate sophisticated mathematical models and computational techniques to accurately represent the physical processes involved:

$$\frac{\partial}{\partial t}\left(\phi\sum_{j=1}^{n_p} x_{cj}\rho_j s_j\right) + \nabla\cdot\sum_{j=1}^{n_p}\left(x_{cj}\rho_j\mathbf{u}_j + s_j\rho_j\mathbf{J}_{cj}\right) + \sum_{j=1}^{n_p} x_{cj}\rho_j\widetilde{q}_j = 0, \quad c = 1,2,\ldots,n_c \tag{7}$$

$$\mathbf{u}_j = -K\frac{k_{rj}}{\mu_j}(\nabla p_j - \rho_j g\nabla z), \quad j = 1,\cdots,n_p \tag{8}$$

$$p_w = p_n - p_c \tag{9}$$

$$\sum_{j=1}^{n_p} s_j = 1 \tag{10}$$

$$\mathbf{J}_{cj} = -\phi D_{cj}\nabla x_{cj} \tag{11}$$

where $\mathbf{u}$, p and s are the Darcy velocity, pressure, and saturation, respectively. D is the effective diffusion coefficient. c and j are the index of component and phase, respectively. These variables denoted by a bar represent parameters at the Darcy scale, obtained through measurement or upscaling techniques. ϕ and $\mathbf{k}$ are formation porosity and permeability. ρ, x_{cj}, k_r, and μ are phase density, component mole fraction in a phase, relative permeability, and kinematic viscosity, respectively. g and z are gravitational acceleration and vertical depth. $\mathbf{J}_{cj}$ is

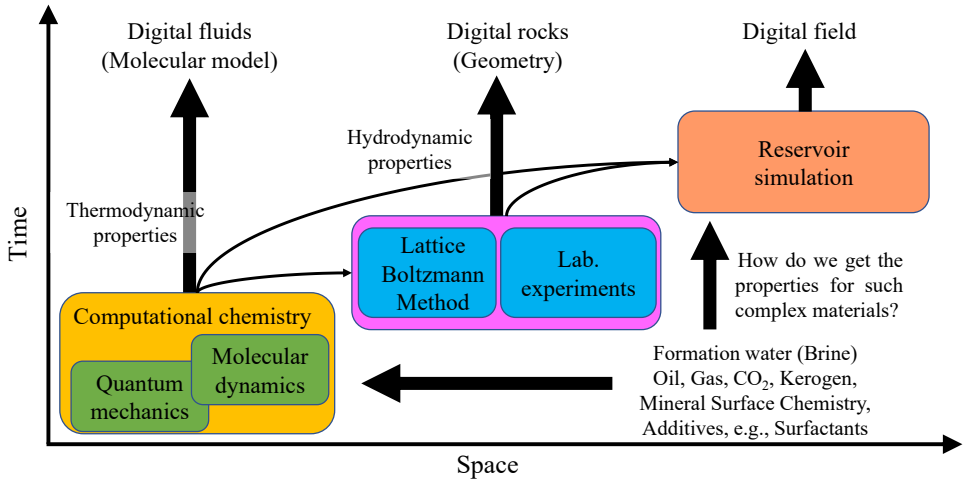

Fig. 3. Schematic diagram of multiscale simulations.

the diffusion-dispersion tensor of component c in phase j.

3. Bridging-scale techniques

3.1 Hybrid multiscale simulation

The transition across scales in porous media modeling remains a fundamental challenge, particularly in linking molecular dynamics with pore-scale representations and further extending these descriptions to continuum-scale models. Hybrid multiscale simulation, which amalgamates continuum and atomistic perspectives, offers a powerful tool for understanding and predicting the behavior of complex systems across different disciplines (Fig. 3). The efficiency of such a hybrid model is significantly influenced by the comparative dimensions of the molecular dynamics and continuum regions, alongside the magnitude of the interface through which data exchange occurs between the two subdomains.

Regarding the advanced simulation approaches for molecular simulation, AB Initio Molecular Dynamics (AIMD) and quantum mechanics/molecular mechanics methods stand out due to their ability to provide a detailed picture of molecular systems at the atomic level. AIMD combines quantum mechanics principles with classical molecular dynamics, allowing for the simulation of molecular systems with electrons explicitly included. This method is particularly useful for studying chemical reactions, material properties at the atomic scale, and the behavior of molecules in various environments. It provides insights that are unattainable through classical molecular-dynamics simulations alone. AIMD and quantum mechanics/molecular mechanics methods embody the forefront of computational chemistry and materials science, enabling the exploration of complex molecular phenomena with remarkable detail and accuracy.

