# Simulated of flow in a three-dimensional porous structure by using the IB-SEM system 

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(Received December 8, 2018, Revised May 23, 2019, Accepted August 22, 2019)


#### Abstract

The IB-SEM numerical method combines the spectral/hp element method and the rigid immersed boundary method. This method avoids the problems of low computational efficiency and errors that are caused by the re-division of the grid when the solids move. Based on the Fourier transformation and the 3D immersed boundary method, the 3D IB-SEM system was established. Then, using the open MPI and the Hamilton HPC service, the computational efficiency was increased substantially. The flows around a cylinder and a sphere were simulated by the system. The surface of the cylinder generates vortices with alternating shedding, and these vortices result in a periodic force acting on the surface of the cylinder. When the shedding vortices enter the flow field behind the cylinder, a recirculation zone is formed. Finally, the three-dimensional pore flow was successfully investigated.


Keywords: Fourier transformation; 3D immersed boundary method; the 3D IB-SEM system; open MPI

## 1. Introduction

The 3D NS equations are Fourier decomposed in the $\theta$ direction to transform the 3D equations into a set of 2D problems, which can be spatially discretized via a spectral/hp element method and temporally discretized via a velocity-correction scheme (Levin et al. 2015).

When the numerical simulation is transformed from two-dimensional to three-dimensional, the amount of calculation is substantially increased. Serial computing cannot satisfy the requirements. Compared with serial computing, parallel computing can solve the same problem more quickly, can use a smaller amount of input to complete the task and can exceed the physical limit. Parallel computing is an effective approach for large-scale numerical simulation. The IB-SEM system uses a common parallel interface standard message passing interface (MPI) (Agapito 2013, Gropp et al. 2014). MPICH is one of the most popular parallel programming standards for MPI standards.

Due to its simple geometry, flow around a cylinder has been a popular topic in the field of hydrodynamics. It is of substantial significance for engineering applications. The characteristics of the flow field depend on the Reynolds number. The variational characteristics of the flow around a cylinder are highly complicated with the change of the

[^0]Reynolds number.
Three-dimensional flow around a sphere is a basic research topic in fluid research in fluid mechanics. Taneda conducted a substantial amount of experimental research (Taneda 1956). When the Reynolds number reached 24, flow separation occurred behind the sphere and symmetric vortex rings began to appear. When the Reynolds number reached 210, steady asymmetric vortex structures began to appear. When the Reynolds number exceeded 270, the vortex began to fall off. When the Reynolds number was 420-800, the tail vortex began to fall irregularly and to rotate. In numerical studies, the assumption of axial symmetry was typically imposed due to the limited computational efficiency of the methods. In this scenario, the computational results were not satisfactory when the Reynolds number exceeded 210. Lee Sungsu used the finite element method to simulate the flow around a sphere when the Reynolds number ranged from 100 to 500 (Lee 2000). In this chapter, the flow around a sphere was investigated using the IB-SEM system and the results were compared with those of other studies (Park et al. 2016).

In the simulation of flow in 3D porous media, little related research has been conducted, which can be divided into the following categories: First, a coupled micromechanical technique for modelling pore water flow and solid-phase deformation of granular soils was proposed. The fluid-particle interactions were investigated and the fluid motion was idealized using averaged Navier-Stokes equations and the discrete element method (DEM) (Siamak et al. 2016, Chen et al. 2016). Second, a particle-fluid coupling scheme with a mixed Lagrangian-Eulerian approach that enables the simulation of coupling problems with large Reynolds numbers was implemented in PFC 2D and PFC 3D (Marina et al. 2015, Wang and Ni 2013).

Third, the three-dimensional response of sandy deposits was investigated using a coupled hydromechanical model when subjected to critical and over-critical upward pore fluid flow (El and Zeghal 2005).

The IB-SEM system was established based on a spectral element method, namely, Semtex, and the rigid immersed boundary method (Wang et al. 2018). This system is used to simulate solid and fluid interactions.

