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Improved pore network models to simulate single-phase flow in porous media by coupling with lattice Boltzmann method

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A B S T R A C T
In this paper, different pore network models to simulate single-phase flow in porous media are built and their accuracy is evaluated. In addition to the conventional pore network model (CPNM) which consists of regular pore bodies and throat bonds, three improved pore network models (IPNMs) are developed allowing to better describing the real pore and throat geometry. The first improved pore network model (IPN1M) replaces the regular throat bond with a throat bond showing the real throat cross section. The second improvement (IPN2M) uses a series of sub-throat bonds with varying cross sections to better describe the real throat geometry, which is firstly proposed in this paper. The third model (IPN3M) extracts the real pore-throat-pore geometry without simplification. The conductance of fluid flow through these more realistic throat bonds is calculated by the lattice Boltzmann method (LBM). The accuracy and computational efficiency of the different pore network models are evaluated taking the LBM simulation over the whole porous medium as reference solution. The global permeability and detailed pressure distributions in the pores for the different pore network models are validated. The results show that the accuracy of the pore network model increases from CPNM to IPN3M, but at the expense of increasing computational cost. This study suggests that IPN3M can replace a whole-domain LBM simulation with similar accuracy but much lower computational cost. As a first-order approximation the newly proposed IPN2M is suggested as good compromise between accuracy and computational cost.

1. Introduction
Permeability is an important property characterizing fluid flow in porous media. It can be obtained mainly in three ways: by experiments, using analytical models or numerical simulation at pore scale. Although experimental testing is straightforward, it has some limitations (Gerke et al., 2018) such as measurement errors and the inability to determine the real flow regime in the porous medium. Analytical models predict the permeability based on physical properties of the porous media. The Kozeny-Carman (K-C) equation (Carman, 1939) is the most-used analytical model for permeability prediction, which is derived through simplifying the complex porous medium into a simple capillary bundle model. The original K-C model has many limitations as it only considers porosity and specific surface area. Later it has been modified for different kinds of porous media taking into account more detailed pore geometry information (Nishiya and Yokoyama, 2017; Xu and Yu, 2008). However, the topology and heterogeneity of the pore structure, which have a significant influence on permeability, cannot be properly accounted for in these analytical models. In recent years, the development of imaging techniques, namely X-ray computer tomography (CT) (Schlüter et al., 2014) has enabled to document the real pore structure of porous media. With this information, pore-scale numerical methods can be used to calculate permeability and study the influence of pore geometry on permeability.

There are different kinds of numerical methods at pore scale to simulate single-phase flow in porous media, mainly including direct numerical methods (DNM), pore network models (PNM) and hybrid methods combining these two in some manner. DNM simulates fluid flow directly in the real porous structure. The lattice Boltzmann method (LBM) is a commonly used direct numerical method for fluid flow in porous media because of the following advantages: (a) ease of programming; (b) natural suitability for parallel computing; (c) ease of dealing with complex solid boundaries (Qin et al., 2019). In pioneering work, Succi et al. (1989) firstly adopted LBM to simulate single-phase flow in three-dimensional complex porous media. As the simulation could recover Darcy’s law, this work was groundbreaking towards using LBM for rocks and other porous media. Since then, LBM has been more widely adopted to simulate fluid flow in different kinds of porous geometries (Nabovati et al., 2009; Okabe and Blunt, 2004). The relationships between permeability and pore structures were widely investigated (Bosl et al., 1998; Kang et al., 2003; Matyka et al., 2008; Nabovati et al., 2009; Van Doormaal and Pharoah, 2009;
Zhao et al., 2020a, 2016), which can be used for macroscopic flow simulations or analysis of flow mechanisms. For example, Sun et al. (2017) proposed to analyze the gas transport patterns in shale rocks based on LBM simulation results. Noteworthy is the work of Pan et al. (2006) reporting that the intrinsic permeability obtained by single-relaxation-time (SRT) LBM is strongly dependent on fluid viscosity, which is unphysical. This deficiency can be significantly controlled by multi-relaxation-time (MRT) LBM. LBM is in fact a Navier-Stokes (N-S) solver as the N-S equation can be recovered by LBM (He and Luo, 1997). For low speed creeping flow, which usually happens in porous media, the N-S equation can be simplified to the Stokes equation.

Another direct numerical method is to solve the N-S equation or Stokes equation directly in porous media using the finite element (FEM) (Borujeni et al., 2013), finite volume (FVM) (Guilbert et al., 2015) or finite difference (Mostaghi et al., 2013; Zhu et al., 2019) methods. The governing equation can be further simplified in order to avoid solving the N-S or Stokes equations and improve the computational efficiency. Shabro et al. (2012) and Chung et al. (2019) characterized the fluid flow resistance or conductivity in each pore voxel using two parameters, namely the distance to the pore wall and the largest inscribed radius of the corresponding pore. Then the simplified elliptic flow equation is solved using the FDM or FVM directly on the micro-CT images. The obtained permeability is within acceptable error compared with that of other more accurate solvers. Arns et al. (2018) used a Laplace solver using only the Euclidean distance map to calculate the local conductivity of each voxel, which is a fast and stable approach even under low spatial resolution. These methods were later combined with dual grid domain decomposition method (Du Wang et al., 2019) or voxel agglomeration method (Chung et al., 2019a) to further improve the computational efficiency. Although such numerical methods are promising in calculating the permeability of single-phase flow, their applicability to two-phase flow simulation is still unclear.

