Study of particle rotation effect in gas-solid flows using direct numerical simulation with a lattice Boltzmann method

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Background

Gas-solid multiphase flows are prevalent in many fossil fuel processes such as gasification and combustion.

Advanced computational technique known as the computational fluid dynamics (CFD) has been recognized as an emerging tool that is able to reduce the time and cost in the design and scale-up of the multiphase reactors involved in those processes, and has been applied in typical equipment such as fluidized bed gasifiers and chemical looping combustion reactors.

The capability of the CFD in correctly predicting multiphase flow dynamics relies heavily on accuracy of sub-models that account for particle-fluid interactions and particle-particle interactions. The overall objective of our proposed research is to improve fundamental understanding of such interactions, and to formulate a new drag model with particle rotation effects that can be applied to reactor scale simulations

Objectives

The emphasis of our proposed work is to address effects of particle rotation in gas-solid flows with the following specific aims:

- direct impact of particle rotation on the average particle-fluid drag force of a particle suspension at various Reynolds numbers.
- indirect impact of particle rotation on the drag force through the change in the particle concentration distribution, or the microstructure of a flow.
- role of particle rotation in energy dissipation of the particle-fluid system.

Research Setup

Hardware

Workstation
Supercomputer

Software

Linux Operating system
Gfortran compiler
MFIX code from DOE/NETL

Human Beings

Developing computer software codes with hardware and software to achieve our objectives

Project Status

One HP workstation computer with 8 CPU cores, 8 gigabytes Random Access Memory (RAM), and 1 trillion bytes hard drive memory was purchased.

The DOE/NETL 2012-version MFIX software has been downloaded onto our recently-purchased workstation computer.

Modification of the existing code for direct numerical simulations of gas-solid flow is in progress. The accuracy of our immersed boundary-lattice Boltzmann method (IB-LBM) has been improved to the second order accuracy in order to achieve high-fidelity simulation results in the near future, whereas the traditional immersed boundary-lattice Boltzmann method only gives first order accuracy.

First Order Accuracy vs. Second Order Accuracy

- Order means how fast the solution will converge as the mesh size, usually denoted as a grid size (dx), approaches zero.

- Usually, higher order methods give more accurate results on the same mesh.

- The traditional immersed boundary-lattice Boltzmann only gives first order accuracy. The second order accurate method is adapted in our modified computer code in order to account for the rotation of particles in the flow and produce results with a higher level of fidelity.

Immersed Boundary Method (IBM) for particulate flow

Advantage

- The no-slip/no-penetration (NS/NP) is easily imposed by adding additional force to the flow in the vicinity of the surface of a particle
- Does not need regridding when particles are moving

Disadvantage

- The approximation of NS/NP is hard to be exactly imposed.
- Traditional IBM only yields first-order accuracy.

Recent improvement of IBM

- Multidirect forcing scheme to reduce the NS/NP error (Luo et al. 2007)
- A slight retraction (Hofler and Schwarzer 2000) of Lagrangian markers from the surface of a particle towards the interior of the particle is used to enhance the accuracy of IBM.
- Breugem (2012) demonstrated that the improved IBM coupled with traditional incompressible NS-solver gives a second order of convergence