## 2. Basic theory for the numerical simulation

### 2.1 Fourier transformation in the azimuthal direction

The velocity components are $2 \pi$ in $\theta$. The three dimensional Navier-Stokes equations can be transformed into a set of two dimensional complex Fourier modes (see Fig. 1).

$$
\begin{equation*}
\widehat{u_{k}}(z, r, t)=\frac{1}{2 \pi} \int_{0}^{2 \pi} u(z, r, \theta, t) e^{-i k \theta} d \theta \tag{1}
\end{equation*}
$$

where k is the integer azimuthal wavenumber. The velocity field can be recovered from these complex modes via Fourier series reconstruction

$$
\begin{equation*}
(z, r, \theta, t)=\sum_{k=-\infty}^{\infty} \widehat{u_{k}}(z, r, t) e^{i k \theta} \tag{2}
\end{equation*}
$$

The cylindrical-coordinate forms of the gradient and Laplacian of a complex scalar mode are

$$
\begin{align*}
& \nabla_{k}=\left(\partial_{z}(\quad), \partial_{r}(\quad), \frac{i k}{r}(\quad)\right)  \tag{3}\\
& \nabla_{k}^{2}=\partial_{z}^{2}+\frac{1}{r} \partial_{r} r(\quad)-\frac{k^{2}}{r^{2}}(\quad) \tag{4}
\end{align*}
$$

And the divergence of a complex vector mode is

$$
\begin{equation*}
\nabla \cdot(\quad)_{k}=\partial_{z}(\quad)+\frac{1}{r} \partial_{r} r(\quad)+\frac{i k}{r}(\quad) \tag{5}
\end{equation*}
$$

The radial and azimuthal velocity components are coupled to divergence the viscous terms by introducing

$$
\begin{equation*}
\widetilde{v_{k}}=\widehat{v_{k}}+i \widehat{w_{k}} \text { and } \widetilde{w_{k}}=\widehat{v_{k}}-i \widehat{w_{k}} \tag{6}
\end{equation*}
$$

The whole set of equations can be symmetrized by premultiplication on both sides by r , leading to

$$
\begin{equation*}
\partial_{r} r \widehat{u_{k}}+r\left[N(u)_{z}\right] \widehat{k}=-r \partial_{z} \widetilde{p_{k}}+\frac{1}{R e}\left(\partial_{z} r \partial_{z}+\partial_{r} r \partial_{r}-\frac{k^{2}}{r}\right) \widehat{u_{k}} \tag{7}
\end{equation*}
$$

$$
\begin{align*}
& \partial_{t} r \widetilde{v_{k}}+r\left[N(u)_{r}\right] \tilde{k}=-\left(r \partial_{r}-k\right) \widehat{p_{k}}+\frac{1}{R e}\left(\partial_{z} r \partial_{z}+\right. \\
& \left.\partial_{r} r \partial_{r}-\frac{[k+1]^{2}}{r}\right) \widetilde{v_{k}}  \tag{8}\\
& \partial_{t} r \widetilde{w_{k}}+r\left[N(u)_{\theta}\right] \widetilde{k} \\
& \quad=-\left(r \partial_{r}+k\right) \widehat{p_{k}}+\frac{1}{R e}\left(\partial_{z} r \partial_{z}\right. \\
& \left.\quad+\partial_{r} r \partial_{r}-\frac{[k-1]^{2}}{r}\right) \widetilde{w_{k}} \tag{9}
\end{align*}
$$

$$
\begin{equation*}
\partial_{z} r \widehat{u_{k}}+\partial_{r} r \widehat{v_{k}}+i k \widehat{w_{k}}=0 \tag{10}
\end{equation*}
$$

Full solution algorithm
For the $\partial_{z} r=0$, the pressure Poisson equation can be


Fig. 1 Fourier transform
written as

$$
\begin{gather*}
\left(\partial_{z} r \partial_{z}+\partial_{r} r \partial_{r}-\frac{k^{2}}{r}\right){\widehat{p p_{k}}}^{n+1}=\frac{1}{\Delta t}\left(\partial_{z} r{\widehat{u_{k}}}^{*}+\partial_{r} r{\widehat{v_{k}}}^{*}+\right.  \tag{11}\\
\left.i m{\widehat{\omega_{k}}}^{*}\right)
\end{gather*}
$$