Pore network models (PNM) belong to another type of pore-scale numerical method, which are much more computationally efficient than direct numerical methods (Blunt et al., 2013). Instead of simulating fluid flow directly in real pore structures, PNM simulates fluid flow in networks of simplified pores, which are constructed based on real pore geometry of porous media. The complex pore structures are simplified into regular pore bodies connected by throat bonds. In conventional PNM, the cross sections of the pore bodies and throat bonds are described by circles, squares, triangles or other regular geometries. The fluid transport properties in such simple pore bodies and throat bonds can be calculated by analytical or empirical expressions (Lal et al., 2019; Oren et al., 1998; Rajaram et al., 1997; Valvatne, 2004). This significantly reduces the computational cost. On the other hand, the conductance predicted with simplified pore bodies and throat bonds is less accurate than with a description based on the real pore geometry, leading to errors in the predicted transport properties of the porous medium.

As described above, DNMs can accurately capture the details of pore structures at the expense of computational efficiency. On the contrary, PNM is computationally less but accurate in accounting for the effect of real pore geometry on fluid flow. In recent years, some hybrid methods have been developed which combine the strengths of both PNM and DNMs. For single-phase flow in porous media, the flow resistance increases in more constricted channels, which means that the throats with smaller cross sections account for most of the flow resistance. Therefore, it is essential to describe the throat geometry as accurate as possible. As a result, different improvements of pore network models have been proposed using a more realistic representation of the throat bonds. Miao et al. (2017) and Rabbani et al. (2019) extracted throat bonds with real throat cross sections instead of using regular shapes for pore network simulation. Then DNMs were used to calculate the conductance of these real throat bonds. In addition, neural network models are developed to derive correlations between throat geometry information and conductance based on a large number of simulations. Sholokhova et al. (2009) and Van Marcke et al. (2010) extracted the pore-throat-pore elements without any geometry simplification and used DNMs to simulate single-phase flow and calculate the conductance in each element. The obtained conductances are in turn introduced into PNM to calculate the permeability of the whole porous medium. This kind of pore network models, which uses more accurate geometry information, yields a more accurate prediction of the permeability compared with CPNM, while the computational cost is lower compared to DNMs. In addition, the improved pore network models can be easily extended to two-phase flow simulations. Recently, Zhao et al. (2020b) extended the improved pore network model with real throat cross section to two-phase drainage flow simulation, which showed better prediction results than the CPNM.

It is true that with modern high performance clusters a highly optimized LBM code can simulate single-phase flow in real porous structures rather fast. One exception is when the porous structure is very tight, it is hard for the LBM to converge. At such conditions, an accurate PNM becomes a good option to calculate the permeability. For example, Song et al. (2016) proposed a unified apparent permeability calculation model for shale gas reservoir by incorporating various transport mechanisms, which was used in PNM simulations. In addition, for two-phase flow in porous media, LBM can be much more computational expensive and the advantage of PNM becomes more significant. The dynamic PNM can be used to simulate two-phase flow in porous media taking into account both the capillary force and viscous force (Joekar-Niasar et al., 2010). In dynamic PNM for two-phase flow, single-phase PNM is used to calculate the pressure distributions in the wetting and non-wetting phases while maintaining a capillary pressure between the two phases (e.g. Joekar-Niasar et al., 2010). Accurate pressure distribution is needed as this information is used to update the phase distribution. However, to our knowledge, there is still no research reporting on the accuracy of using single-phase PNM to simulate pressure distribution. Therefore, we focus on improved pore network models to simulate single-phase flow in porous media in this work. We not only evaluate the improvements in terms of calculating the permeability but also the detailed fluid pressure distribution.

Four pore network models are evaluated in this work including the conventional PNM and three improved PNsMs. For the improved pore network models, in addition to using throat bonds showing real throat cross section and the real pore-throat-pore geometry without simplification, we propose a third option with a new hybrid PNM approach, which uses serial sub-throat bonds with real throat cross sections to describe the cross section variation between two pore bodies. The paper is arranged as follows. In Section 2, we introduce different pore network extraction methods. In Section 3, the numerical methods are introduced, including the multi-relaxation-time lattice Boltzmann model, the conventional pore network model and the three improved pore network models. The coupling procedure between LBM and PNsMs is described in detail. In Section 4, the performance of the different PNsMs to predict the permeability and pressure distributions is discussed in detail. Finally, conclusions are summarized in Section 5.

2. Pore network extraction

There are different methods to extract a pore network from a real porous geometry, such as the medial axis based method (Lindquist et al., 1996), maximum ball based method (Dong and Blunt, 2009), watershed based method (Gostick, 2017; Rabbani et al., 2014). In this work, we use the watershed method to decompose the porous media into sub-pore regions and extract the pore network.

In addition to the conventional pore network model, three different improved pore network models are presented in this work, as shown in Fig. 1. Firstly, the porous medium is decomposed into sub-pore regions using the watershed method, which has been implemented in the open-source algorithm SNOW (Gostick, 2017). This algorithm includes four steps. First step is to obtain the distance map and apply a Gaussian filter to remove some fake watershed ridge lines. Then a maximum filter is
applied to eliminate peaks on saddles and plateaus. We set the standard deviation of Gaussian filter as 0.4 and the radius of structuring element as 5 in this work. Next, the peaks close to each other are merged into one peak. Finally, the porous medium is segmented into sub-pore regions. More details about this algorithm can be found in (Gostick, 2017). Using the watershed method, the pore space is split into sub-pore regions, as illustrated in Fig. 1(b). Each identified sub-pore region corresponds to a pore body in the extracted pore network. The sub-pore regions are connected with narrow interfaces, which correspond to the throat bonds in the pore network.