Multiscale simulation, integrating molecular simulation with the LBM or Computational Fluid Dynamics (CFD) methods, represents a cutting-edge approach in computational physics and engineering to study complex fluid dynamics and transport phenomena across different scales (Smith and Theodorakis, 2024). In this hybrid framework, molecular simulation provides detailed insights into the microscopic interactions and behaviors of individual particles or molecules (Fig. 4). This microscopic information is essential for accurately capturing phenomena at the nanoscale, where the specific interactions between molecules significantly influence the overall behavior of the system. On the other hand, the LBM, a mesoscopic approach, excels at simulating fluid flows at larger scales by treating the fluid as a collection of discrete particles and tracking their distribution functions over a lattice mesh. By coupling these two methodologies, the multiscale simulation leverages the strengths of both: the detailed representation of particle interactions in molecular simulation for accurate boundary and initial condition definitions, and the efficient handling of fluid flow at larger scales in LBM. This synergistic integration allows for the simulation of complex systems with high fidelity, spanning from the molecular up to the macroscopic level, thus bridging the gap between microscopic mechanisms and their macroscopic manifestations in fluid dynamics and material science. Similarly, the algebraic multiscale solver, initially used for continuum scale, leverages an algebraic approach that requires only the fine-scale system and a superimposed multiscale coarse grid, allowing it to be applied to arbitrary geological models without additional preprocessing (Hajibeygi et al., 2011; Hajibeygi and Tchelepi, 2014; Wang et al., 2014). A key innovation is its hybrid two-stage strategy: a global solver operates exclusively at the coarse scale, reducing computational costs, while various fine-scale local preconditioners, including correction functions, block incomplete lower–upper factorization, and ILU, enhance convergence and numerical stability. Notably, algebraic multiscale solver demonstrates superior efficiency and flexibility, particularly in handling complex geological heterogeneity, making it a significant advancement in multiscale reservoir simulation techniques.

Combining pore-scale modeling with reservoir simulation allows for more comprehensive and accurate descriptions of fluid flow and transport phenomena. By integrating these two scales, one can leverage the detailed insights gained from pore-scale models to inform and enhance the parameterization

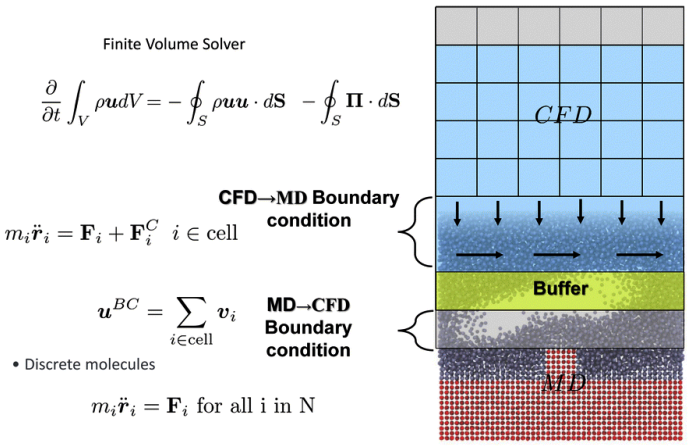

Fig. 4. A domain decomposition coupling arrangement, which includes: (1) an averaged region at the bottom boundary to determine the CFD boundary, and (2) a constrained region at the top boundary of the domain where a termination force is applied to prevent molecules from escaping. Additionally, a buffer zone is incorporated to ensure that the constrained molecular region does not directly interact with the averaged region used for boundary determination (Smith and Theodorakis, 2024).

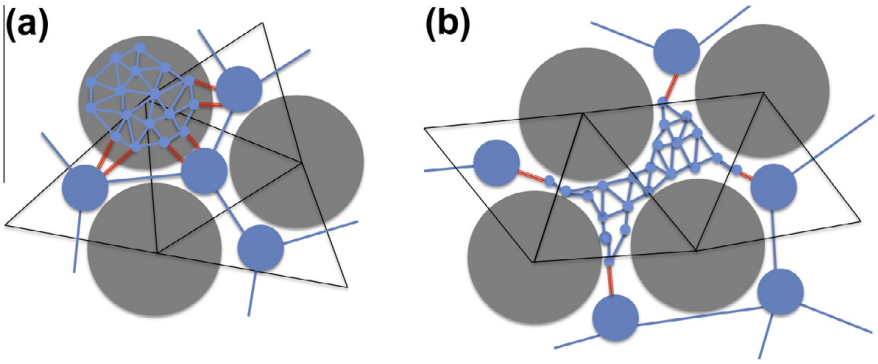

Fig. 5. Schematic of two-scale pore network construction for (a) grain-filling and (b) pore-filling microporosity (Mehmani and Prodanović, 2014).

of Darcy-scale models. For example, pore-scale simulations can be used to calculate effective permeability and relative permeability curves, which are then upscaled and incorporated into Darcy-scale simulations to improve their accuracy in predicting macroscopic flow behavior. One notable study that highlights the potential of this multi-scale approach is the work by Blunt et al. (2013), which utilized pore-scale imaging and modeling to derive petrophysical properties of carbonate rocks. Their findings demonstrated that pore-scale simulations could provide detailed characterizations of pore connectivity and distribution, which are critical for accurate Darcy-scale modeling. Another significant contribution is the research by Bijeljic et al. (2013), where they employed multi-scale imaging techniques to capture the pore structure and subsequently performed flow simulations to understand the impact of pore-scale heterogeneities on macroscopic transport properties. The integration of pore-scale and Darcy-scale models has also been effectively applied in studying multiphase flow in porous media (Fig. 5). For instance, a method is developed to compute relative permeability from pore-scale simulations and demonstrated that incorporating these detailed pore-scale data into Darcy-scale models could significantly enhance the predictive capabilities for two-phase flow systems (Raeini et al., 2012; Mehmani and Prodanović, 2014).