Each component was appeared in the right hand side divergence term

$$
\begin{align*}
& r{\widehat{u_{m}}}^{*}=-\sum_{q=1}^{J} \alpha_{q} r \hat{u}^{(n-q)}-\Delta t \int_{q=0}^{J-1} \beta_{q} r\left[N\left(u^{(n-q)}\right)_{z}\right] \hat{k}  \tag{12}\\
& r{\widehat{v_{m}}}^{*}=-\sum_{q=1}^{J} \alpha_{q} r \hat{v}^{(n-q)}-\Delta t \int_{q=0}^{J-1} \beta_{q} r\left[N\left(v^{(n-q)}\right)_{z}\right] \hat{k}  \tag{13}\\
& r{\widehat{\omega_{m}}}^{*}=-\sum_{q=1}^{J} \alpha_{q} r \widehat{\omega}^{(n-q)}-\Delta t \int_{q=0}^{J-1} \beta_{q} r\left[N\left(\omega^{(n-q)}\right)_{z}\right] \hat{k} \tag{14}
\end{align*}
$$

### 2.2 Discretization of 3D Navier-Stokes equations

The Navier-Stokes equations must be discretized prior to being applied to computational fluid dynamics. The discretization methods include the spatial discretization method for the spectral/hp element method and the temporal discretization method for the velocity-correction scheme.
The NS equation can be expressed in the cylindrical coordinate system $(z, r, \theta)$ as follows

$$
\begin{gather*}
\partial_{t^{*}} u^{*}=-\left(u^{*} \cdot \nabla\right) u^{*}-\frac{1}{\rho} \nabla p^{*}+v \nabla^{2} u^{*}  \tag{15}\\
\nabla \cdot u^{*}=0 \tag{16}
\end{gather*}
$$

Z represents the stream-wise coordinate
where $u^{*}\left(z^{*}, r^{*}, \theta, t^{*}\right)$ is the velocity field, in which $z$ represents the streamwise coordinate; $p^{*}\left(z^{*}, r^{*}, \theta, t^{*}\right)$ is the pressure; $\rho$ is the density; and v is the viscosity. The equations for the corresponding nondimensionalized variables (without superscript *) are as follows

$$
\begin{gather*}
\partial_{t} u=-(u \cdot \nabla) u-\nabla p+\frac{1}{R e} \nabla^{2} u  \tag{17}\\
\nabla \cdot u=0 \tag{18}
\end{gather*}
$$

where,

$$
\begin{equation*}
r=\frac{r^{*}}{L} \tag{19}
\end{equation*}
$$



Fig. 2 The simulation process of IB-SEM system

$$
\begin{gather*}
z=\frac{z^{*}}{L}  \tag{20}\\
t=\frac{t^{*} u_{\infty}}{L}  \tag{21}\\
u(z, r, \theta, t)=(u, v, w)(t)=\frac{u^{*}}{u_{\infty}}  \tag{22}\\
p=\frac{p^{*}-p^{\infty}}{\rho u_{\infty}^{2}}  \tag{23}\\
\operatorname{Re}=\frac{u_{\infty} L}{v} \tag{24}
\end{gather*}
$$

Here, $\mathrm{L}, u_{\infty}$ and $p_{\infty}$ are characteristic length, velocity and pressure respectively.

## 3. Concurrent execution for the 3D IB-SEM

The IB-SEM system was established based on the Spectral element method and the rigid immersed boundary method. This system is used to simulate the interaction of the solid and fluid which are shown in Fig. 2 (Li et al. 2019).

In the pre-processing, the modelling software of the IB-SEM system is established. This software was used to realize two dimensional and three dimensional immerse boundary modelling and the elements and nodes of fluid domain generating.

For the large-scale three-dimensional simulation, the computation time of the serial algorithm is too long. A message passing interface is required for parallelizing the above algorithms. For the three-dimensional NS equation, the MPI method is used to parallelize the distributed memory cluster.

Table 1 Computational scale $\mathrm{N}=5123$, Single step calculation time and speed-up ratio analysis

| Number of processors | Single step time <br> (second) | Speed-up ratio |
| :---: | :---: | :---: |
| 8 | 31.5 | 1 |
| 16 | 16.4 | 1.9 |
| 32 | 9.0 | 3.5 |
| 64 | 4.9 | 6.5 |
| 128 | 3.5 | 9 |
| 256 | 2.2 | 14.1 |

Running of the three dimensional IB-SEM system
The code supports concurrent execution for 3D simulations, with MPI used as the message-passing kernel. Compile using make MPI=1 to produce dns_mp. (When compiling femlib, it will also be necessary to compile in the appropriate message-passing routines by switching to the femlib directory and using the following commands: make clean; make MPI=1; and make install MPI=1.) Nonlinear terms are not dealiased if running in parallel but are dealiased in the Fourier direction if running on one process or running the serial code. To obtain a serial code that does not perform dealiasing on Fourier terms (e.g., for crosschecking), compile the serial code using make ALIAS $=1$ to produce dns_alias (after deleting nonlinear.o; see Table 1).