2.1. Conventional pore network extraction with simplified pore and throat geometry

In the conventional pore network model (CPNM), both pore bodies and throat bonds are simplified into regular geometries under some constraints, as shown in Fig. 1(c). In this work, all the pore bodies are taken as cubes, with the volume equal to that of the corresponding sub-pore region. Throats usually account for most of the flow resistance as they have much smaller cross sections than the pore bodies. Therefore, it is assumed that the pore bodies have no flow resistance and that all flow resistance is located at the throat bonds. Similar assumptions have been used in other research (Joekar-Niasar et al., 2010). The inscribed radius \( r_{in} \) and shape factor \( G \) of the throat cross sections are adopted to simplify the real throat cross sections into regular geometries such as circle, square and triangle (Valvatne, 2004). The inscribed radius \( r_{in} \) is defined as the radius of inscribed circle in the throat cross section. The shape factor \( G \) is defined as \( A/P^2 \), where \( A \) and \( P \) are the area and perimeter of the throat cross section, respectively. Based on \( G \), the throat cross sections can be simplified into triangle \((G \leq \sqrt{3}/36)\), square \((\sqrt{3}/36 < G \leq 1/16)\) and circle \((G > 1/16)\), respectively. After the geometry simplification, the parameters \( A \) and \( P \) of the throat bonds are recalculated based on the simplified cross sections. The length of throat bonds is calculated by \( L_{ij} = r_{ni} - r_{nj} \), where \( L_{ij} \) is the distance between the centroids of the connecting two pore bodies, \( r_{ni} \) and \( r_{nj} \) are the inscribed radii of these two pore bodies.

2.2. Improved pore network extraction with real throat cross section

One way to improve the accuracy of pore network model is to replace the regular throat bonds with throat bonds with real throat cross sections, as shown in Fig. 1(d). This improvement has also been studied recently by (Miao et al., 2017; Rabbani and Babaei, 2019). We refer to this first improved pore network model as IPNM1 hereafter. To obtain the real cross section of the throat bonds, we firstly connect the centroids of the connecting two pore bodies with a straight line, shown as dashed blue line in Fig. 1(b). Then a plane perpendicular to this line is inserted and moved from centroid 2 to 3 and the varying cross sections along this line are obtained. We select the cross section with minimum inscribed radius as the real throat cross section because the minimum cross section has most significant influence on the flow resistance. The lengths of the throat bonds are calculated in the same manner as those in CPNM. As there is no analytical or empirical equations to calculate the conductances of these real throat bonds, LBM is used to calculate such conductance, as described in Section 3.2.

2.3. Improved pore network extraction with real pore and throat geometry

To retain as much geometrical information as possible, the best way is to extract the real pore-throat-pore element without any geometry simplification, as shown in Fig. 1(f). To extract the pore-throat-pore element, first a straight line connecting the two pore bodies is also determined. Then two planes perpendicular to this line are inserted at the pore centroids 2 and 3 and all pore voxels in between these two planes are extracted, while the other voxels between these two planes are considered as solids. The extracted pore-throat-pore element is placed in a cubic simulation domain to calculate the conductance, as shown in Figs. 1(f) and 4.

2.4. Improved pore network extraction with serial sub-throat bonds

As more geometrical information is maintained in the improved pore network model in previous section, the computational efficiency becomes much lower, as demonstrated in Section 4.2. To reach a balance between the accuracy and computational efficiency we propose a new improved pore network model. For a real throat connecting two pore bodies, the shape of the cross section varies from one pore centroid to the other. However, both the CPNM and IPNM1 use only one throat cross section to calculate the flow resistance, which means that the variation of throat cross section between the two pore bodies is not captured. To capture this information, we propose a new pore network model, which uses several throat bonds in series between the two pore bodies, as shown in Fig. 1(e). To determine the shapes of the bonds, the procedure is similar to the one in Section 2.2. First a straight line is set connecting two pore bodies. Then the total throat bond is divided into several sub-throat bonds each with length \( L_{sub} \). The cross section retained for each sub-throat bond is the one with minimum inscribed radius, as shown in Fig. 1(e), and its flow resistance is determined. The overall flow resistance is calculated by the harmonic mean of the conductances of all sub-throat bonds, which will be further elaborated in Section 3.2.3. As the accuracy and the computer efficiency of this model lie in between those of IPNM1 and of the IPNM presented in Section 2.3, we call this improved pore network model 2 (IPNM2) in the following analysis, while the model described in Section 2.3 as improved pore network model 3 (IPNM3).

3. Numerical methods

3.1. Lattice Boltzmann method

A multi-relaxation-time (MRT) single-phase LB model is used to simulate fluid flow in the throat bonds and calculate their conductances. It is also used to simulate fluid flow in the whole porous medium to provide a reference solution for evaluating the accuracy of the different pore network models. Here the LB model is briefly introduced. The evolution equation is shown below:
\[ \left| f(r + e_a \delta_t t + \delta_i) \right| - |f(r, t)| = -M^{-1} \dot{\mathbf{S}} \left[ |m(r, t)| - |m^0(r, t)| \right] \]
\[ + M^{-1} \left( I - \frac{\dot{S}}{2} \right) M(F) \delta_i, \]  
where \( |f| = (f_0, f_1, ..., f_{18})^T \) and \( f_0 \) is the density distribution function of a direction; \( r \) is the spatial location; \( e_a \) is the velocity of the \( a \) direction; \( t \) is the time; \( I \) is the identity matrix; \( \delta_i \) is the time step. The D3Q19 velocity model is adopted in this work. \( F \) is the external body force which acts as the driven force in IPNM1 and 2 to calculate the throat conductance, and it can be expressed as:
\[ F = (F_0, F_1, ..., F_{18})^T. \]
\[ F_a = \rho u_a \left( \frac{e_a \cdot a}{c_i^2} a + \frac{u_a}{c_i^2} (e_a e_a - c_i^2 I) \right) \delta_i, \]
where \( \rho_0 \) is the weight factor in the \( a \) direction; \( \rho \) is the macroscopic density; \( u \) is the acceleration due to external forces; \( c_i = 1/\sqrt{3} \) is the speed of sound.