Coupling reservoir simulation and molecular simulation on massively parallel High-Performance-Computing (HPC) systems represents a sophisticated computational approach designed to bridge the gap between macroscopic reservoir behaviors and microscopic fluid interactions (Bao et al., 2016). This approach leverages the immense computational power of HPC systems to simultaneously run large-scale reservoir simulations, which predict fluid flow and phase behavior on the scale of kilometers, and molecular simulation simulations, which model the physical and chemical interactions between molecules at the nanometer scale (Fig. 6). By integrating these two levels of simulation, a more comprehensive understanding of subsurface fluid dynamics can be achieved, encompassing both the large-scale effects of reservoir geometry and heterogeneity, as well as the microscopic influences of fluid viscosity and wettability. The parallel nature of HPC systems allows for the distribution of computational tasks across thousands of processors, significantly reducing the time required for simulations and enabling the handling of complex models that were previously infeasible, thus providing insights into

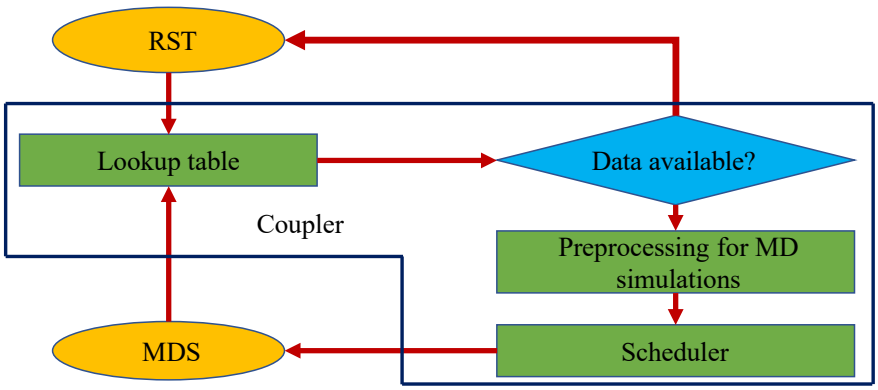

Fig. 6. Flow chart of the computational framework for molecular simulation and reservoir-simulation toolbox (modified from Bao et al. (2016)).

optimizing carbon sequestration strategies with unprecedented detail and accuracy.

3.2 Approximated physics and advanced nonlinear solvers

Due to the highly nonlinear properties across different scales of time and space, one useful technique is to simplify the complex, underlying physical laws governing small-scale interactions to make large-scale simulations computationally feasible without significantly sacrificing accuracy. Upscaling techniques, aiming to derive macroscopic properties from microscopic behavior, help in bridging the gap between pore-scale phenomena and field-scale applications, ensuring that the detailed interactions at the pore level are adequately represented in larger-scale models. For instance, homogenization techniques and volume averaging are commonly employed to obtain effective parameters, e.g., porosity, permeability, and reactive surface areas that can be used in Darcy-scale models (Zhang et al., 2021). Another improvement in reactive mass transport is the development of a nonlinear element balance formulation that seamlessly integrates thermodynamic and chemical equilibria within a reactive-compositional flow model (Kala and Voskov, 2020; Ahusborde et al., 2024; de Hoop et al., 2024). Unlike traditional molar-based formulations, which often struggle with numerical instability and inefficiencies in handling complex phase behavior, this approach leverages the consistent reduction of component conservation equations to element conservation equations, ensuring a more robust and computationally efficient framework. A key innovation is the incorporation of chemical equilibrium constraints directly into the multiphase multicomponent negative flash calculations, enabling the simultaneous solution of phase and chemical equilibria. By introducing the Equilibrium Rate Annihilation matrix and modifying the multiphase flash equations to work with element mole fractions, the method provides a generalized treatment of precipitation and dissolution reactions in multiphase flow systems. In addition, some reactive transport simulators couple solute transport equations with chemical kinetics. These simulators often implement approximations such as local equilibrium assumptions, where it is presumed that chemical reactions reach equilibrium instantaneously compared to the timescale of transport processes (Steefel et al., 2015). This significantly reduces the computational burden as it avoids the need to solve complex differential equations governing reaction kinetics. These techniques have proven effective in various applications, from groundwater contamination remediation to enhanced oil recovery.

The hybrid analytical-numerical method, developed by Flyer and Fokas (2008), offers another possibility to solve complex problems in multiphase flow and reactive mass transport. This technique is particularly valuable in scenarios where exact solutions are available for specific parts of a problem domain, or where boundary conditions and singularities pose challenges that purely numerical methods might struggle to handle efficiently. By integrating analytical solutions for parts of the domain where they are applicable, this approach can significantly enhance the accuracy and efficiency of the simulation. It provides a way to impose rigorous solutions to subsets of a problem, ensuring that the overall numerical solution adheres more closely to the physical reality. Furthermore, this method can reduce computational costs by simplifying aspects of the model where high precision is crucial but difficult to achieve numerically (Meunier et al., 2017; De Barros et al., 2019).