## 4. Flow around the cylinder and the sphere

### 4.1 Calculation of the vorticity and velocity magnitude

Vorticity is a concept in fluid mechanics that describes the rotation of a fluid. In continuum mechanics, the vorticity is a pseudo vector field that describes the local spinning motion of a continuum near a specified point, as would be viewed by an observer who is located at that point


Fig. 3 Schematic diagram of calculation and grid


Fig. 4 The simulation results of flow around cylinder


Fig. 5 The curve of $u$ along the $y$ direction near wake region
and travelling along with the flow. It is defined as the curl of the fluid velocity vector. The unit of vorticity is one second (s-1).

Vortex lines are defined by the relation

$$
\begin{equation*}
\frac{d_{x}}{\omega_{x}}=\frac{d_{y}}{\omega_{y}}=\frac{d_{z}}{\omega_{z}} \tag{25}
\end{equation*}
$$

where, $\omega=\left(\omega_{x}, \omega_{y}, \omega_{z}\right)$ is the vorticity in Cartesian coordinates.

$$
\begin{equation*}
\omega_{x}=\frac{\partial \omega}{\partial y}-\frac{\partial v}{\partial z} \tag{26}
\end{equation*}
$$



Fig. 6 The immerse boundary nodes

$$
\begin{align*}
& \omega_{y}=\frac{\partial u}{\partial z}-\frac{\partial w}{\partial x}  \tag{27}\\
& \omega_{z}=\frac{\partial v}{\partial x}-\frac{\partial u}{\partial y} \tag{28}
\end{align*}
$$

The velocity magnitude is

$$
\begin{equation*}
v_{m}=\sqrt{\left(u_{x}\right)^{2}+\left(u_{y}\right)^{2}+\left(u_{z}\right)^{2}} \tag{29}
\end{equation*}
$$

After the simulation, the vorticity was calculated in Tecplot. U, V and W represent the velocity in the threedimensional flow. The vorticity, which is denoted as (wx, $\mathrm{wy}, \mathrm{wz})$, is expressed by the following equations:.

$$
\begin{align*}
& \{w x\}=d d y(\{w\})-d d z(\{v\})  \tag{30}\\
& \{w y\}=d d z(\{u\})-d d x(\{w\})  \tag{31}\\
& \{w z\}=d d x(\{v\})-d d y(\{u\}) \tag{32}
\end{align*}
$$

The velocity magnitude can be calculated as

$$
\begin{equation*}
\{\text { VelocityMagnitude }\}=\operatorname{sqrt}(\{u\} * * 2)+\{v\} * * 2+\{w\} * * 2 \tag{33}
\end{equation*}
$$

### 4.2 Flow around a cylinder (Semtex ${ }^{3 D}$ )

In this section, a cylinder with diameter $D=1$ is considered as the research object and Semtex3D is used to simulate the flow field around the cylinder. The domain and meshes are shown in Fig. 7. The diameter of the cylinder is equal to the characteristic length. The length, width and height of the computational domain are 25,10 and 4 . The numbers of the elements and nodes are 74 and 94 . The number of curves is 52 .

Boundary conditions and initial conditions
The velocity of the inlet is $u=1$. The inlet and outlet are set on the left and right sides of the domain. The other four surfaces and the cylinder surface are non-slip wall boundaries. The Reynolds number is 200 .

The computational domain is illustrated in Fig. 3
The simulation of $\omega_{z}$ is shown in Fig. 4.
The distribution of along the $y$-direction in the nearwake region behind the cylinder is plotted in Fig. 5. When $\frac{y}{D}=0, \mathrm{u}$ attains its minimum value of -0.247 . When $y / D$ is in the range of $(-1,0)$ and $(0,1)$, the speed increases substantially with the absolute value of $y / D$. Then, the speed decreases slowly as the absolute value of $y / D$ increases.

