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Research paper

Multi-thread parallel algorithm for reconstructing 3D large-scale porous structures

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ABSTRACT

Geomaterials inherently contain many discontinuous, multi-scale, geometrically irregular pores, forming a complex porous structure that governs their mechanical and transport properties. The development of an efficient reconstruction method for representing porous structures can significantly contribute toward providing a better understanding of the governing effects of porous structures on the properties of porous materials. In order to improve the efficiency of reconstructing large-scale porous structures, a multi-thread parallel scheme was incorporated into the simulated annealing reconstruction method. In the method, four correlation functions, which include the two-point probability function, the linear-path functions for the pore phase and the solid phase, and the fractal system function for the solid phase, were employed for better reproduction of the complex well-connected porous structures. In addition, a random sphere packing method and a self-developed pre-conditioning method were incorporated to cast the initial reconstructed model and select independent interchanging pairs for parallel multi-thread calculation, respectively. The accuracy of the proposed algorithm was evaluated by examining the similarity between the reconstructed structure and a prototype in terms of their geometrical, topological, and mechanical properties. Comparisons of the reconstruction efficiency of porous models with various scales indicated that the parallel multi-thread scheme significantly shortened the execution time for reconstruction of a large-scale well-connected porous model compared to a sequential single-thread procedure.

1. Introduction

Geomaterials inherently contain many discontinuous, multi-scale, geometrically irregular pores, forming a complex porous structure that governs their mechanical properties and transport behavior. For example, in the fields of geoscience and environmental engineering, the porous structures of geomaterials significantly influence the pressure accumulation and evolution in the earth's crust and are thus important for understanding tectonic processes such as earthquakes (David et al., 1994). The porous structure of reservoir rock determines its porosity and permeability, which are fundamental parameters for designing the strategies of natural oil and gas extraction (Cui et al., 2007; Hidajat et al., 2002; Van Bergen et al., 2004; Walls et al., 1982), CO_2 geological sequestration (Rutqvist and Tsang, 2002), and nuclear waste disposal (Tsang et al., 2005). Therefore, the development of an effective approach to specify and predict the properties of porous materials is of great significance.

In geoscience as well as geotechnical and mining engineering, experimental methods such as in-situ detection and laboratory investigation are usually employed to determine the specifications of porous geomaterials (Cai and Huai, 2010; Kainourgiakis et al., 2005; Liu et al., 2009). To achieve high accuracy in these determinations, sufficient rock samples must be acquired from geological formations and tested thoroughly. However, drilling rock samples from underground geological formations is technically challenging and expensive (Pilotti, 2000; Spanne et al., 1994). These experimental limitations make it difficult to accurately specify the deformation and failure of porous structures as well as their relation with the macroscopic properties of the geomater-

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ials (Cai and Huai, 2010; Kainourgiakis et al., 2005; Liu et al., 2009).

In order to overcome these experimental limitations, scientists and engineers have been seeking alternative specification and prediction methods, such as digital rock models to characterize the effects of porous structures on the properties of geomaterials. Such research has attracted considerable attention because it could enable one to probe and elucidate the physical properties of porous materials and their intrinsic mechanisms. A reliable 3D digital porous rock model would be a prerequisite for such studies. Many numerical reconstruction models are based on data from porous systems that are extracted using innovative techniques, such as an integrated focused ion beam and high-resolution scanning electron microscopy (FIB-SEM) (Chalmers et al., 2012; Keller et al., 2011b; Liu et al., 2010) and X-ray computed tomography (CT) (Karacan and Okandan, 2001; Masad et al., 1999; Werth et al., 2010; Wildenschild and Sheppard, 2013). However, performing these methods for three-dimensional (3D) porous model acquisition is expensive and time-consuming, which is usually unacceptable in engineering applications (Ju et al., 2014a, 2014b).

As supplementary methods for experimentally obtaining the porous structure, several computer reconstruction methods have been proposed, such as statistical information-based methods (Bodla et al., 2014; Fullwood et al., 2008; Okabe and Blunt, 2005; Torquato, 2002; Yeong and Torquato, 1998b), process-based methods (Arns et al., 2003; Øren and Bakke, 2002), hybrid method (Politis et al., 2008), fractal-theory-based methods (Latief et al., 2010), and pore network models (Jiang et al., 2013, 2012). Among the existing 3D reconstruction methods, the method proposed by Yeong-Torquato (Y-T) (Yeong and Torquato, 1998a), which combines correlation functions with simulated annealing algorithms (SAA), has been adopted by many researchers to reconstruct 3D porous structures. This method facilitates the reconstruction of different types of rock models with specific statistical functions (Čapek et al., 2011; Gerke and Karsanina, 2015; Gerke et al., 2015, 2014; Havelka et al., 2016; Jiao et al., 2007, 2009, 2008; Karsanina et al., 2015; Torquato, 2002). The drawback of this method is that it struggles to represent porous structures with high connectivity if only low-order correlation functions are applied, such as the porosity function or the two-point probability function. To address this problem and to improve the accuracy and efficiency of the reconstructed models, some investigators have incorporated high-order statistical functions into the reconstructions, including the linear-path function for the pore phase in orthogonal directions (Yeong and Torquato, 1998b), a more directional linear-path function for both phases (Gerke and Karsanina, 2015; Gerke et al., 2014; Karsanina et al., 2015), chord-length distributions (Kainourgiakis et al., 2005), the pore size distribution function (Eschricht et al., 2005), the fractal system correlation function (Ju et al., 2014b), and the two-point cluster function (Jiao et al., 2009; Karsanina et al., 2015). Incorporation of these correlation functions improves the reconstruction accuracy to some extent.