\( M \) is a 19x19 transformation matrix to map the vector \( f \) in the discrete velocity space to the vector \( m \) in the moment space. \( \dot{S} \) is the diagonal collision matrix. The sub-throat boundary condition is adopted on solid surfaces which will generate no-slip velocities. The accuracy of using LBM to simulate single-phase flow is verified by comparing simulation results with analytical solutions in simple geometries, as illustrated in the Appendix.

In all simulations and analyses of the following paragraphs, lattice units are used unless otherwise specified. The lattice units can be easily converted into physical units given the time scale \( T_0 \), length scale \( L_0 \) and mass scale \( M_0 \) (Zhao et al., 2018). For example, the viscosity in lattice units can be converted into physical units by \( \mu^{(L)} = \mu^{LBM} \frac{M_0}{T_0^2} \).

### 3.2. Pore network model

For single-phase flow through a throat bond connecting two pore bodies \( i \) and \( j \), the volume flux \( q_{ij} \) is proportional to the pressure difference in the two pore bodies, which can be expressed by:
\[ q_{ij} = g_{ij} (p_i - p_j), \]  
where \( g_{ij} \) is the throat conductance; \( p_i \) and \( p_j \) are the pressures in pores \( i \) and \( j \), respectively. Under steady state, the mass balance equation in each pore body \( i \) should be satisfied, which means:
\[ \sum_j q_{ij} = \sum_j g_{ij} (p_i - p_j) = 0 \]  

For pressure driven fluid flow, the pressures at the inlet and outlet pores are constant:
\[ p_i|_{\text{inlet}} = p_i, \]
\[ p_i|_{\text{outlet}} = p_j. \]  

Combining Eqs. (3)-(5), we can solve the pressure field in the whole pore network. Then the volume flux across the pore network and the corresponding permeability can be calculated. It is obvious that the accuracy of single-phase pore network model depends on the throat conductance \( g_{ij} \). The difference of different pore network models lies in the calculation of \( g_{ij} \), which will be described in following paragraphs.

### 3.2.1. Conventional pore network model (CPNM)

As introduced in Section 2.2, in CPNM, the complex throat cross sections are simplified into regular shapes such as circle, square and triangle. For single-phase flow in such regular throats, the throat conductance can be calculated by (Valvatne, 2004):
\[ g = \frac{A^2 G}{\mu L}. \]  
where \( c \) is a modification coefficient and \( c = 0.5, 0.5623 \) and 0.6 respectively for circular, square and triangular throat bonds; \( L \) is the throat length; \( A \) is the cross section area of the throat bond and \( \mu \) is the dynamic fluid viscosity.

As there is no analytical or empirical expressions to calculate the throat conductance in the improved pore network models, LBM is used to simulate single-phase flow in these real throat bonds and calculate their conductances.

### 3.2.2. Improved pore network model 1 (IPNM1)

In IPNM1, the throat bond with real cross section is considered. To calculate the conductance, the model shown in Fig. 2(a) is developed by extending the real throat cross section in \( x \) direction with a short distance, namely 3 lattices in this work. This throat cross section is extracted from the pore-throat-pore element shown in Fig. 4. In the LBM simulation, the fluid density is set as 1.0 and the kinetic viscosity is set as 0.5. A small external acceleration \( a_x = 1.0 \times 10^{-3} \) is imposed in \( x \) direction and periodic boundary conditions are considered. The volume flux \( q \) across this throat bond can be calculated by integrating the velocity distribution in the slice at \( x = 0 \). When the relative volume flux change in 100 consecutive iteration (time) steps is less than \( 10^{-6} \), conditions referred to as the stop criterion, the simulation is assumed to have reached the steady state. This simulation can reach steady state in a short time as there is no velocity gradient in \( x \) direction and the simulation domain is small. The throat conductance is then given by:
\[ g_{ij} = \frac{q_j}{\rho a_x L} \frac{\mu^{LBM}}{\mu}. \]  

where \( \rho \) is the fluid density in the LBM simulation; \( L \) is the length of throat bond. As the throat conductance is related to the fluid viscosity, the last term of Eq. (6) above is used to rescale the throat conductance calculated in LBM simulation with the dynamic viscosity \( \mu^{LBM} \) to the one in PN simulation with the dynamic viscosity \( \mu \). As this work considers single-phase flow, the dynamic viscosity has no influence on the calculation of permeability and pressure distribution, and we set \( \mu = \mu^{LBM} = 0.5 \) in lattice units.

### 3.2.3. Improved pore network model 2 (IPNM2)

In IPNM2, we assume two pore bodies are connected through several sub-throat bonds in series. The cross section of each sub-throat bond is extracted from the digital rock with its real geometry. The length \( L_{ij} \) between two pore centroids of connecting pore bodies \( i \) and \( j \) is divided into \( N_{sub} = L_{ij}/L_{sub} \) sub-throat bonds. To check the influence of \( L_{sub} \) on the throat conductance, we calculate the conductances of different pore-throat-pore elements with different \( L_{sub} \) ranging from 8 to 3. It is found
that there is very minor change in throat conductance after $L_{sub} = 5$. Therefore, we set $L_{sub} = 4$ in the following simulation and analysis. As an example, for the pore-throat-pore element shown in Fig. 4, we obtain 6 sub-throat bonds with $L_{sub} = 4$. The cross section of each sub-throat bond is shown in Fig. 3. Then LBM is used to simulate single-phase flow and flow resistance for each sub-throat bond (Eq. (7b)). The overall flow resistance is calculated as the harmonic mean of the conductances of all sub-throat bonds:

$$\delta = \frac{1}{\sum \delta_{k,u}}$$

$$\delta_{k,u} = \frac{q_k}{\rho c_k L_k \mu LBM \mu},$$

where $\delta_{k,u}$ is the conductance of sub-throat bond $k$; $L_k$ is the length of sub-throat bond $k$.

