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Perspective

Multi-scale molecular simulation methods in energy storage systems

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Abstract:
Multi-scale molecular simulation methods, integrating Molecular Dynamics (MD) and Monte Carlo (MC) techniques, have emerged as transformative tools for studying complex fluid behaviors in nanoporous media. This perspective highlights the synergy between MD's atomistic precision and MC's statistical efficiency, enabling accelerated simulations of rare events and large-scale systems. Applications span energy storage (shale gas adsorption, CO_2 sequestration, hydrogen leakage mitigation), demonstrating the versatility of these methods. Key innovations include spatial-temporal coarsening strategies and novel state definitions that balance computational speed with accuracy. Challenges such as error propagation in coarsening and force field limitations are discussed, alongside future directions leveraging machine learning and multi-physics integration.

1. Introduction

Molecular-scale phenomena underpin critical challenges in energy storage engineering, from underground carbon sequestration to hydrogen gas leakage (Feng et al., 2024). Traditional Molecular Dynamics (MD) simulations provide unparalleled atomic resolution but falter when simulating rare events or large systems due to high computational costs. Monte Carlo (MC) methods, while efficient in sampling equilibrium states, lack the dynamics needed to model non-equilibrium processes. The integration of MD and MC into a Multi-Scale Monte Carlo Markov Chain (MDMC) framework addresses these limitations by synergizing MD's precision with MC's statistical efficiency (Liu et al., 2022).

MDMC promotes the understanding of fluid behavior in confined geometries, such as shale nanopores, where pore sizes and surface chemistry dictate gas storage and transport. For instance, methane adsorption in kerogen, a process spanning picosecond-scale molecular vibrations to large scale diffusion, requires a multi-scale approach to resolve both atomic interactions and macroscale trends. Similarly, hydrogen leakage through caprock defects, governed by nanoscale water-clay interactions and micrometer-scale defect geometries, demands a multi-scale simulation strategy. Recent advances in spatial-temporal coarsening and adaptive state definitions have further enhanced the framework's versatility. By dynamically merging states or aggregating time steps, the method achieves orders-of-magnitude speed-ups while preserving essential physics. This perspective explores the algorithmic innovations behind these advances and applications in energy storage, and emerging opportunities to tackle unresolved challenges in computational molecular science.

2. Multi-scale MDMC framework

The Multi-Scale MDMC framework is a computational paradigm that seamlessly integrates the precision of MD with the statistical efficiency of MC methods, enabling the simulation of complex molecular behaviors across spatial and temporal scales (Liu et al., 2022). The framework begins with MD simulations to generate high-resolution trajectories of molecular interactions, capturing phenomena such as van der

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Waals forces, electrostatic interactions, and hydrogen bonding with femtosecond-level accuracy. For instance, in studies of shale gas adsorption, MD models the intricate behavior of methane molecules within kerogen nanopores, revealing how they adhere to hydrophobic aromatic clusters or compete with CO_2 for binding sites. These atomistic trajectories are then discretized into discrete states defined by spatial coordinates, energy minimum, or velocity directions. In hydrogen leakage studies, states might classify molecules as ”trapped in water clusters,” ”adsorbed on clay surfaces,” or ”free in bulk gas,” allowing precise tracking of H_2 migration through caprock defects. The transition probabilities between these states are extracted from MD trajectories to construct a probability transition matrix, which forms the basis of the MC phase. Spatial coarsening merges adjacent states-such as combining multiple nanopores into a single mesoscale region-to reduce computational complexity while preserving critical dynamics. Temporal coarsening aggregates steps by raising the transition matrix to a power, enabling predictions of rare events like CO_2 diffusion over geological timescales. Validation is achieved through rigorous comparisons: residence times of methane in kerogen pores or spatial distributions of CO_2 derived from MD and MC simulations must align within a 5% error margin. Adaptive algorithms further refine the framework by dynamically adjusting coarsening levels-retaining atomic resolution in high-stakes regions while employing coarser grids in larger pores to optimize computational efficiency. This approach bridges the gap between nanosecond-scale molecular vibrations and macroscopic system behaviors, offering a unified tool to explore phenomena that span orders of magnitude in space and time.

3. Energy storage applications

The Multi-Scale MDMC framework has revolutionized the design and optimization of energy storage systems, particularly in subsurface environments where nanoscale interactions dictate macroscopic performance. In shale gas reservoirs, the method unravels how methane molecules diffuse into the pores of kerogen-a process governed by hydrophobic interactions and pore-size heterogeneity. MD simulations reveal that methane preferentially adsorbs to aromatic clusters in kerogen, while MC models predict long residence times in sub-2-nm pores, identifying these regions as ”trapping zones” critical for storage. By spatially coarsening atomic-scale states into mesoscale states, the framework reduces simulation time for hundreds of times without sacrificing accuracy, enabling to map methane distribution to larger scales. Similarly, in CO_2 sequestration (Cao et al., 2024), the framework captures how CO_2 injection compresses kerogen matrices, increasing porosity and homogenizing pore size distributions (Liu et al., 2024a). MD simulations show that CO_2 disrupts kerogen's hydrophobic networks, creating 0.5–1 nm pores, while MC models project CO_2 migration pathways over large scales, highlighting that high temperatures enhance mobility but destabilize storage by promoting thermal expansion. Practical insights emerge injecting CO_2 minimizes leakage while maximizing storage density. For hydrogen storage, the framework addresses the challenge of H_2's ultra-small molecular size, which allows rapid leakage through caprock defects (Liu et al., 2024b; Wu et al., 2024). MD simulations identify that water clusters, stabilized by hydrogen bonds, physically block 0.5-nm pores, while MC models quantify how residual methane forms adsorption layers on clay surfaces, reducing H_2 leakage. These findings translate to actionable strategies-mixing H_2 with water during injection seals nanopores, cutting leakage and enabling safe storage in depleted shale formations. By resolving atomic-scale interactions and scaling to system-level predictions, the framework empowers the design of efficient, stable energy storage systems, from unconventional gas reservoirs to next-generation hydrogen caverns.

4. Conclusions

Multi-scale molecular simulations have revolutionized our ability to probe intricate processes in energy, from gas adsorption in shale nanopores to hydrogen storage integrity. By harmonizing MD's resolution with MC's efficiency, these methods unlock insights into previously intractable problems. Future advancements hinge on overcoming coarsening artifacts and integrating multi-physics phenomena. As computational power grows and algorithms evolve, multi-scale approaches will remain pivotal in addressing global challenges in sustainable energy engineering. The challenges can be summarized as follows two aspects.

1) Coarsening introduces approximation errors, particularly in heterogeneous systems. Adaptive coarsening algorithms, guided by machine learning, could dynamically optimize spatial-temporal resolution.
2) Coupling fluid dynamics, thermal effects, and geomechanical stresses (e.g., in subsurface reservoirs) requires scalable multi-scale frameworks.

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Conflict of interest

The authors declare no competing interest.

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