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SIMULATION OF MOTION OF MULTIPLE PARTICLES IN A CLOSED CONDUIT USING THE LBM BASED APPROACH

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Abstract: *The two-dimensional numerical model of motion of multiple circular particles in fluid flow based on the lattice Boltzmann method (LBM) is presented. The flow is driven by the power-law velocity profile at the inlet in a closed horizontal conduit. Motion of particles consists of free motion in the flow, particle-bed and particle-particle collisions. The simulation for both movements of particles and velocity field of the flow is developed. Stability issues of the simulation are considered and a resolution using the entropic LBM and extension of computational resources is proposed. Finally, an enhancement of the simulation for more complex processes is suggested.*

Keywords: Motion of particles, Hydrodynamic forces, Lattice Boltzmann method, Entropic LBM.

1. Introduction

The motion of multiple particles in the flow in a closed horizontal conduit is examined. It consists of free motion in the flow, mutual collisions of particles and collisions with the bed. Simulation – based on the LBM – of both motion of particles and velocity field of the flow is developed. It is shown that the simulation produces results comparable to the outputs derivable from the explicit expressions for hydrodynamic forces.

The mathematical model consists of equations for the fluid flow (e.g., Navier-Stokes), equations of motion for particles in the flow (Newton equations) and equations for velocities before and after (both particle-bed and particle-particle) collisions which can be derived from relations for impulse forces. Typically, the fluid flow and the particle motion are solved separately and coupled every time step. The fluid flow equations are usually solved by some of the CFD methods while the motion of particles can be treated for example by the discrete element method (DEM).

In contrast, the methods based on the lattice Boltzmann equation (LBM) represent a numerical strategy which allows to solve particle-fluid systems within a unique frame (e.g., Yu & Fan, 2010). The LBM is a two decade old numerical approach originating from the lattice gas automata methods (LGCA) used for the simulation of complex fluid flows (e.g., Succi, 2001). The LBM represents a second order, efficient computational scheme due to its inherent locality and explicitness. Moreover, the possibility of straightforward parallelization yields another considerable advantage of the traditional numerical approaches to fluid flow problems.

2. Mathematical Model

The flow is driven by the power-law velocity profile at the inlet in a closed horizontal conduit with smooth boundaries. The flow field is described by the incompressible Navier-Stokes equations. The two-dimensional conduit has boundaries of two types: open boundaries (inlet and outflow) and solid boundaries. Each type of boundaries is represented by a different boundary condition.

The no-slip boundary condition – identification of the fluid velocity adjacent to the surface with the velocity of the surface – is supposed at the boundaries of the conduit $\mathbf{u}(\mathbf{x}_{con}) = 0$ as well as on the surface of the moving particles $\mathbf{u}(\mathbf{x}_{part}) = \mathbf{v}(\mathbf{x}_{part})$. At the outflow, the Neumann free flow – the so called "do

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nothing" – boundary condition is imposed which corresponds to the normal gradients of the velocity set to zero (e.g., Heywood, 1996).

The motion of a number (up to ten) of non-deformable particles in the flow is determined by actions of body and hydrodynamic forces. They are summed into the resultant net force

$$\mathbf{F}_{net} = -(m - m_f)\mathbf{g} + \rho A \frac{C_D}{2} v_r \mathbf{v}_r + m_f C_m \frac{d\mathbf{v}_r}{dt} + \rho A \frac{C_L}{2}(v_{rT}^2 - v_{rB}^2)\mathbf{e}_L \qquad (1)$$

where the first term stands for the gravitational force $\mathbf{F}_g$, the second term represents the drag force $\mathbf{F}_d$, the third term represents the force due to added mass $\mathbf{F}_m$ and the last term corresponds to the lift force $\mathbf{F}_L$ (Wiberg & Smith, 1985). The net force also develops a torque on the particles which determines their angular velocities ω.

Both the particle-bed and particle-particle collision models are derived from impulse equations of the form $m(\mathbf{v}' - \mathbf{v}) = \mathbf{J}$ which use the impulse force $\mathbf{J}$ as the measure of change of momentum (the quote mark distinguishes velocities before and after collisions). It is supposed that collisions take place in a very short time and all external forces can be neglected. If rotation is taken into account the corresponding impulse equation for the angular velocities before and after the collision reads as $I(\omega' - \omega) = r J_t$ where I stands for momentum of inertia. The above relations enable to derive expressions for new velocities after collisions for both the particle-bed and particle-particle collisions (Czernuszenko, 2009; Lukerchenko et al., 2006, 2009).