3.2.4. Improved pore network model 3 (IPNM3)  

In IPNM3, the complete pore-throat-pore element is extracted. Fig. 4 shows one pore-throat-pore element randomly selected and extracted from a Fontainebleau sandstone digital rock shown in Fig. 5(c). LBM is used to determine the pressure driven single-phase flow imposing an inlet pressure $p_{in}$ at the left boundary and an outlet pressure $p_{out}$ at the right boundary. The volume flux $q$ across this pore-throat-pore element is calculated by integrating the velocity at the inlet/outlet boundary. The same stop criterion as in Section 3.2.2 is adopted. To minimize the compressible effect, we use a small inlet-outlet pressure ratio (1.01) in the simulation. In addition, the average volume flux across the inlet and outlet boundaries is used. In this simulation, more time steps are needed to reach steady state as the simulation domain is much larger and more complex. The conductance of this pore-throat-pore element is calculated by:

$$\delta_{p} = \frac{q}{p_{in} - p_{out}} \mu LBM \mu$$

4. Results and analysis

The three different models combining PNM and LBM are run on three different digital porous materials and the results of permeability, pressure distribution and throat conductance are compared with results of simulations with conventional PNM and whole-domain LBM.

4.1. Digital rocks and pore networks

The different PNM models used to simulate single-phase flow are based on three different digital rocks: a Berea sandstone (Berea Sandstone, 2008), a Fontainebleau sandstone (Berg, 2016) and a Bentheimer sandstone (Muljadi, 2015), as shown in Fig. 5(a)-(c). The three digital rocks are available from online resources. To save computational time and for better comparison, a subdomain of size of 300 $\times$ 200 $\times$ 200 voxels is extracted from each of the digital rock. Voxels are then directly considered as lattices/grids to build the computational domain in the LBM simulation. Two buffer zones of 10 lattices are added at the inlet and outlet of each domain. The corresponding digital rock samples are shown in Fig. 5(d)-(f), and figures (g)-(i) show the extracted pore networks. For each pore network, the number of pore bodies are 854, 653 and 812, and the number of throat bonds are 1791, 1480 and 1489, respectively. It should be mentioned that the Bentheimer sandstone digital rock is upscaled from 1000 $\times$ 1000 $\times$ 1000 voxels to 500 $\times$ 500 $\times$ 500 voxels in order to include more pore bodies in the extracted pore network, which means eight neighboring voxels in the original dataset are merged into one voxel in the rescaled digital rock. In the rescaling process, the upscaled voxel is assigned as pore voxel if the fraction of pore voxels in original dataset is larger than 50%. The main goal of this work is to evaluate the accuracy and efficiency of different PNM models to simulate single-phase flow in porous media through comparing with whole-domain LBM simulation. If the prediction results of PNM are already accurate for smaller domains, it will produce even more accurate results for larger domains. Therefore, we do not implement the representative element volume (REV) test here.

First, LBM is used to simulate fluid flow in the whole digital rocks shown in Fig. 5(d-i). The left boundary is considered as inlet and right as outlet and pressure boundary conditions are imposed on both sides. At initial condition, a linear pressure distribution from inlet to outlet is considered. When the same stop criterion as above is met, it is assumed that the steady state is reached. Then the permeability is calculated based on Darcy equation. These LBM simulation results are considered as reference solutions in the following analysis. Next, the different pore network models are extracted, the conductance of each throat bond is calculated, and the fluid flow and permeability of the porous medium is determined.
Fig. 5. Different sandstone digital rocks. Black indicates the solid phase and white the pore space. (a) Berea sandstone (400 × 400 × 400, 5.345 μm/voxel) (Berea Sandstone, 2008); (b) Fontainebleau sandstone 18 (480 × 480 × 480, 5.7 μm/voxel) (Berg, 2016); (c) Rescaled Bentheimer sandstone (500 × 500 × 500, 6.007 μm/voxel) (Muljadi, 2015). (d)-(f) Extracted subdomains (320 × 200 × 200, resolutions remain unchanged) of the digital rocks used in this work. (g)-(i) Corresponding pore networks. Pore bodies are represented by balls while throat bonds by tubes. The color and size of balls/tubes indicate the pore/throat radii in voxels.

Table 1

<table>
<thead>
<tr>
<th>rock type</th>
<th># PN pores</th>
<th># PN throats</th>
<th>numerical model</th>
<th>permeability (D)</th>
<th>relative error (%)</th>
<th>time (h)</th>
</tr>
</thead>
<tbody>
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<td>Berea</td>
<td>854</td>
<td>1791</td>
<td>LBM (reference)</td>
<td>1.702</td>
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<tr>
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<td>-</td>
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<td>1.143</td>
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<tr>
<td></td>
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<td>1.143</td>
<td>0.322</td>
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<tr>
<td>Fontainebleau</td>
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<td>1480</td>
<td>LBM (reference)</td>
<td>2.236</td>
<td>-</td>
<td>3660.373</td>
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<tr>
<td>653 pores</td>
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<td>-</td>
<td>-35.88</td>
<td>0.322</td>
<td>0.069</td>
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<tr>
<td>1480 throats</td>
<td>IPNM1</td>
<td>1.217</td>
<td>-</td>
<td>1.78</td>
<td>1.143</td>
<td>0.322</td>
</tr>
<tr>
<td></td>
<td>IPNM2</td>
<td>1.941</td>
<td>-</td>
<td>2.01</td>
<td>1.143</td>
<td>0.322</td>
</tr>
<tr>
<td></td>
<td>IPNM3</td>
<td>2.236</td>
<td>-</td>
<td>2.01</td>
<td>1.143</td>
<td>0.322</td>
</tr>
<tr>
<td>Bentheimer</td>
<td>812</td>
<td>1899</td>
<td>LBM (reference)</td>
<td>2.869</td>
<td>-</td>
<td>3921.726</td>
</tr>
<tr>
<td>812 pores</td>
<td>CPNM</td>
<td>0.505</td>
<td>-</td>
<td>-35.88</td>
<td>0.322</td>
<td>0.069</td>
</tr>
<tr>
<td>1899 throats</td>
<td>IPNM1</td>
<td>2.011</td>
<td>-</td>
<td>1.78</td>
<td>1.143</td>
<td>0.322</td>
</tr>
<tr>
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<td>-</td>
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<td>0.322</td>
</tr>
<tr>
<td></td>
<td>IPNM3</td>
<td>2.915</td>
<td>-</td>
<td>2.01</td>
<td>1.143</td>
<td>0.322</td>
</tr>
</tbody>
</table>