Though these approximations can predict the phase dynamics in porous media, the underlying physics is expressed either by empirical correlations or simple models to reduce the nonlinearity, which may cause discrepancies in the predictions. One accurate and efficient approach, named Operator-Based Linearization (OBL), is proven to solve the coupled problems efficiently and accurately (Voskov, 2017; Lyu et al., 2021a). Conventionally, the simulations require assessing physical properties and their derivatives in relation to nonlinear variables, which is a process known for its complexity and time consumption. However, the OBL approach introduces a novel tactic for simplifying the calculation of nonlinear physics by parameterizing the state-dependent properties in the physical space either during the preprocessing process or adaptively with a few supporting points (Khait and Voskov, 2018; Lyu and Voskov, 2023). In the course of a simulation, the physical properties at the current timestep are assessed using a multilinear interpolation method (Fig. 7). This approach enhances

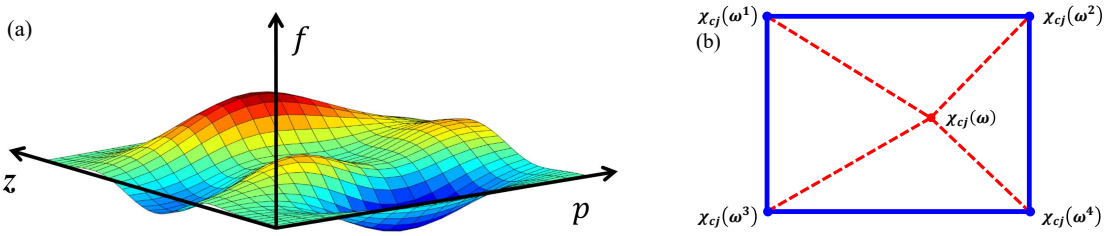

Fig. 7. Schematic description of operator parameterization and interpolation process for χ operators with a predefined OBL resolution (modified from Voskov (2017); Lyu et al. (2021a)). ω^1 to ω^4 are four supporting points, and ω is the current thermodynamic state of a given control volume at a given timestep in the simulation. (a) Operator distribution and (b) interpolation.

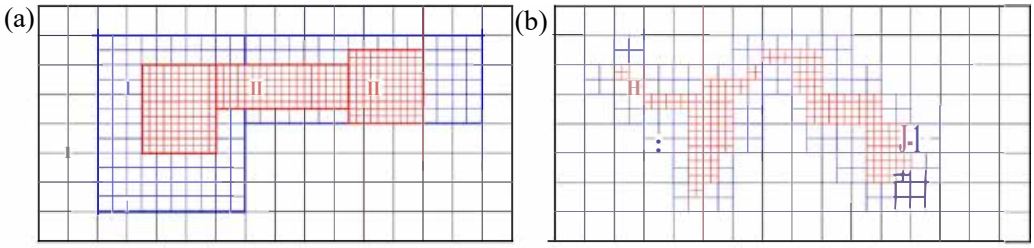

Fig. 8. Examples of data structures used by AMR codes. (a) Block-structured and (b) point-structured (modified from Cant et al. (2022)).

the efficiency of the linearization process (Voskov, 2017). By simplifying the assembly of the Jacobian matrix, it utilizes partial derivatives of the physical properties with respect to nonlinear variables, which are then directly calculated as coefficients in the multi-linear interpolation process. One can find more details about the applications of the OBL approach for multi-phase multi-component systems with gravity (Khait and Voskov, 2018), capillarity (Lyu et al., 2021a), thermal (Wang et al., 2020), and diffusion effects (Lyu et al., 2021c). This approach can bridge the gap between detailed microscopic descriptions and emergent macroscopic behaviors. Approximated physics enables the exploration of a vast range of applications, providing insights into the behavior of complex systems across multiple levels of organization.

Nonlinear solvers address the inherent nonlinearity in the governing equations of fluid flow and transport in porous media. These equations, such as the Navier-Stokes equations or the Richards equation, exhibit strong nonlinearities due to coupling between pressure, saturation, and permeability. Advanced nonlinear solvers are designed to handle these complexities effectively when the classical Newton-Raphson approach suffers from convergence issues. Adaptive Mesh Refinement (AMR) techniques dynamically adjust the computational grid to resolve fine-scale features where they are most needed, such as near sharp fronts or interfaces in porous media (Fig. 8). By refining the mesh adaptively, AMR methods can achieve high resolution in critical regions while maintaining coarser grids elsewhere, thus optimizing computational resources. Nonlinear solvers combined with AMR, such as the nonlinear multigrid-AMR methods, have demonstrated substantial improvements in both accuracy and efficiency for multiscale simulations (Berger and Oliger, 1984; Cusini et al., 2018; de Hoop et al., 2021).