3. D2Q9 Lattice Model

The numerical model based on the LBM corresponding to the mathematical description above is designed for the set of nine discrete velocities $\mathbf{c}_i$ on two-dimensional square lattice – such a lattice is denoted by D2Q9. In the LBM the fluid is composed of fictive particles which propagate along the lattice links and interact in nodes. The fictive particles are represented by particle distribution functions $f(\mathbf{x}, \mathbf{c}_i, t)$ which give probabilities of finding of a fictive particle in a node $\mathbf{x}$ with a certain discrete velocity $\mathbf{c}_i$ in time t. The collision and propagation process follows from the lattice Boltzmann equation

$$f_i(\mathbf{x} + \mathbf{c}_i\Delta t, t + \Delta t) - f(x,t) = \frac{1}{\tau}(f_i^{eq} - f_i)$$

where the Bhatnagar-Gross-Krook (BGK) collision operator on the right-hand side is applied on particle distributions f_i in nodes and expresses the tendency to local equilibriums f_i^{eq} (Δt is lattice time step). The collision operator has to fulfill the first law of thermodynamics, i.e., conservation of mass and momentum.

In the case of the BGK approximation the LBM is subject to numerical instabilities at the sub-grid scale caused dramatic fluctuations of distributions f_i in neighboring nodes (e.g., due to very low/high viscosity/Reynolds number). However, if the parameter τ (which expresses the rate of tendency to the local equilibrium f_i^{eq}) is replaced by the factor $\alpha/2\tau$ where the parameter α represents a non-trivial root of equation $H(f + \alpha(f_i^{eq} - f)) = H(f)$, and H is the Boltzmann H-function of the form $H(f) = \Sigma f_i \ln(f_i / w_i)$ and w_i represents weights of respective discrete velocities $\mathbf{c}_i$ (Karlin et al., 2002, 2006). The collision term is then modified as $\alpha/2\tau(f_i^{eq} - f)$ which results in unconditionally stability of the method – even for high Reynolds number cases – while still retaining its locality and efficiency.

Boundary conditions mentioned above – for open boundaries of the inlet and the outflow, and the solid boundaries of the conduit – require the usage of different numerical schemes. Thus for the solid surface the so called bounce-back scheme is used $f_i(\mathbf{x}_{con}, t + 1) = f_{-i}(\mathbf{x}_{con}, t + 1/2)$ which consists in simple inversion of distributions along the directions incident to the boundary nodes. In the case of the moving surface the term $2w_i\,\rho(\mathbf{x}_{part}, t) / c_s^2\,(\mathbf{c}_i . \mathbf{v})$ corresponding to the exchange of momentum between fictive particles and the moving macroscopic particle is added to the inverted distributions. The specified velocity profile at the inlet is implemented by the Zou-He boundary scheme (Zou & He, 1996) which allows to impose velocity $\mathbf{u}(\mathbf{x}_{in}, t)$ or pressure $p(\mathbf{x}_{in}, t)$ on the boundary. In this case, only the non-equilibrium parts of distributions are bounced-back in the normal direction with respect to the boundary.

In the LBM frame motion of macroscopic particles in the flow is the effect of interaction of fictive particles with the solid surface of the macroscopic objects. The action of the objects on the flow is modeled as a special – moving – case of bounce-back boundary conditions considered above. Motion of macroscopic objects is caused by the momentum transfer $\Delta\mathbf{p}$ from the fictive particles to these objects. Time rate of this momentum transfer $\Delta\mathbf{p}\,/\Delta t$ defines the hydrodynamic forces by which the flow acts on the objects. The hydrodynamic forces are calculated as a sum over momentum contributions from all fictive particles incident to the boundary nodes of the objects

$$\mathbf{F}_{part} = \frac{\Delta\mathbf{p}}{\Delta t} = \sum_{bn}\sum_i 2\mathbf{c}_{-i}\left[f_{-i}^{c}\left(\mathbf{x}_{part},t\right) + w_i\frac{\rho\left(\mathbf{x}_{part},t\right)}{c_s^2}\left(\mathbf{c}_i\cdot\mathbf{v}(\mathbf{x}_{part},t)\right)\right] \tag{2}$$

with Δt = 1 (Aidun et al., 1998). Another two contributions to the hydrodynamic forces must be mentioned which comes from nodes covered (the force $\mathbf{F}_{cov}$ is exerted on the particle) or uncovered (the force $\mathbf{F}_{ucov}$ forms the negative impulse force increment.) by motion of a particle. Thus the hydrodynamic forces can be expressed as the sum $\mathbf{F}_{net} - \mathbf{F}_{g} = \mathbf{F}_{bn} + \mathbf{F}_{cov} + \mathbf{F}_{ucov}$, compare with equation (1). To update the particle position $\mathbf{x}(t)$ and its velocity $\mathbf{v}(t)$ the left-hand side of the Newton equations has to be integrated every time step. For this purpose, the leap-frog algorithm is chosen as it is simple, possesses second order accuracy, is invariant under time reversal and has other favorable global properties (Allen & Tildeley, 1987).