The results are analyzed in following sections. When comparing the simulation results of different models, we use the same digital rock, thus the same resolution.

4.2. Performance comparison of different numerical methods

Table 1 summarizes the performances of the different PNsMs introduced in Section 3. The relative error of different pore network models is calculated by $E_r(\%) = (k_{PNM} - k_{LBM}) / k_{LBM} \times 100$, with $k$ the permeability. All the LBM simulations are executed on the PIZ DAINT from the Swiss National Supercomputing Centre. The computational times shown in the table are transformed to equivalent one-CPU time by multiplying the time for simulation with the number of CPUs. In general, for the improved pore network models, the simulation time increases with the throat number. It should be noted that both the time for pore network extraction and the time for conductance calculation using LBM
are included in the computational time for the different pore network models. As shown in Table 1, all the IPNMs improve the prediction of permeability of the digital rocks compared to the CPNM results because they capture more accurate information on the pore geometry than CPNM. Both the CPNM and IPNM1 underestimate the permeability. Although IPNM1 shows a better performance than CPNM in predicting permeability, its relative error is still around -25% to -45%. The main reason for the underestimation is that the first two pore network models assume only the minimum cross section of the throat between the two pore bodies. When considering also the cross section variation of the throats between the two pore bodies in IPNM2, the accuracy significantly improves, with only a little increase in computational cost compared to IPNM1. As IPNM3 considers the real pore-throat-pore geometry, it shows the best accuracy predicting similar results as the reference LBM, however at a much higher computational cost compared to IPNM1 and IPNM2. Compared with the reference LBM, IPNM3 shows a much lower computational cost. Therefore, IPNM3 can be considered to replace whole-domain LBM simulation for predicting the permeability of a digital rock with almost the same accuracy, while requiring much lower computational cost. However, to obtain a first-order prediction of the permeability, the newly proposed IPNM2 is considered as the best choice showing the best compromise between accuracy and computational cost.

We also observe that the predicted permeability of IPNM2 for the Fontainebleau sandstone is less accurate than those predicted for the Berea and Bentheimer sandstones. Analyzing the porous structures and the pore network extraction processes for the different digital rocks, we found that the accuracy of IPNM2 is related to the structure of the extracted pore network. The numbers of extracted pore bodies and throat bonds change with the standard deviation of Gaussian filter and the radius of structuring element in the watershed method. The accuracy of IPNM2 can be improved if optimal pore network extraction parameters are selected. However, even with a less favorable extracted pore network, as shown in Table 1, the accuracy of IPNM2 is still much higher than those of CPNM and IPNM1. An analysis of the sensitivity of pore network extraction process on the accuracy of the permeability calculation by the different pore network models is, although an important topic, not the focus of the present paper and should be studied in future.

4.3. Pressure distribution comparison of different models

As stated in the introduction, it is important to obtain accurate prediction of the pressure distribution when simulating dynamic two-phase flow in porous media. In this section, we evaluate the accuracy of the different pore network models to simulate the pressure distribution. Fig. 6(a-c) show the dimensionless pressure distributions in different digital rocks obtained by LBM simulations. Fig. 6(d-f) show the corresponding simulation results obtained by IPNM3. As all the pore network models yield visually similar results, we only plot the pressure distribution for IPNM3 for illustration.

To quantitatively compare the results, for LBM simulations, the fluid pressure in each pore body is calculated by volume averaging as:

\[
p_i^{\text{LBM}} = \frac{\sum_r p_{i,r}^{\text{LBM}}(r)}{V_i}, \tag{9}
\]

where \(p_{i,r}^{\text{LBM}}\) is the volume averaged fluid pressure in pore body \(i\), \(p_{i,r}^{\text{LBM}}(r)\) is the fluid pressure in position \(r\), \(R_i\) is the coordinate set of region \(i\), \(V_i\) is the total volume of pore region \(i\).

We take the LBM simulation results as reference value and compare the pressure distributions for the different rocks and PNMs, as shown in Fig. 7. In all the figures, \(x\) represents the fluid pressure obtained by LBM, \(y\) represents the corresponding pressure obtained by the pore network model. From top to bottom, the pore network models are CPNM, IPNM1, IPNM2 and IPNM3, respectively. From left to right, the rock types are Berea sandstone, Fontainebleau sandstone and Bentheimer sandstone, respectively. The mean absolute relative error (MARE) for each case is calculated as:

\[
\text{MARE} = \frac{1}{N_p} \sum_{i=1}^{N_p} \left| \frac{p_i^{\text{PNM}} - p_i^{\text{LBM}}}{p_{in} - p_{out}} \right| \times 100\%, \tag{10}
\]

where \(p_i^{\text{PNM}}\) is the reference pressure of pore \(i\) obtained by LBM, \(p_i^{\text{PNM}}\) is the pressure of pore \(i\) simulated by PNMs, \(N_p\) is the total number of pore bodies for evaluation, \(p_{in}\) and \(p_{out}\) are the inlet and outlet pressures, respectively. The MARE values for different cases are shown in Table 2.

