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Machine learning accelerated molecular simulation: Implications for oil and gas problems

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In the last few decades, deep learning (DL) has afforded solutions to macroscopic problems in petroleum engineering, but mechanistic problems at the microscale have not benefited from it. Mechanism studies have been the strong demands for the emerging projects, such as the gas storage and hydrate production, and for some problems encountered in the storage process, which are common found as the chemical interaction between injected gas and mineral, and the formation of hydrate. Emerging advances in DL technology enable solving molecular dynamics (MD) with quantum accuracy. The conventional quantum chemical method is computational expensive, whereas the classical MD method cannot guarantee high accuracy because of its empirical force field parameters. With the help of the DL force field, precision at the quantum chemistry level can be achieved in MD. Moreover, the DL force field promotes the computational speed compared with first-principles calculations. In this study, the basic knowledge of the molecular force field and deep neural network (DNN) is first introduced. Then, three representative open-source packages relevant to the DL force field are introduced. As the most common components in the development of oil and gas reservoirs, water and methane are studied from the aspects of computational efficiency and Chemical reaction respectively, providing the foundation of oil and gas researches. However, in the oil and gas problems, the complex molecular topo structures and various element types set a high challenge for the DL techniques in MD. Regarding the computational efficiency, it needs improvement via GPU and parallel accelerations to compete with classical MD. Even with such difficulties, the booming of this technique in the area of petroleum engineering can be predictable.

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References

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