Domain decomposition methods partition the computational domain into smaller subdomains, solving the nonlinear equations within each subdomain either sequentially or in parallel. These methods, including the Schwarz alternating method and the balancing domain decomposition by constraints, facilitate scalable and efficient solutions for large-scale multiscale simulations. By addressing nonlinearity within localized regions, domain decomposition methods can handle complex boundary conditions and heterogeneous properties more effectively. Another efficient technique, named Operator splitting method, decomposes the original problem into simpler sub-problems that can be solved sequentially. For instance, the adomian decomposition method splits nonlinear Partial Differential Equations (PDEs) into linear and nonlinear parts, solving them iteratively. These methods are particularly useful for handling stiff reactions and transport processes in porous media. Nonlinear solvers applied within each sub-problem ensure that the overall solution remains accurate and stable (Estep et al., 2008; Lu et al., 2022; Vasilyeva, 2023).

3.3 High-performance computing and machine-learning-assisted multiscale simulation

HPC has become an indispensable tool in modern scientific and engineering research, enabling the solution of complex and computationally intensive problems. HPC involves the use of supercomputers and parallel processing techniques to perform computations at speeds far beyond that of standard computing systems. The ability to process vast amounts of data and perform numerous calculations simultaneously makes HPC crucial in multiscale simulations (Gauthier et al., 2021;

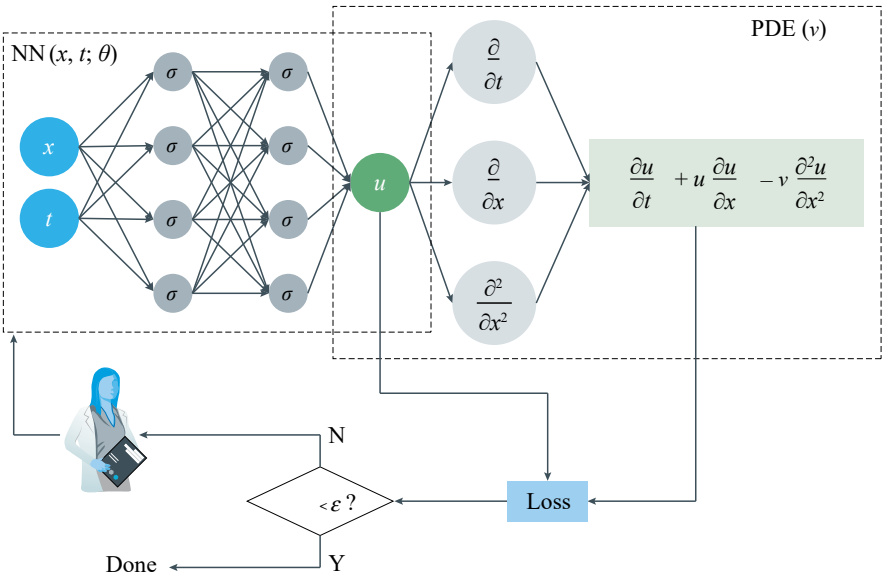

Fig. 9. The physics-informed neural network algorithm (Karniadakis et al., 2021).

Ghassemzadeh et al., 2021). One of the primary components of HPC is the architecture of supercomputers, which includes thousands of interconnected processors working in parallel. These processors can perform quadrillions of calculations per second. For instance, the Graphics Processing Units (GPUs) offer substantial improvements in computational speed and efficiency. GPUs are designed to handle parallel tasks efficiently, making them particularly well-suited for the large-scale simulations and matrix operations inherent in reservoir modeling. Studies have shown that GPUs can accelerate computational tasks by an order of magnitude compared to CPUs, which translates into more timely and cost-effective decision-making processes in reservoir management (Esler et al., 2022).

Even with significant advancements in simulating multiphysics challenges through the numerical breakdown of PDEs, integrating noisy data into current algorithms still poses difficulties. In addition, it is intricate to address high-dimensional issues steered by parameterized PDEs. Furthermore, addressing inverse problems that involve undiscovered physical principles is frequently exorbitantly costly. This necessitates distinct approaches and complex codes. Machine-learning-assisted multiscale simulation has emerged as a transformative approach for analyzing multiphase flow and reactive mass transport in porous media, e.g., CNNs (Han and Jentzen, 2017; Zha et al., 2022; Zhuang et al., 2024a). These neural networks enhance the efficiency and accuracy of simulations that span multiple scales, from atomic to macroscopic levels, by learning patterns and predicting outcomes from vast datasets. Recurrent neural networks, with their ability to handle sequential data, are invaluable for simulations involving time-dependent processes. On the other hand, CNNs excel in analyzing spatial data, making them ideal for simulations related to image recognition, material science, and fluid dynamics, where the spatial distribution of elements is crucial. By integrating these ML models into multiscale simulations, one can tackle complex, real-world problems more effectively, leading to breakthroughs for multiscale phenomena (Zhuang et al., 2024b).