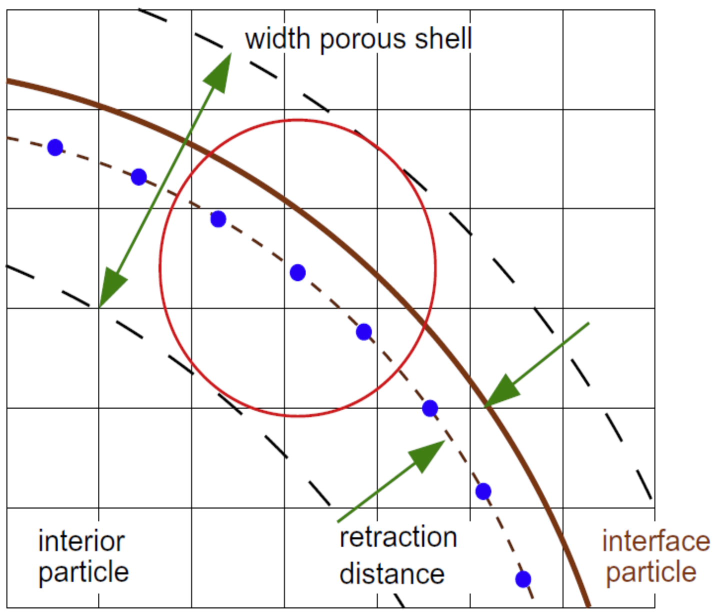


Fig. 3. Illustration of the porous shell covering a solid particle. The dots indicate the position of Lagrangian grid points, which are retracted from the actual interface (the solid line) with a fraction of the Eulerian grid spacing (about $0.3\Delta x$ in this case). The circle depicts the range of action of the regularized Dirac delta function.

Our Present work: embed the improved IBM into LBM

- Use relaxation technique to further reduce the NS/NP errors in the multi-direct forcing procedure

change $\mathbf{u}^{**,s} = \mathbf{u}^{*} + \Delta t \mathbf{f}^{s}$ *to* $\mathbf{u}^{**,s} = \mathbf{u}^{*} + \Delta t(\mathbf{f}^{s-1} + \omega(\mathbf{f}^{s} - \mathbf{f}^{s-1}))$

- Use classic fourth order Runge-Kutta scheme to advance the position, the linear momentum and angular momentum of a particle.

In the framework of the improved IBM-LBM, we can not directly get the flow information in the fractional time step between *nΔt and (n+1) Δt* . We get the flow information by simple extrapolation:

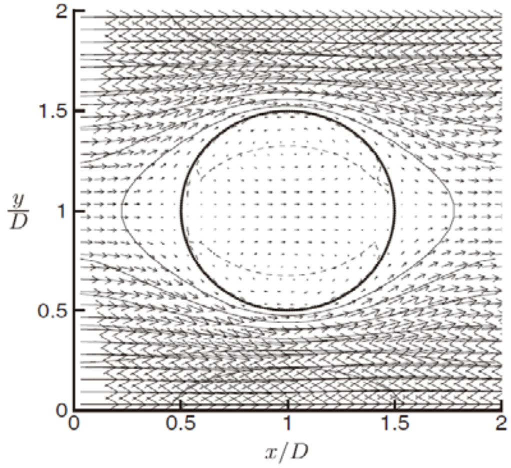
$$\mathbf{u}^{*} = \mathbf{u}^{n} + \alpha \Delta t (rsh^{n})$$

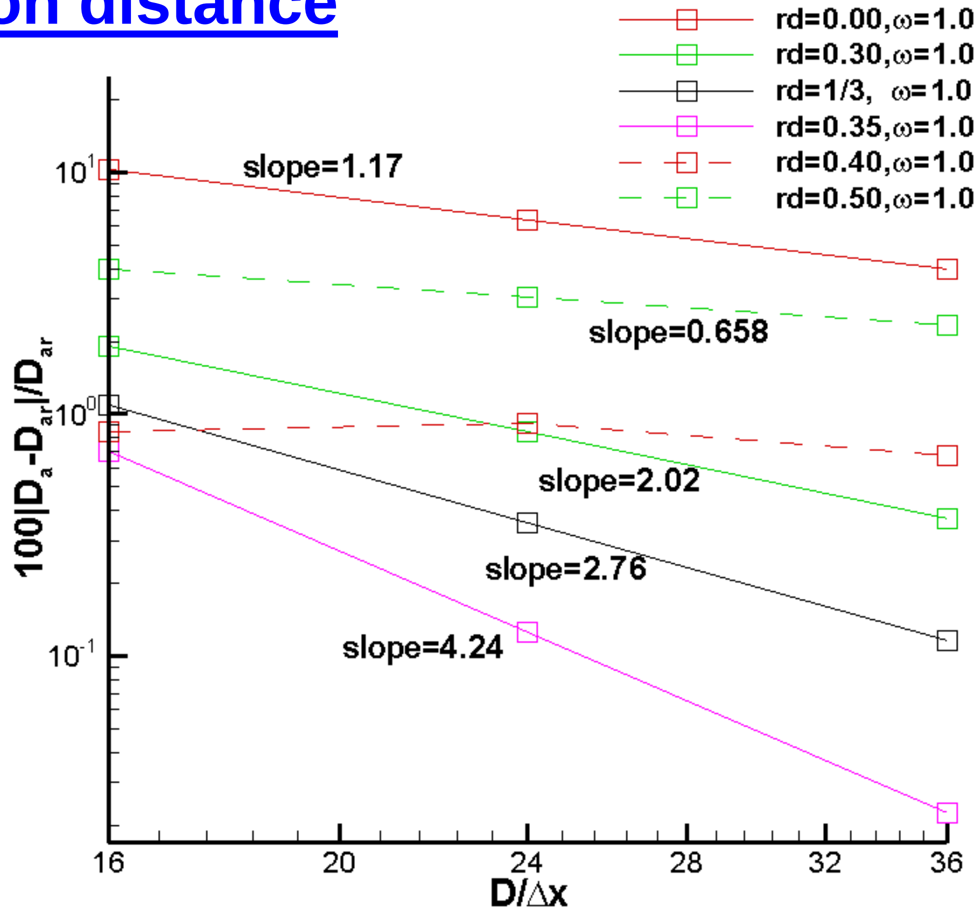
Numerical Test 1:Darcy problem (3D)