As can be seen from the top two rows of Fig. 7, the pressure distributions obtained by both CPNM and IPNM1 deviate more from the reference LBM results, compared to IPNM2 and IPNM3, shown in the
Fig. 7. Pore-to-pore comparison of fluid pressure distributions. Pressure determined by reference LBM on x-axis, pressure determined by different PNM on y-axis. From left to right, the digital rocks are Berea sandstone, Fontainebleau sandstone and Bentheimer sandstone, respectively. From top to bottom, CPNM, IPNM1, IPNM2 and IPNM3, respectively.
Fig. 8. Comparison of conductance of each throat bond calculated by different pore network models. $x$ represents the value calculated by IPNM3, $y$ represents the values calculated by other pore network models. From left to right, the digital rocks are Berea sandstone, Fontainebleau sandstone and Bentheimer sandstone, respectively. From top to bottom, CPNM, IPNM1 and IPNM2, respectively. The conductances are in lattice units.

bottom two rows. Although IPNM1 was found to be more accurate in predicting the permeability compared to CPNM, the MAREs of pressure for IPNM1 are even worse, as shown in Table 2, meaning more errors for IPNM1 in predicting the pressure distribution. The reason for this observation will be analyzed in the next section. As the IPNM2 and IPNM3 capture more geometry information, they yield more accurate pressure distributions. The MAREs for these two pore network models are much smaller, especially for IPNM3. This comparison also confirms the conclusion obtained in previous section that the IPNM3 can replace whole-domain LBM simulation for single-phase flow in porous media, while the IPNM2 is a good first-order approximation for single-phase flow in porous media.
4.4. Throat conductance comparison of different pore network models

As mentioned in Section 3.2, the accuracy of single-phase pore network model depends highly on the throat conductance. According to the results in Sections 4.2 and 4.3, IPNM3 can produce results similar to the ones of the reference LBM, in terms of both permeability and pressure distribution. This means that the prediction of the throat conductance by IPNM3 is most accurate compared with the other three pore network models, reason being that IPNM3 uses the real pore-throat-pore geometry. In this section, we consider the throat conductance of IPNM3 as reference values and compare these with the throat conductances predicted by the other pore network models. The comparison results are shown in Fig. 8.

As can be seen from Fig. 8, for CPNM, most throat bonds yield an underestimated value of the throat conductance, especially for small throat bonds. Accordingly, the permeability of the whole porous medium is underestimated. In general, the throat conductances calculated by IPNM1 are higher than those obtained by CPNM. Therefore, IPNM1 predicts a higher permeability than CPNM, obtaining values closer to the reference values obtained by LBM. However, there is a crossover for the conductance calculated by IPNM1 and the reference values calculated by IPNM3. For small throat bonds, IPNM1 underestimates the throat conductance, while for large throat bonds, IPNM1 overestimates the throat conductance. Due to this phenomenon, the pressure distribution obtained by IPNM1 deviates substantially from those obtained by IPNM3 and LBM. Compared with the first two pore network models, the data obtained by IPNM2 are less scattered, predicting throat conductances similar to those of IPNM3 for both small throat bonds and large throat bonds. Therefore, IPNM2 gives much better prediction results than CPNM and IPNM1, in terms of both permeability and pressure distribution.

We take the Fontainebleau sandstone as an example to further analyze the crossover of throat conductance for IPNM1 observed in Fig. 8. In IPNM1, the flow resistance between two pore bodies is determined only by the throat conductance as the flow resistances in the pore bodies are neglected. For a certain throat bond, its conductance depends on two parameters: its cross section and length. Fig. 9 shows schematically two different pore-throat-pore structures and the resulting extracted pore network. In IPNM1, the cross section of a throat bond is taken as the minimum cross section between two connecting pore bodies and the length of the throat bond is calculated by $L_{ij} = r_{mi} - r_{mj}$ as stated in Section 2.1. We use three parameters to describe the structure of the throat bond and its relationship with the connecting pore bodies, which are the radius ratio between throat bond and the connecting pore bodies ($r_{throat}/r_{pore}$), the ratio between throat length and the distance connecting the centroids of the two pore bodies ($L_{throat}/L_{ij}$), and the ratio between throat length and throat diameter ($L_{throat}/d_{throat}$). These throat characteristics are plotted for all throat bonds of the Fontainebleau sandstone pore network versus throat conductance in Fig. 10. In Fig. 10(a), the ratio $r_{throat}/r_{pore}$ generally increases with throat conductance, meaning that throat bond much smaller that connecting pore bodies results in lower conductance. In contrast, both the ratio’s $L_{throat}/L_{ij}$ and $L_{throat}/d_{throat}$ generally decrease with increasing throat conductance, thus a relatively shorter throat bond results in larger throat conductance, as shown in Fig. 10(b) and (c). Using the schematic of Fig. 9(b), for throat bonds with small conductance, e.g. throat bond $T_{1,2}$, the inscribed radius of this throat bond is much smaller than those of the connecting pore bodies $P_1$ and $P_2$. Therefore, the ratio $r_{throat}/r_{pore}$ is small and the flow resistance in the connecting pore bodies can be neglected. Remark that the cross section varies along the long throat bond, while it is assumed in IPNM1 that it equals the minimum throat cross section in the throat bond $T_{1,2}$. Accordingly, the throat bond $T_{1,2}$ underestimates the real throat conductance. While a large throat bond, as illustrated by the throat bond $T_{2,3}$ in Fig. 9(b), has an inscribed radius similar to the radii of the connecting pore bodies $P_2$ and $P_3$. In addition, the $L_{throat}/L_{ij}$ is relative small,
meaning that the radii of the pore bodies are similar to the length of throat bond. Therefore, the flow resistances in the throat bond and the connecting pore bodies are of the similar magnitude. However, the flow resistances in the connecting pore bodies are ignored in IPNM1, resulting in an overestimation of the throat conductance. The above description provides an explanation for the crossover of throat conductance for IPNM1. As IPNM2 considers the cross section variation between the centroids of the connecting two pore bodies, it actually adjust for this crossover and predicts throat conductance more accurately.