Training deep neural networks often hinges on the availability of large datasets, which may not always be accessible for specific scientific inquiries. As an alternative, these networks can be effectively trained by leveraging supplementary information derived from the application of physical laws. This innovative technique is called the PINNs, which integrate traditional physical models with advanced ML algorithms (Wang and Lin, 2020; Karniadakis et al., 2021). PINNs ensure that simulations are not only data-driven but also adhere to fundamental physical laws, enabling more accurate and efficient predictions of complex phenomena (Fig. 9). By capturing the intricate behaviors and interactions within porous materials at multiple scales, this approach significantly enhances our ability to design and optimize energy storage processes. Recently, Physics-Informed Kolmogorov-Arnold Networks (PIKANs) have attracted attention due to their advantages over traditional PINNs, making them a powerful alternative for solving complex physics-governed problems (Jacob et al., 2024; Rigas et al., 2024; Toscano et al., 2024). The primary strength of PIKANs lies in their architecture, which is inspired by the Kolmogorov-Arnold representation theorem. Unlike standard PINNs that rely on deep fully connected networks to approximate solutions to differential equations, PIKANs decompose the solution space into a hierarchical structure, enabling a more interpretable and efficient representation of complex functions. This decomposition reduces the number of required parameters, leading to faster convergence and improved generalization, particularly in high-dimensional problems where PINNs often struggle due to the curse of dimensionality. Traditional PINNs operate as black-box models, where the learned functions lack transparency and do not explicitly reveal the underlying structure of the solution (Toscano et al., 2024). PIKANs, however, leverage the Kolmogorov-Arnold structure to provide a more modular and hierarchical break-

Table 1. Comparison of different approaches for multiscale modeling.

Approach	Advantages	Limitations	Potential Applications
Hybrid multiscale Simulation	- Captures physics across multiple scales - Accurate representation of pore- and continuum-scale processes	- High computational cost - Requires sophisticated coupling strategies	- Multiphase flow in porous media - CO_2 sequestration - Hydrocarbon recovery modeling
Approximated physics	- Reduces computational complexity - Provides stable solutions for complex nonlinear systems	- Potential loss of physical fidelity - May require calibration with full-physics models	- Reactive transport modeling - Enhanced oil recovery simulations - Large-scale reservoir modeling
HPC	- Enables large-scale, high-resolution simulations - Supports real-time data processing	- Requires significant computational resources - Can be expensive and energy-intensive	- High-resolution energy storage simulations - Large-scale multiphase flow modeling
ML-assisted simulation	- Accelerates computation using surrogate models - Can learn complex patterns from data	- Requires large training datasets - Limited interpretability in some cases	- Data-driven reservoir modeling - Uncertainty quantification - CO_2 and hydrogen storage forecasting

down of the target function, allowing for better physical insight and easier identification of dominant patterns in the learned representations. This aspect is particularly beneficial in fields like porous media flow, subsurface transport, and geophysical modeling, where understanding the interactions between variables is crucial for improving predictive accuracy. In addition, computational efficiency is another area where PIKANs outperform PINNs. The hierarchical nature of PIKANs ensures that the network learns low-dimensional representations effectively before reconstructing the full function, leading to better-conditioned optimization problems and reducing the likelihood of vanishing or exploding gradients that commonly hinder deep PINNs architectures. Furthermore, PIKANs demonstrate improved robustness in handling multiscale problems, a domain where PINNs often require extensive tuning of hyperparameters and network depth to capture small-scale features. Since PIKANs break down complex mappings into simpler sub-functions, they naturally accommodate multiscale structures without excessive parameterization.

Table 1 shows the comparison of different approaches for multiscale modeling for multiphase flow and reactive mass transport in porous media. Hybrid multiscale simulations provide a rigorous framework for capturing physics across multiple scales, accurately representing pore- and continuum-scale interactions. However, their high computational cost and the necessity for sophisticated coupling strategies make them challenging to implement for large-scale reservoir simulations. In contrast, the approximated physics approach aims to reduce computational complexity by simplifying governing equations while maintaining stability and accuracy. Although these methods enhance computational efficiency, they may sacrifice physical fidelity and often require calibration with full-physics models to ensure reliability.

HPC has significantly expanded the capabilities of multiscale simulations by enabling high-resolution, large-scale modeling through parallel computing and GPU acceleration. While HPC facilitates real-time data processing and enhances the accuracy of multiphase flow and reactive transport simulations, it demands substantial computational resources, making it costly and energy-intensive. Meanwhile, machine-learning-assisted multiscale simulations offer a promising alternative by leveraging surrogate models and data-driven approaches to accelerate computations. These methods excel in pattern recognition, uncertainty quantification, and real-time forecasting but require extensive training datasets and may suffer from limited interpretability. Ultimately, the choice of modeling approach depends on the specific application, balancing accuracy, computational efficiency, and scalability for challenges such as CO_2 sequestration, hydrogen storage, and enhanced oil recovery.

4. Challenges and perspectives

Although significant advancements have been made in multiscale modeling for multiphase flow and reactive transport in porous media, several critical challenges persist. Addressing these issues is essential to improving model accuracy, computational efficiency, and practical applicability in subsurface energy storage and carbon sequestration.