influence of retraction distance

- laminar flow through a simple cubic lattice of a fixed sphere (Breugem (2012))
- The sphere is fixed in the center of the domain.

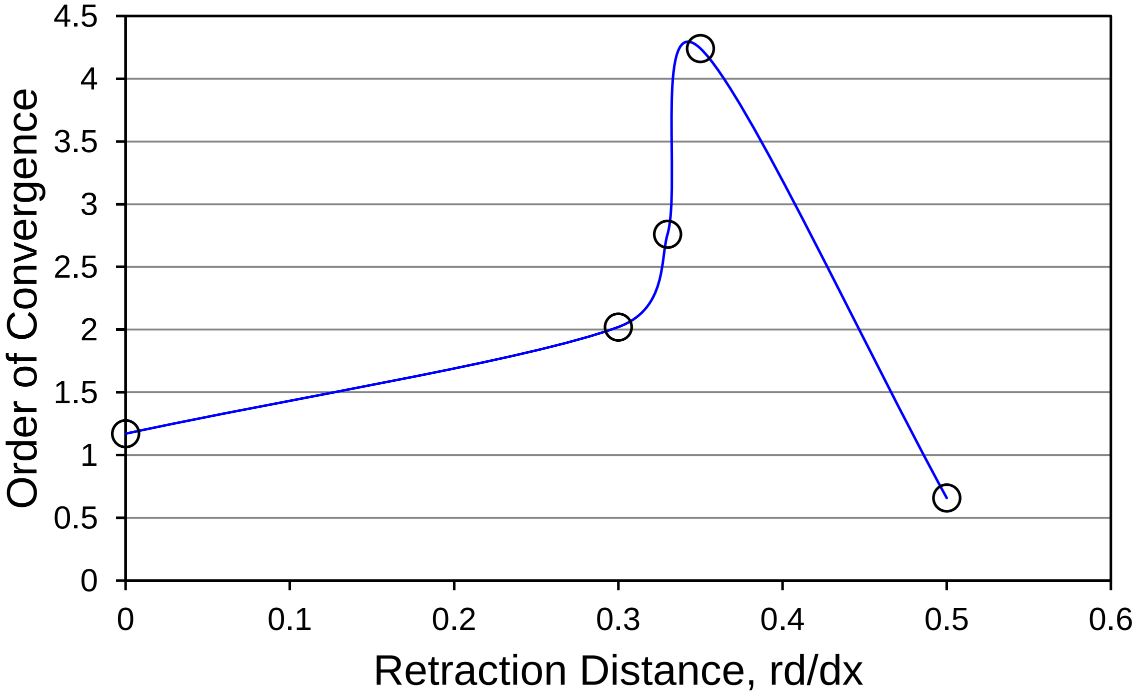
$$Da = \frac{\mu_f U_b}{(-dp_e/dx)D^2}.$$