4.5. Velocity distribution comparison of different pore network models

Pore network models have been often used to simulate solute transport for which the single-phase PNM is used to provide the flux or velocity distribution (Köhne et al., 2011; Qin and Hassanizadeh, 2015). In this section we analyze the velocity distributions obtained by different PNs. We take the simulation results in the Berea sandstone digital rock as an example. The velocity distributions obtained by different models are shown in Fig. 11. The velocity in each throat bond in the pore network model is calculated by \( v_s = \frac{q_s}{A_t} \), where \( q_s \) and \( A_t \) are the volume flux across the throat bond and the area of throat cross section, respectively. We remark that the different PNs only display the mean velocities across the throats with minimum cross section which are larger than the ones in other cross sections. Therefore, it is reasonable that the velocity magnitude of IPNM3 shown in Fig. 11(e) is visually larger than that of the LBM simulation results shown in Fig. 11(a).

Simulation results between LBM and PNM cannot be compared throat by throat as the LBM velocities are not uniform over the throat. Alternatively, we take the simulation result of IPNM3 as the reference value and compare the velocity distributions obtained by the different PNs. As shown in Fig. 11(b)–(e), the velocity distributions obtained by IPNM2 and IPNM3 are roughly similar, but the velocity distributions obtained by IPNM1 and CPNM are significantly different with the ones obtained by IPNM3, especially for CPNM, which produces much smaller velocities than the IPNMs. Taking the velocity distribution obtained by IPNM3 as the reference value, we further compare the velocity distributions obtained by the other PNs throat by throat in the plots of Fig. 12. We note that a few data points with values smaller than 1.0E-8 are excluded from this figure for better view. According to the comparison results, the CPNM significantly underestimates the velocity in each throat bond due to the fact that the CPNM predicts smaller throat conductance than IPNM3. The IPNM1 predicts better the velocities than CPNM. The dataset of IPNM2 is least scattered and shows the best agreement with IPNM3. The comparison results are
similar to those of throat conductance shown in Fig. 8, as the velocity distribution is determined by the throat conductance.

5. Conclusion

In this paper, we performed a comprehensive investigation of the accuracy of different pore network models to simulate single-phase flow in porous media. Four different pore networks are extracted based on the watershed method. The conventional pore network model (CPNM) uses regular shaped pore bodies and throat bonds. The first improved pore network model (IPNM1) replaces the regular shaped throat bonds with throat bonds showing their real minimal throat cross sections. The second improved model (IPNM2), which is firstly proposed in this work, uses a series of sub-throat bonds to describe the cross section variation between two pore bodies. The improved pore network model 3 (IPNM3) directly extracts the real pore-throat-pore element without any geometry simplification. The throat conductance of the three improved pore network models is calculated by LBM. The performance of different PNsMs to simulate single-phase flow in porous media is evaluated taking the LBM simulation results in the whole porous media as reference solutions. From CPNM to IPNM3, the accuracy to predict the permeability increases, as more accurate information on pore geometry is used, at the expense of computational efficiency. In addition to the permeability, the pressure distribution obtained by different PNsMs is compared pore by pore with the reference LBM results. The results show that IPNM2 and IPNM3 achieve more accurate pressure distributions compared with those obtained by CPNM and IPNM1. Although IPNM1 can predict more accurate permeability than CPNM, the relative errors in predicting the pressure distributions are even worse. It was shown that CPNM underestimates the throat conductance for most of the throat bonds as compared to those calculated by IPNM3. IPNM1 underestimates the throat conductance for small throat bonds and overestimates the throat conductance for large throat bonds, due to the structure difference for small throat bonds and large ones. IPNM2, which takes into account the cross section variation between the connecting pore bodies, obtains very similar throat conductance values as those determined by IPNM3. In summary, IPNM3 can replace LBM to simulate single-phase flow in porous media with almost the same accuracy, but at much lower computational cost. However, to obtain a first-order approximation of single-phase flow in porous media in terms of both permeability and pressure distribution, the newly proposed IPNM2 is a better choice, with the best balance between accuracy and computational cost. The results presented in this work by comparing different pore network models can help researchers and engineers to choose the adequate pore network model for their specific purpose. In addition, the different improvements presented here for single-phase pore network models can be incorporated into other pore network models for more complicated flow or transport processes, such as multiphase flow, solute transport, etc, which should be studied in future work.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests.

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![Fig. 13. Comparison of permeability through circular tubes with different radii. The properties are in lattice units.](https://www.digitalrockportal.org/projects/57)

Appendix

We conduct external force driven single-phase flow through circular tubes with different radii to verify the accuracy of using LBM to calculate the conductance. The simulation domain is similar to that shown in Fig. 2 and we replace the cross section with circles of different radii. A small external acceleration $a_e = 1.0 \times 10^{-4}$ is imposed in $x$ direction and periodic boundary condition is considered. When the relative volume flux change in 100 consecutive iteration (time) steps is less than $10^{-6}$, the simulation is assumed to have reached the steady state. Then the permeability of fluid flow through this tube can be calculated by:

$$k_{LBM} = \frac{q \mu}{\pi r_a^3 a_e}$$

The calculated permeability by LBM is plotted in Fig. 13 as red squares, where the solid line shows the theoretical solution which is $k_{\text{theory}} = r_e^2 / 8$. As can be seen, the simulation results match well with theoretical solutions, demonstrating the accuracy of using LBM to calculate conductance of single-phase flow.

References