4.1 Robust coupling techniques

A key difficulty in coupling techniques arises from the inherent scale separation between microscopic and macroscopic processes. Traditional numerical methods, such as finite difference or finite element approaches, struggle to resolve fine-scale details without significantly increasing computational expense (Soulaine, 2024). On the other hand, upscaling techniques like volume averaging or homogenization simplify fine-scale processes but often fail to preserve essential microscale heterogeneities, leading to errors in macroscopic predictions (Zhang et al., 2021). The complexity is further exacerbated in reactive transport problems, where chemical reactions occurring at the pore scale can have a significant impact on macroscopic flow behavior. If these interactions are not accurately accounted for, the model may fail to capture important phenomena such as mineral precipitation, dissolution, or wettability alteration, all of which influence the long-term performance of subsurface energy storage systems.

In addition, the nonlinearity is introduced by multiphase interactions, phase changes, and geochemical reactions (Cai et al., 2024). In highly heterogeneous reservoirs, fluid flow and reaction kinetics vary significantly across different rock formations, requiring adaptive modeling approaches. However, ensuring numerical stability while capturing these complex interactions remains a major hurdle, particularly when dealing with large-scale simulations with millions of computational grid cells.

To overcome these challenges, research efforts are focused on developing more robust and efficient coupling strategies that balance computational feasibility with model accuracy. Hybrid multiscale simulation techniques offer a promising solution by integrating continuum-based approaches with discrete models, allowing for localized fine-scale resolution while maintaining computational efficiency. For example, hybrid schemes can employ pore-network models to resolve microscale interactions in specific regions of interest while using continuum-based solvers for large-scale flow simulations. This approach reduces computational costs while preserving critical fine-scale details. The study by Korneev and Battiato (2016) on the homogenization of pore-scale reactive transport models is an example of how advanced mathematical techniques can be used to derive effective parameters for Darcy-scale simulations from detailed pore-scale data. In addition, the advancement of adaptive multiscale methods, where model resolution dynamically changes based on local conditions, also provides one possibility to resolve these challenges. For instance, fine-scale simulations can be triggered in regions experiencing rapid phase transitions or chemical reactions, while coarser grids are used in less dynamic regions. This adaptive refinement approach ensures that computational resources are allocated efficiently without sacrificing accuracy in critical areas. Despite advancements in modeling frameworks, bridging the gap between scales while preserving the fidelity of the underlying physics remains an ongoing research frontier (Blunt et al., 2013; Lasseux et al., 2016; Soulaine, 2024).

4.2 Balancing model complexity and computational feasibility

High-fidelity models strive to capture detailed physics, such as interfacial tension effects, pore-scale transport phenomena, geochemical reactions, and phase behavior, to enhance predictive accuracy. However, incorporating such intricate details into large-scale reservoir simulations leads to significant computational demands, often rendering these models impractical for real-world applications. A major challenge arises from the need to resolve fine-scale heterogeneities in porous media, such as fractures, grain boundaries, and capillary interactions, while maintaining computational efficiency at the reservoir scale (Duran et al., 2021). Traditional fully coupled numerical methods, including finite element and finite volume approaches, become prohibitively expensive when applied to large domains with high resolution. Additionally, reactive transport processes introduce strong nonlinearities due to coupled chemical reactions, which further increase the computational cost by requiring small time steps and fine spatial discretization (Abd and Abushaikha, 2021; Baqer and Chen, 2022).

Approximated physics methods offer a way to alleviate the computational burden by simplifying governing equations, reducing the number of variables, or employing surrogate models to approximate fine-scale processes. However, the challenge lies in ensuring that these approximations do not introduce significant errors that undermine model reliability. Simplified reaction networks, for example, may fail to capture critical reaction pathways that influence long-term system behavior (Abd and Abushaikha, 2021; Ladd and Szymczak, 2021). Similarly, reduced-order models, while computationally efficient, often struggle to generalize beyond the conditions under which they were trained (Ardakani et al., 2024). Finding the right balance between model simplification and physical realism remains a key challenge in multiscale modeling. Moreover, real-world applications require models to be adaptable to different reservoir conditions, such as variations in rock properties, fluid compositions, and operating conditions. Fixed-resolution models may either be too computationally expensive for large-scale simulations or too simplistic to capture essential dynamics. Developing a modeling framework that dynamically adjusts its complexity based on local conditions is crucial for improving both efficiency and accuracy.

Adaptive resolution techniques, where model complexity varies depending on local flow conditions and reaction rates, is one possible way to achieve this goal (Liu and Zhang, 2021; Yang et al., 2021). For example, fine-scale resolution can be selectively applied to regions experiencing rapid phase transitions or strong chemical reactions, while coarser grids are used in less dynamic regions. This approach significantly reduces computational costs without sacrificing accuracy in critical areas. Adaptive meshing techniques, such as dynamic grid refinement and coarsening, offer a practical way to implement this concept in large-scale simulations. Hybrid modeling, another promising approach, combines high-fidelity and reduced-order models in a single framework (De Santis et al., 2021; Li and Voskov, 2021). In this strategy, detailed physics-based models are used in regions where high accuracy is required, while simplified surrogate models approximate less critical areas. Hybrid multiscale methods, such as domain decomposition techniques, enable the seamless transition between different levels of model complexity, ensuring computational efficiency without compromising essential physical details (Tang et al., 2021a).