The results are consistent with previous results. Using Semtex ${ }^{3 D}$, the flow around the cylinder can be accurately simulated at various Reynolds numbers.

When the fluid flows through the surface of the cylinder, most of the pressure on its surface is negative. Then, due to the combined effect of the negative pressure difference and the fluid viscosity, the fluid is separated from the cylinder surface. The surface of the cylinder generates vortices with alternating shedding, which results in a periodic force that acts on the surface of the cylinder. When the shedding vortices enter the flow field behind the cylinder, a recirculation zone forms near the surface of the cylinder.

### 4.3 Flow around a sphere (IB-SEM)

Calculation of the vector force of the sphere
$\tau$ is the viscous shear stress and

$$
\tau \cdot n=\operatorname{Re}^{-1}\left[\begin{array}{ccc}
2 \partial_{x} u_{x} & \partial_{x} u_{x}+\partial_{x} u_{y} & \partial_{z} u_{x}+\partial_{x} u_{z}  \tag{34}\\
\partial_{y} u_{x}+\partial_{x} u_{y} & 2 \partial_{y} u_{y} & \partial_{z} u_{y}+\partial_{y} u_{z} \\
\partial_{z} u_{x}+\partial_{x} u_{z} & \partial_{z} u_{y}+\partial_{y} u_{z} & 2 \partial_{z} u_{z}
\end{array}\right] \cdot\left[\begin{array}{c}
n_{x} \\
n_{y} \\
n_{z}
\end{array}\right]
$$

The force of viscous force in $\mathrm{x}, \mathrm{y}$ and z directions are respectively


Fig. 7 The computational domain

$$
\begin{gather*}
\tau_{x}=\mathrm{Re}^{-1}\left(2 \partial_{x} u_{x} * n_{x}+\partial_{y} u_{x} * n_{y}+\partial_{x} u_{y} * n_{y}+\right.  \tag{35}\\
\left.\partial_{z} u_{x} * n_{z}+\partial_{x} u_{z} * n_{z}\right) \\
\tau_{y}=\mathrm{Re}^{-1}\left(\partial_{y} u_{x} * n_{x}+\partial_{x} u_{y} * n_{x}+2 \partial_{y} u_{y} * n_{y}\right. \\
\left.+\partial_{z} u_{y} * n_{z}+\partial_{y} u_{z} * n_{z}\right)  \tag{36}\\
\tau_{z}=\operatorname{Re}^{-1}\left(\partial_{z} u_{x} * n_{x}+\partial_{x} u_{z} * n_{x}+\partial_{z} u_{y} * n_{y}+\partial_{y} u_{z}\right. \\
\left.* n_{y}+2 \partial_{z} u_{z} * n_{z}\right) \tag{37}
\end{gather*}
$$

In fluid dynamics, the drag coefficient, which is denoted as $C_{d}$, is a dimensionless quantity that is used to quantify the drag or resistance of an object in a fluid environment, such as air or water. It is used in the drag equation, in which a smaller drag coefficient corresponds to the object having less aerodynamic or hydrodynamic drag. The drag coefficient is always associated with a specified surface area.

$$
\begin{equation*}
C_{d}=\frac{2 F_{d}}{\rho u^{2} A}=\frac{8 F_{d}}{\rho u^{2} \pi D^{2}} \tag{38}
\end{equation*}
$$

where $F_{d}$ is the drag force, the $F_{d}$ is defined as

$$
\begin{align*}
F_{d} & =\int_{\Gamma} f_{x}^{B} d \Gamma  \tag{39}\\
F_{d x} & =\tau_{x}+p_{x}  \tag{40}\\
F_{d y} & =\tau_{y}+p_{y} \tag{41}
\end{align*}
$$

$$
\begin{equation*}
F_{d z}=\tau_{z}+p_{z} \tag{42}
\end{equation*}
$$

$\rho$ is the mass density of the fluid, $u$ is the mean freestream velocity. $A$ is the reference area.

$$
\begin{equation*}
A=\pi D^{2} / 4 \tag{43}
\end{equation*}
$$

To evaluate the accuracy of the three-dimensional IBSEM system for the simulation of moving spheres, we use it to simulate the laminar flow around a sphere for Reynold numbers from 50 to 300 . In this study, the sensitivity of the drag to boundary perturbations in the three-dimensional flow past a sphere is investigated. The sphere was simulated via the immersed boundary method. The surface of the sphere is considered the perturbation boundary.