Our preliminary study had indicated that incorporating fractal system correlation functions in the Y-T method could improve the reconstruction accuracy of well-connected 3D porous structures having a size of 352×352×70 voxels (Ju et al., 2014b). A comparison of the reconstructed and reference models shows a high degree of consistency in terms of their correlation functions, geometry, topology, and mechanical properties. However, the problem of time-consuming reconstruction persists. In spite of improvements in the initial model casting and later stage control over point selection, the major part of the Y-T method controlling the interchanging of points requires a considerable amount of time. In addition, an increasing in the reconstructed model size leads to a sharp increase in the computational time. Because the model is updated with two points in the interchanged positions at each instance, the statistical correlation functions must be updated to determine whether the interchange can be accepted. As the model size increases, the interchanging time increases exponentially.

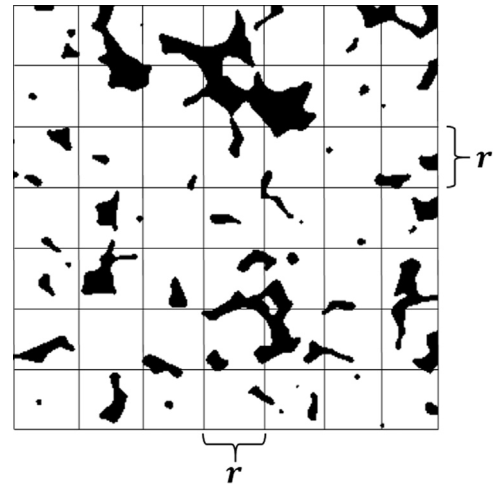

Fig. 1. Determination of fractal correlation function using box-counting method.

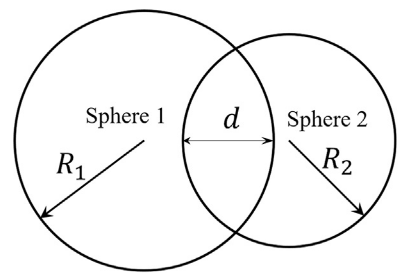

Fig. 2. Overlapping spheres in the random sphere packing method, $d \le 1.5R_2$ ($R_2 \le R_1$).

The low efficiency of the Y-T method in these situations has become a major obstacle to reproducing large-scale well-connected porous rock models.

In this study, we aim to improve the reconstruction efficiency of the Y-T method by using a parallel computing scheme. In the Y-T method, numerous interchanges of voxel pairs are performed sequentially to evolve the reconstructed model. Whether the interchanging of a pair of voxels is accepted is determined by its influence on the statistical correlation function values. The most time-consuming part in the reconstruction is the determination of the correlation function values. In most previous model reconstructions, the correlation function values have been calculated in certain directions for simplicity (Gerke and Karsanina, 2015; Gerke et al., 2014; Ju et al., 2014b; Karsanina et al., 2015; Yeong and Torquato, 1998b). Similarly, the correlation function values have been calculated in orthogonal directions in our previous study (Ju et al., 2014b). In this case, interchanging points with different coordinates in the X, Y, and Z directions have independent effects on the correlation function values. In other words, their effects can be superimposed to determine the changes in the correlation function values of the system status. This is the cornerstone of developing our parallel algorithm. Based on this fact, the multi-thread technique is used to compute the effects of different pairs of interchanging points on the system status in a parallel manner; then, these effects are superimposed. This method exploits modern multicore computers to speed up the reconstruction process.

The computational efficiency of the newly developed parallel algorithm is compared with that of the program using the standard sequential algorithm. Moreover, the reliability of the reconstructed model is evaluated by comparing it with a prototype model obtained from CT scanning, in terms of their statistical properties, geometrical parameters, and mechanical properties.

The remainder of this paper is organized as follows. Section 2 details the general reconstruction procedure. Section 3 introduces the