4. Results

Particle motions are simulated by means of two different techniques. First approach employs the LBM scheme as a fluid solver which is coupled to exactly evaluated hydrodynamic forces based on explicit relations (1). In the second approach the forces are evaluated within the LBM frame as sum of contributions from momentum transfers of fictive particles (2). The trajectories resulting from both techniques are compared to test robustness and applicability of the LBM approach for simulating motion of multiple particles.

It is supposed that the process is performed in a horizontal conduit of the length L = 1 m and height $L/20$. The flow is driven by the power-law velocity profile with maximal value $u(0, L/10)$ = 0.3 m.s^{-1} at the inlet. The radii of the moving particles are assumed to be in range $r \in (L/400, L/200)$. The particles are released from different vertical positions of the conduit with zero translational and rotational initial velocity $(v_{x0}, v_{y0}) = (0, 0)$ and $\omega = 0$. The process is examined with the sand-like particle of density ρ_p = 2.5× ρ_w. However, most of the input parameters are adjustable within a range of values, e.g., maximal inlet velocity, radii of the moving particles, density of both the fluid and the particle or viscosity.

Segments of three particle trajectories $\mathbf{x}(t)$ with respect to the length and height of the conduit expressed in lattice space units are depicted in Fig. 1. The particles undergo both translational and rotational motion, collide with each other (collisions are illustrated by arrows connecting centers) and collide with the bed. Although the trajectories calculated in two ways (described above) are similar they also differ partially. This can be caused for example by presence of experimentally determined coefficients in exact expressions (1) or by insufficient refinement of the lattice grid.

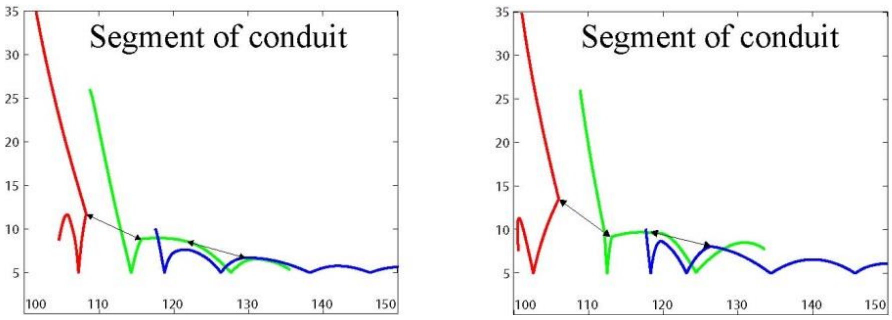

Fig. 1: Trajectories determined by forces: a) within the LBM frame or b) derived from exact expressions.

The low kinematic viscosity of water results in high Reynolds number $Re = uL/\nu \approx 10^5$ of the flow. The low value of the corresponding lattice viscosity ν^* means that the relaxation parameter $\tau \equiv \nu^*/c_s^2 + ½ \rightarrow ½$, and therefore the LBE method becomes potentially unstable because of incapability to dissipate the energy due to very large velocity gradients. The instability issues can be eliminated in various ways.

The entropic LBM represents a resolution of these issues due to its property of unconditional stability. However, calculation of the parameter α in each (potentially disruptive) node means solving the mentioned non-linear equation. This equation is usually solved by combination of the bisection and Newton-Raphson method. To eliminate computational demands the parameter α is evaluated only in nodes exceeding a tolerance value for the deviation $|(f_i^{eq} - f_i) \;/\; f_i\;| < 10^{-2}$, i.e., in nodes with large deviations of the population f_i from local equilibrium f_i^{eq}. Thus the entropic approach is applied at quite larger scale (than in Dolanský, 2013) because of better usage of mentioned parallel features of the LBM.

Except the above considered entropic LBM better stability can be also achieved by refining the lattice grid. However, such a refinement also yields a significant grow in demands on computational resources. Due to the inherently parallel nature of the LBM it can be handled by employing the Parallel Computing Toolbox (MATLAB) and other transformations enabling usage of the CUDA GPU computing technology.

5. Conclusions

The LBM based two-dimensional simulation for movements of particles and velocity field of the flow in a closed horizontal conduit is described. The robustness of the method is tested by comparison of trajectories and hydrodynamic forces evaluated either within the LBM frame (2) or calculated from explicit expressions (1). It is shown that in both cases trajectories and forces are similar though there are differences which can be caused by various reasons and will be subject to other considerations. Stability issues of the simulation are considered and a resolution using an extended LBE model and enhancement of computational resources is proposed. The LBM is extended into the so called entropic LBM to guarantee the stability of the computation. The need for increase of computational resources results in employing the parallel features of the LBM. Thus, regarding stability and accuracy the LBM is shown to be suitable for ongoing development of the simulation. It is planned to extend it to motion of cluster of interacting particles in the fluid to observe mutual influence of the flow and the cloud of particles.

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