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Controllable generation of porous media hybrid multiple-point statistics and sliced Wasserstein metric

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Porous media have a wide range of applications in various engineering fields. Accurate modeling microstructure of porous media is the basis for subsequent numerical analyses and structure–property relationship researches. Computational reconstruction methods play an important role in these studies, can address limitations of some imaging techniques that are difficult to directly model three-dimensional (3D) structures, such as 2D-to-3D microstructure reconstruction and specific structure generation, and provide a fast and efficient way to model microstructures. Current computational reconstruction methods include traditional methods and machine learning-based (or deep learning-based) methods. Compared with traditional methods, machine learning-based computational reconstruction methods show advantages in reconstruction accuracy and speed. However, such machine learning-based methods also have limitations in interpretability, controllability, generalization, and small data sample application, which make it difficult to deal with various reconstruction tasks. In the previous study, we developed a hybrid method combining multiple-point statistics and machine learning, which is capable of handling 2D-to-2D, 2D-to-3D, and 3D-to-3D reconstruction tasks. Whereas, there are still some limitations in dealing with controllable and conditional generation tasks.

To further improve the reconstruction performance, we propose a novel controllable generation method hybrid multiple-point statistics and sliced Wasserstein metric, design a controlled sampling strategy and a conditional reconstruction strategy, and make progresses in dealing with controllable and conditional generation tasks. In this method, multipoint statistical information is adopted for microstructure characterization and sliced Wasserstein metric and gradient optimization are used for microstructure reconstruction. The controlled sampling strategy enables microstructure generation for any given phase volume fraction, by sampling with purpose from multipoint statistical information of training images. While the conditional reconstruction strategy can generate different microstructures satisfying the condition data. In addition, the proposed method only requires a single data sample (a 2D image or a 3D structure) to complete the above tasks, which has advantages in controllability, generalization, and small sample data application. Finally, to verify the reconstruction performance of our method, multiple sets of experiments are performed on a variety of porous media images (e.g., porous rocks, silica materials, battery electrode materials, and synthetic ceramics), by generating microstructures with different phase volume fractions and condition data from a single data sample. Comparisons of visualization, statistical parameters such as two-point probability function and linear path function, and numerical analysis are adopted to further show the effectiveness of our reconstruction results.

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