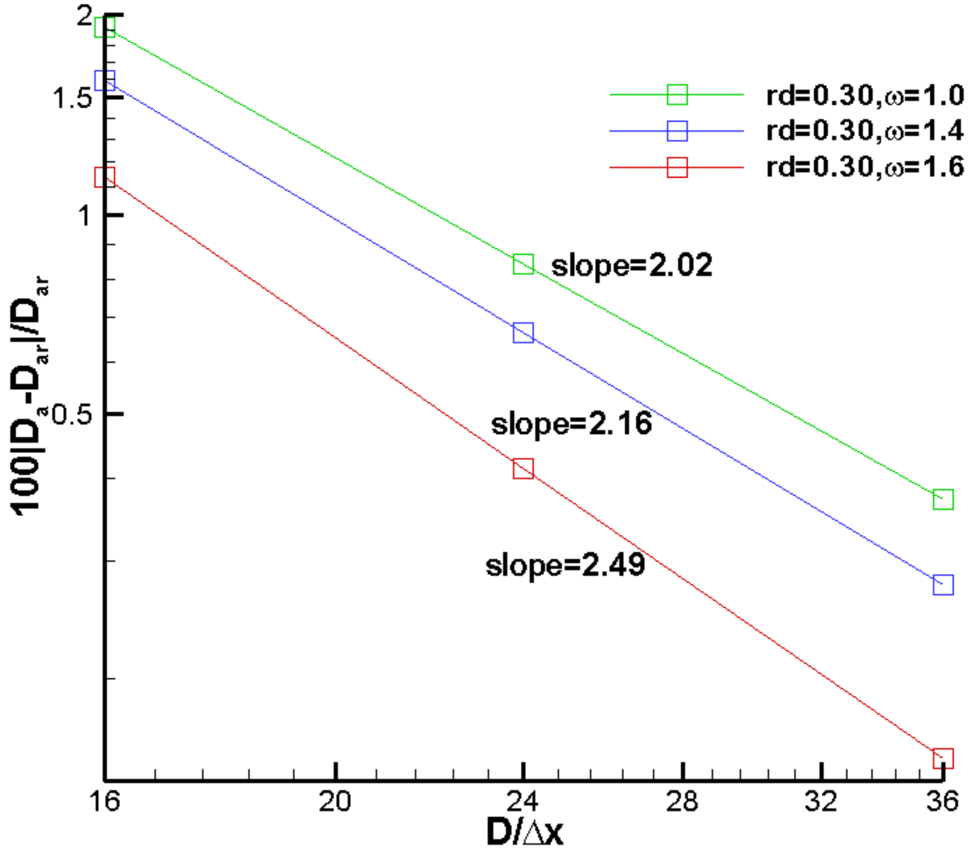


Convergence of the Darcy number

Convergence order of the Darcy number at various retraction distance and the relaxation coefficient ω=1