The numerical model integrates the three-dimensional, time-dependent, incompressible, Navier-Stokes, continuity equations and non-dimensionalizes the result according to the diameter of the sphere and the free-stream velocity.

For comparison with other studies, the diameter of the sphere is set to 1 . The size of the domain is $25 * 20 * 20$ in the $\mathrm{x}-\mathrm{y}$ y- and z -directions. The sphere is centred at $(10,10,10)$ in the Cartesian coordinate system.

The density of the fluid is set as 1.0 . The inflow and out flow are located at $x=0$ and $x=25$, respectively. Free stream boundary conditions with $u=1.0, v=1.0$ and $w=1.0$ are applied to the inflow boundary. The far-field boundaries are located at $\mathrm{y}=0$ and $\mathrm{y}=20$. Two typical Reynolds numbers, namely, 100 and 200, are considered.

The three-dimensional computational domain is decomposed into 2000 spectral elements and 2091 nodes in the $x$ - and $y$-directions, in each of which piecewise continuous nodal-based polynomial expansions with polynomial order $\mathrm{P}=6$ are applied. Time integration is conducted using a velocity-correction scheme. The same numerical methods are used to integrate the Navier-Stokes equations and the adjoint equation using a well-validated numerical code that has been used in DNS and hydrodynamic stability studies of vortex flow and flow around immersed boundaries.

The number of rigid immersed boundary nodes is 441 , as shown in Fig. 11. The feedback forcing coefficients were set to $\alpha=-400000$ and $\beta=-600$. For the feedback forcing method, the stability limit for the time step was approximated by

$$
\begin{equation*}
\Delta t<\frac{-\beta-\sqrt{\left(\beta^{2}-2 \alpha k\right)}}{\alpha} \tag{44}
\end{equation*}
$$

where $k$ is a problem-dependent constant of order one. Hence, the time step $\Delta t$ was set to 0.001 in our simulation. The computational domain and the immersed boundary are illustrated in Fig. 6 and 7.

There are three main methods for calculating the vertical structures: (1) $Q$ - citerion, (2) $\Delta$ - citerion, and (3) $\lambda_{2}$ - citerion

The first three-dimensional vortex criterion that uses (1.1) is the $Q$ - citerion of Hunt, Wray \& Moin, which defines a vortex as a spatial region (Hunt et al. 1988).

$$
\begin{equation*}
Q \equiv \frac{1}{2}\left(u_{i, i}^{2}-u_{i, j} u_{j, i}\right)=-\frac{1}{2} u_{i, j} u_{j, i}=\frac{1}{2}\left[|\Omega|^{2}-|S|^{2}\right]>0 \tag{45}
\end{equation*}
$$

where, $S$ is the rate of strain tensor which is defined as


Fig. 8 ISO-surface of velocity magnitude


Fig. 9 3D vertical structures of sphere for planar symmetric flows

$$
\begin{equation*}
S=\frac{J+J^{T}}{2} \tag{46}
\end{equation*}
$$

$\Omega$ is the vorticity tensor which is defined as

$$
\begin{equation*}
\Omega=\frac{J-J^{T}}{2} \tag{47}
\end{equation*}
$$

We define the gradient velocity tensor $J$

$$
J \equiv \nabla \vec{u}\left[\begin{array}{lll}
\partial_{x} u_{x} & \partial_{y} u_{x} & \partial_{z} u_{x}  \tag{48}\\
\partial_{x} u_{y} & \partial_{y} u_{y} & \partial_{z} u_{y} \\
\partial_{x} u_{z} & \partial_{y} u_{z} & \partial_{z} u_{z}
\end{array}\right]
$$

Another well-known Galilean-invariant definition is the of Chong, Perry \& Cantwell (1990), who define vortices as regions with

$$
\begin{equation*}
\Delta=\left(\frac{Q}{3}\right)^{3}+\left(\frac{\operatorname{det} \nabla \vec{u}}{2}\right)^{2}>0 \tag{49}
\end{equation*}
$$

In these regions, the velocity gradient $\nabla \vec{u}$ admits complex eigenvalues, thus local instantaneous stirring is a plausible assumption.