4.3 Machine-learning integration

The integration of ML into multiscale modeling for subsurface flow and reactive transport has emerged as a powerful tool to enhance computational efficiency and predictive accuracy. However, several fundamental challenges must be addressed to ensure the reliability and practical application of ML in large-scale subsurface simulations.

One of the primary challenges is the lack of interpretability in deep learning models. Traditional physics-based models are built on well-established equations governing multiphase flow and transport processes, providing transparency and explainability in their predictions (Yan et al., 2022). In contrast, ML models, especially neural networks, function as black boxes, making it difficult to understand their decision-making process. This opacity raises concerns regarding their applicability in critical scenarios, such as reservoir management, carbon sequestration, or groundwater remediation, where incorrect predictions could lead to costly or even hazardous consequences (Amini et al., 2022; Wu et al., 2023a; Jacob et al., 2024). Meanwhile, another major obstacle is the need

for extensive and high-quality training data. ML models require large datasets covering a wide range of conditions to generalize well to unseen scenarios. In subsurface modeling, generating such datasets is expensive and time-consuming, as it often involves running high-fidelity numerical simulations or collecting real-world experimental data. Moreover, many subsurface processes involve rare or extreme events, such as sudden permeability changes due to mineral precipitation or breakthrough of injected fluids, which are difficult to capture in training datasets. Data sparsity and distribution shifts between training and real-world conditions further degrade the predictive performance of the model (Wang et al., 2021a; Xu et al., 2022).

Additionally, ensuring generalizability across different geological formations, fluid properties, and operational conditions remains a significant challenge. ML models trained on a specific set of geological features may fail to extrapolate to reservoirs with different permeability distributions, fracture networks, or fluid compositions. Unlike traditional numerical solvers that incorporate governing equations applicable to a broad range of conditions, ML-based models often struggle with scenarios that deviate from the training distribution, leading to unreliable predictions. Hybridizing ML with traditional physics-based approaches introduces new complexities. While PINNs and other hybrid models aim to incorporate fundamental physical principles into ML architectures, designing such models requires balancing data-driven learning with equation-driven constraints. Ensuring numerical stability and convergence in these hybrid approaches is still an active area of research.

One possible way to overcome this challenge is to develop physics-informed and hybrid machine-learning models that integrate prior physical knowledge into data-driven frameworks (Zhu et al., 2022; Wu et al., 2023b). PINNs and other constrained ML techniques enforce governing equations as part of the learning process, reducing reliance on extensive training data and improving generalizability. By embedding physics-based loss functions, these models can ensure that predictions adhere to fundamental conservation laws, enhancing their reliability in real-world applications. In this process, we also can develop the adaptive fusion of ML models with numerical solvers, where ML accelerates certain computationally expensive components (such as subgrid-scale physics or iterative solvers), while traditional numerical techniques ensure robustness and accuracy (Kochkov et al., 2021). For example, ML can be used to rapidly approximate fine-scale permeability fields or reaction rates, while finite-volume or finite-element solvers handle macroscopic flow and transport equations. This approach retains the interpretability of physics-based models while benefiting from ML's efficiency.

Transferring learning and domain adaptation strategies to enhance model generalizability is also one promising way to improve the performance of ML (Oyewole et al., 2022). By pre-training ML models on a diverse set of simulated or experimental datasets and fine-tuning them for specific reservoirs, ML-assisted simulations can become more adaptable to varying geological conditions. Synthetic data augmentation techniques, such as generative adversarial networks, can also be explored to enrich training datasets and improve the robustness of ML predictions. Moreover, uncertainty quantification techniques must be incorporated into ML-assisted subsurface models to assess the confidence level of predictions. Bayesian neural networks and ensemble learning methods can help quantify uncertainties, providing insights into when ML predictions are reliable and when they require correction via traditional numerical solvers (Yin et al., 2021; Abbaszadeh Shahri et al., 2022).

5. Summary

Multiscale modeling techniques tailored for the comprehensive understanding of multiphase flow and reactive mass transport phenomena within porous media are crucial for subsurface energy storage. Great advances have been achieved in recent years, e.g., hybrid multiscale simulation, approximated physics, and machine-learning-assisted multiscale simulation, elucidating their respective merits and challenges in enhancing both the precision and computational efficiency of modeling endeavors. Despite significant strides, persistent hurdles such as the refinement of coupling methodologies, the delicate equilibrium between model intricacy and computational tractability, and the fusion of ML algorithms with physical models are acknowledged. Consequently, prospective avenues for surmounting these challenges, with the ultimate goal of expanding the horizons of multiscale modeling capabilities, are still to be resolved.

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Conflict of interest

The authors declare no competing interest.

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