Numerical Test 1:Darcy problem (3D)
influence of relaxation coefficient

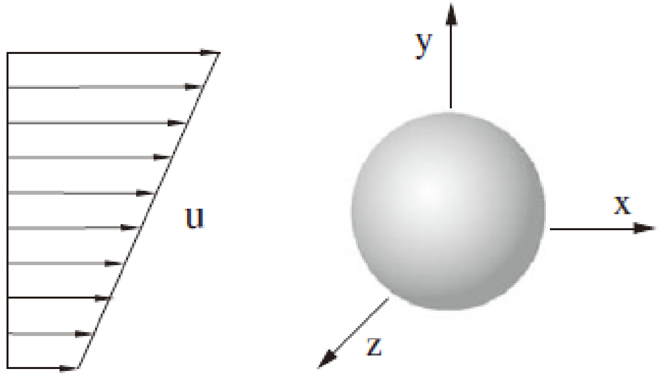


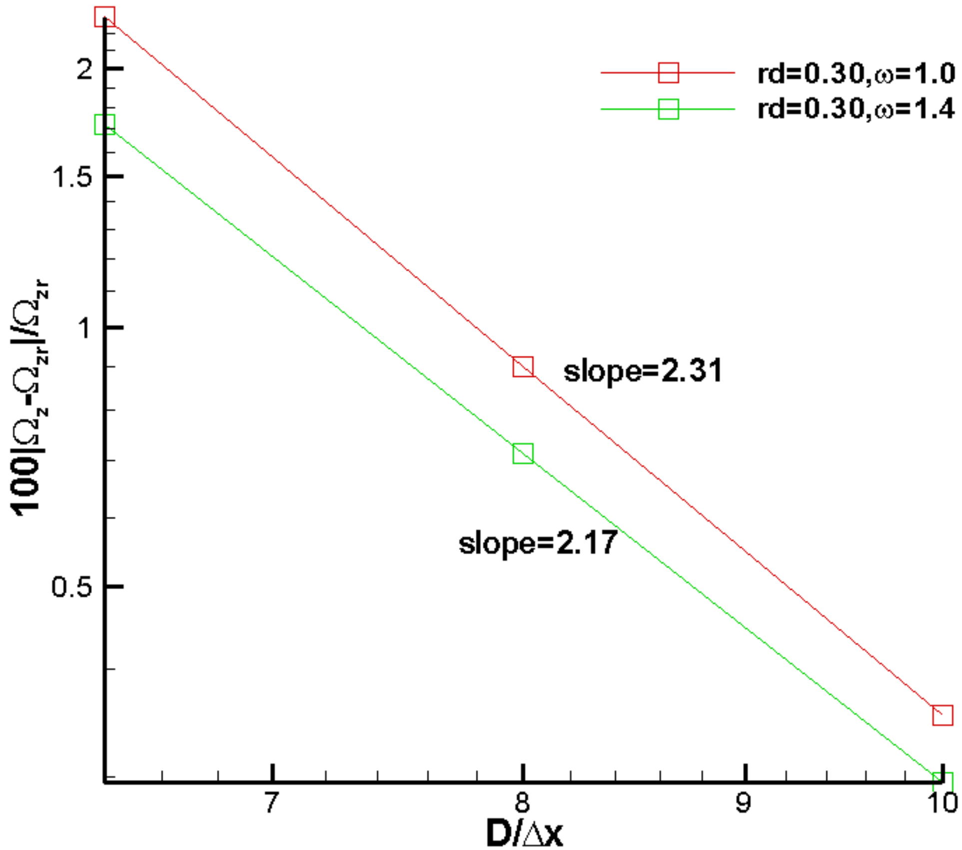
Convergence of the Darcy number

Numerical Test 2:Particle rotation in a simple shear flow

- Rotation-free but fixed in the position (Kempe and Frohlich (2012))