Finally, according to the $\lambda_{2}$ - citerion of Jeong \& Hussain (1995), vortices are defined as

$$
\begin{equation*}
\lambda_{2}\left(S^{2}+\Omega^{2}\right)<0 \tag{50}
\end{equation*}
$$

Table 2 Comparison of drag coefficients at $\mathrm{Re}=100$ and Re=200

| Case | Drag coefficient Cd |  |
| :---: | :---: | :---: |
|  | $\mathrm{Re}=100$ | $\mathrm{Re}=200$ |
| Johnson et al. | 1.112 | 0.79 |
| A. Gilmanov et al. | 1.153 | - |
| Write et al. | 1.128 | 0.8 |
| present | 1.132 | 0.8 |
| 256 | 2.2 | 14.1 |



Fig. 10 Comparison of separation length
where $\lambda_{2}(A)$ denotes the intermediate eigenvalue of a symmetric tensor $A$.

Fig. 8 shows the velocity field in 2D section on $\mathrm{z}=5$. This image shows in detail the direction of the velocity field in the middle plane of the sphere.

A hairpin vortex is formed in the wake. It can be observed from Fig. 9 that the vertical structures are symmetric to the $\mathrm{x}-\mathrm{z}$ plane at this Reynolds number, although the axisymmetric is lost.

The drag coefficients in the numerical simulation via IB-SEM are compared with the previous numerical and experimental results in Table 2 (Johnson and Patel 1999, Gilmanov et al. 2003, White 1974). According to Table 2, the numerical result well accords with the previous results.

The results were compared with results from the literature (Johnson and Patel 1999, Gilmanov et al. 2003). Satisfactory agreement is observed in Fig. 10.

## 5. Flow around a 3D porous structure

The three-dimensional pore flow simulation better accords with the actual conditions than the two-dimensional simulation. However, many problems are encountered with the three-dimensional simulation, such as high modelling and computational complexities. Based on the MPI and the Hamilton HPC, the calculation speed and efficiency are substantially improved with the required accuracy. The water flow in the pores between three dimensional particles is studied in this section. The simulation model is established as follows (see Fig. 11):

The flow was directly simulated in the void space of the resulting models using an IB-SEM system at various Reynolds numbers to investigate the effects of the particle


Fig. 11 Comparison of separation length


Fig. 12 The size of domain and distribution of particles
shape and grain size polydispersity on the hydraulic gradient. Fig. 12 (a) shows the pressure drop from front (red) to back (blue) of the porous medium that was created by IBM.

The simulation parameters are as follows: The number of particles is 27 . The size of the domain and the distribution of particles are shown in Fig. 12. The Reynolds number is 100 . Free-stream boundary conditions with $=$ $1.0, v=1.0$, and $w=0$ are applied to the inflow boundary. The time step is $d_{t}=0.001$. The threedimensional computational domain is decomposed into 1600 spectral elements and 1681 nodes in the $x$ - and $y$ directions, in each of which piecewise continuous nodalbased polynomial expansions with polynomial order $\mathrm{P}=4$ are applied.

From Fig.13, the results of simulation show that three IB-SEM system can reflect the pressure and velocity of water in three dimensions porous. In the three dimensional pore media, the water pressure presents obvious stratification phenomenon. And the pore medium has obvious hindrance to the fluid velocity. This simulation prepared for the three dimensional water inrush simulation. With the gradual increase of the seepage pressure, the threedimensional pore media is gradually destroyed from the inside to the outside, until the large-scale water inrush channel is formed and water inrush occurs.


Fig. 13 The simulation results of flow in porous media

This kind of water inrush usually occurs under the condition of large water pressure and loose filling medium. When the karst pipeline is exposed with excavation, the water and the filling medium will gush together and have a strong burst. Therefore, the prediction work must be done ahead of time before excavation.

## 6. Conclusions

The 3D IB-SEM system is established through the theory of Fourier transformation and the discretization of the 3D Navier-Stokes equations. Compared with previous research, this system yields accurate results.

Then, by using the open MPI and the Hamilton HPC service, the computing efficiency is increased substantially. Three-dimensional pore flow is successfully investigated.

## Acknowledgments

The work is supported by National Natural Science Foundation of China (Grant No. 51809158, 51809157), Shandong Provincial Natural Science Foundation, China (Grant No. ZR2018BEE045), China Postdoctoral Science Foundation (2018M630780).

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