$$\mathbf{u}(y) = U_0 + Sy$$

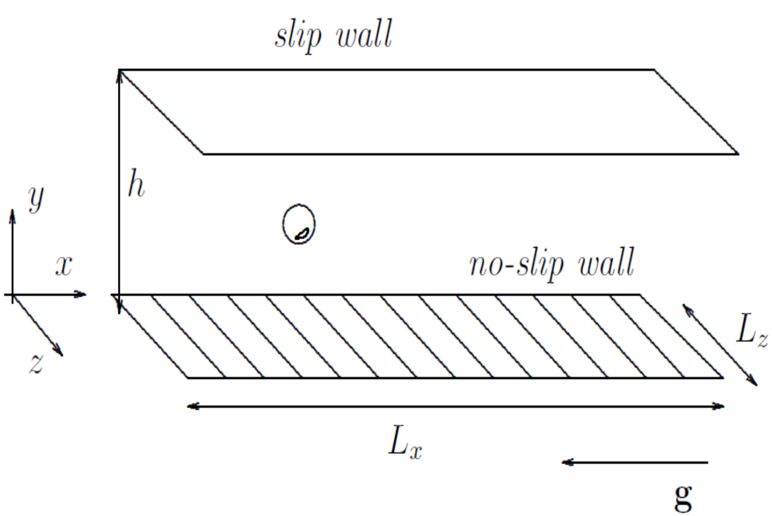




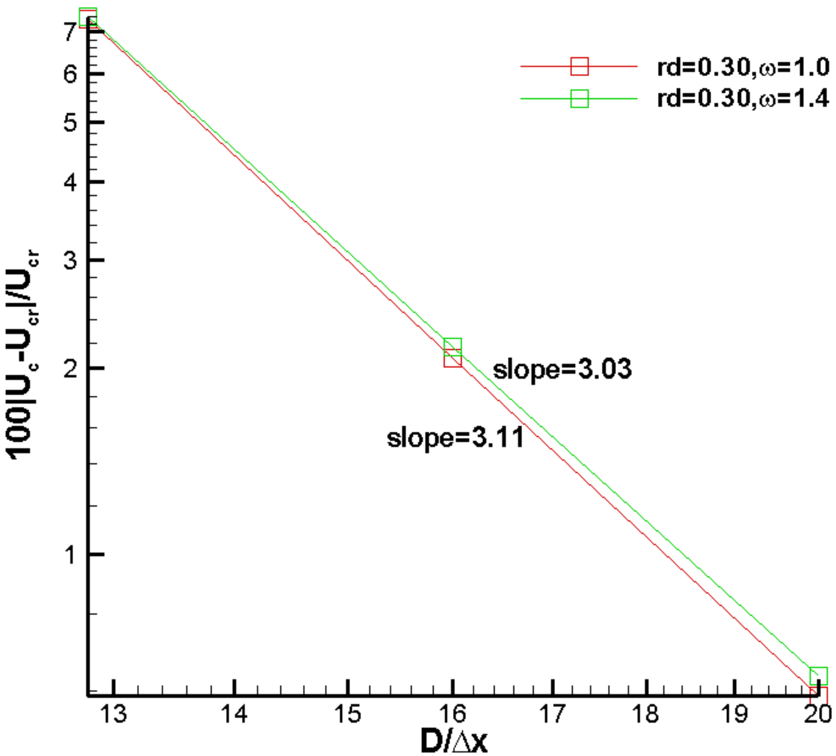
Convergence of the angular velocity

Numerical Test 3: Freely moving sphere in plane Poiseuille flow

- Free to translate and rotate (Uhlmann (2006))



Schematic of the geometry for the case of particulate flow in a plane half-channel.



Convergence of the sphere velocity in x direction at the dimensionless time t=0.999

- Through the numerical tests shown above, we can see that LBM and IBM is coupled sucessfully through the classical fourth order Runge-kutta scheme.
- The overall accuracy reaches second-order. Super-convergence can be achieved (up to fourth-order) when retraction distance (0.30dx—0.35dx) and relaxation coefficient (1.4-1.6) are chosen properly.
- The increase of the accuracy from first-order to second can save us lots of computation time in the near future when massive computation is performed in the sense that less grid points can be used to reach the satisfying computational results

Technical approach to achieving the project goals

- Our work will be carried out by using direct numerical simulation (DNS) of particle-fluid systems with a novel lattice Boltzmann method. The immersed boundary condition LBM (IB-LBM) technique with the no-slip condition on particle surfaces will adopted for our research project.

- The direct-forcing method adopted in our study provides a smoother computational boundary for particles and is capable of achieving results at higher Reynolds number flows in comparison with the conventional LBM.

- The OSU research group's ongoing effort in parallelization of the code will enable simulation of a large number of particles. With the IB-LBM approach and the hard sphere collision model, the DNS will be conducted for particle-fluid systems with $10^2 \sim 10^3$ particles. Particularly, freely-evolving particles will be investigated to analyze effects of collision on particle distribution, averaged drag force, and energy dissipation.

Main advantages of the IB-LBM

- Memory and Central Processing Unit (CPU) savings
- Easy grid generation compared to unstructured grid methods.
- Bodies of almost arbitrary shape can be handled with the immersed boundary condition LBM (IB-LBM) technique.

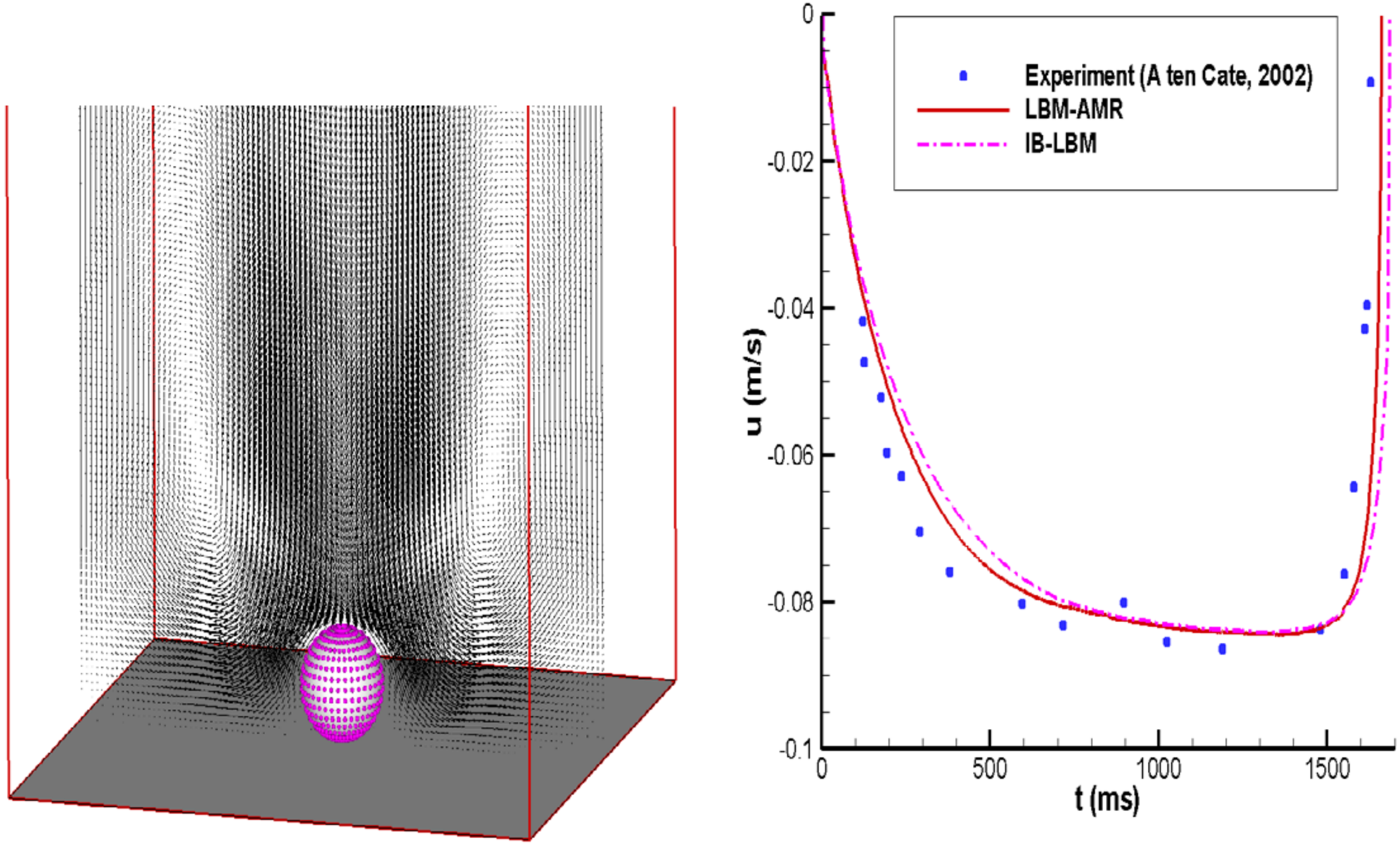
Capability of the existing IB-LBM code

- The OSU research group (see Figure 1(a)) demonstrates the simulated velocity field during the sedimentation of a 15 mm spherical particle in silicon oil.

- The simulated particle velocity is compared with the experimental result and the adaptive mesh refinement (AMR) simulation result.

- The simulation with the IB-LBM method proves its accuracy in capturing the fluid-particle drag force as well as the interaction between the particle and the bottom wall, which are both critical for the proposed purpose in fluid-particle system simulations (see Figure 1(b)).

Figure 1 (a) A slice of the velocity field in the symmetry plane when the particle touches the bottom of the container. (b) Particle velocity simulated by the IB-LBM and LBM-AMR approaches is compared with the experimental data taken at *Re* = 11.6.



(a) (b)

Future Work

Direct numerical simulations of gas-solid flow

- modification of the existing code
- simulations with particles frozen in suspensions
- simulations in freely evolving suspensions

Analysis of simulation results

- Micro-structures of particles
- Translational and rotational fluctuations

Validation using Eulerian-Eulerian simulations

- Install new drag models into MFIX
- Perform simulations of selected experimental gas-solid risers
- Compare new drag models with existing drag models