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Supplementary Information

Inertial focusing of spherical particles in rectangular microchannels over a wide range of Reynolds numbers

Chao Liu,[a] Guoqing Hu,*[a] Xingyu Jiang,[b] Jiashu Sun*[b]

[a] *State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China. E-mail: Guoqing.hu@imech.ac.cn*

[b] *Beijing Engineering Research Center for BioNanotechnology & CAS Key Labtorary for Biological Effects of Nanomaterials and Nanosafety, National Center for Nanoscience and Technology, Beijing 100190, China. E-mail: sunjs@nanoctr.cn*

S1 Governing equations and numerical methods

The governing equations for the incompressible flow of a Newtonian fluid are

$$\nabla \cdot \mathbf{u} = 0 \tag{S1a}$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho_f}\nabla p + \nu \nabla^2 \mathbf{u} \tag{S1b}$$

where $\mathbf{u}$ is the fluid velocity and the gravitational force is neglected in the present study.

The force on a particle is calculated by integrating the total stress across the particle. The motion of a rigid spherical particle follows Newton's second law of motion

$$m_p \frac{d\mathbf{U}_p}{dt} = \int_{\Sigma} (-p\mathbf{1} + \boldsymbol{\tau}) \cdot \mathbf{n} d\sigma + m_p \mathbf{g} \tag{S2a}$$

$$\frac{d(\mathbf{I} \cdot \boldsymbol{\Omega}_p)}{dt} = \int_{\Sigma} (\mathbf{x} - \mathbf{x}_{cm}) \times [(-p\mathbf{1} + \boldsymbol{\tau}) \cdot \mathbf{n}] d\sigma \tag{S2b}$$

where m_p is the mass of the particle, $\mathbf{1}$ the unit tensor, $\mathbf{I} = diag(8\pi\rho_p a^5/15)$ the moment of inertia tensor of the particle, and $\mathbf{x}_{cm}$ the position of the center of mass. The nondimensional force coefficient, C_L, is given as

$$C_L = \frac{F_L}{(\rho_f U_{\max}^2 a^4 / H^2)} \tag{S3}$$

The governing equations are then discretized and numerically solved on structured overlapping grids in the Overture C++ framework[1]. The present computational domain consists of four structured component grids: a Cartesian background, orthographic patches at two poles of a sphere and the sphere with its poles removed to avoid coordinate singularities (Fig. 1(b)). The solutions between different component grids are coupled by interpolating the flow variables of the grid points at the boundary of a component grid from the variables of other component grids. The body fitted grids marching outward the particle surface match well with the background grid in size to obtain a high quality of interpolation. During the motion of the sphere, the overlapping grids are updated at every time step to maintain high quality.

The no-slip wall boundary conditions are imposed on the channel walls and the surface of particle. The Poiseuille-flow velocity profile for a rectangular cross-section is imposed on the inlet

$$u(y,z)=\frac{4H^2\Delta p}{\pi^3\mu L}\sum_{n,odd}^{\infty}\frac{1}{n^3}\left[1-\frac{\cosh\left(n\pi\frac{z}{H}\right)}{\cosh\left(n\pi\frac{W}{2H}\right)}\right]\sin\left[n\pi\left(\frac{y}{H}+\frac{1}{2}\right)\right] \qquad \text{(S4)}$$

where L is the channel length and Δp the pressure difference between the inlet and the outlet. The outflow boundary condition assuming fully developed flow with the constriction of $p+\partial p/\partial n=0$ is imposed on the outlet.

A second-order Adams predictor-corrector method is used for time stepping in solving the incompressible N-S equations[2]. The N-S equations is briefly written to facilitate discussion as follows

$$\frac{\partial \mathbf{u}}{\partial t}=f(\mathbf{u},p) \qquad \text{(S5a)}$$

$$f(\mathbf{u},p)=-(\mathbf{u}\cdot\nabla\mathbf{u})-\nabla p+\nu\Delta\mathbf{u} \qquad \text{(S5b)}$$

In the time stepping, the viscous term is treated implicitly with an implicit factor of 0.5 (Crank-Nicolson method) and other terms are explicitly treated. The function $f(\mathbf{u},p)$ is split into explicit and implicit parts, $f_E=-(\mathbf{u}\cdot\nabla\mathbf{u})-\nabla p$ and $f_I=\nu\Delta\mathbf{u}$.

The predictor and corrector steps are defined as

$$\frac{\mathbf{u}^{p}-\mathbf{u}^{n}}{\Delta t}=\frac{3}{2}f_{E}^{n}-\frac{1}{2}f_{E}^{n-1}+\frac{1}{2}f_{I}^{p}+\frac{1}{2}f_{I}^{n} \quad \text{(S6a)}$$

$$\frac{\mathbf{u}^{n+1}-\mathbf{u}^{n}}{\Delta t}=\frac{1}{2}f_{E}^{p}+\frac{1}{2}f_{E}^{n}+\frac{1}{2}f_{I}^{n+1}+\frac{1}{2}f_{I}^{n} \quad \text{(S6b)}$$

where the superiors p, $n-1$, n and $n+1$ represent the time level at which the equations are solved. The CFL number is set to be 0.75 for all cases to guarantee the stability of numeric solutions. A second-order accurate centered difference scheme is applied to the spatial discretize the convective and viscous terms.

The Poisson equation for pressure is implicitly solved to obtain vanishing divergence. The linear system derived from the pressure equation is iteratively solved using the stabilized bi-conjugate gradient method (BiCG-Stab) with the incomplete LU preconditioner (ILU). The solving process is done by PETSc software package, which has an interface to the Overture framework[3]. The elliptic type pressure equation is efficiently solved on the overlapping grid using the multigrids method.

S2 Entrance effect

The entrance length L_e, which refers to the channel length that needed to achieve a fully developed velocity profile, is expressed as:[R2]

$$L_e = 0.06D\,\mathrm{Re} \quad \text{(S7)}$$

where D is the hydraulic diameter, D = 2HW/(H+W) (H is the channel height, W is the channel width). For the case of AR = 6 (the hydraulic diameter D = 85.7 μm) and Re = 300, the entrance length L_e is:

$$L_e \approx 1.54\ \mathrm{mm}$$

The length that has developing velocity profile is a small portion of the whole channel length of 60 mm. Therefore, the developing velocity profile has little influence on the particle migration.

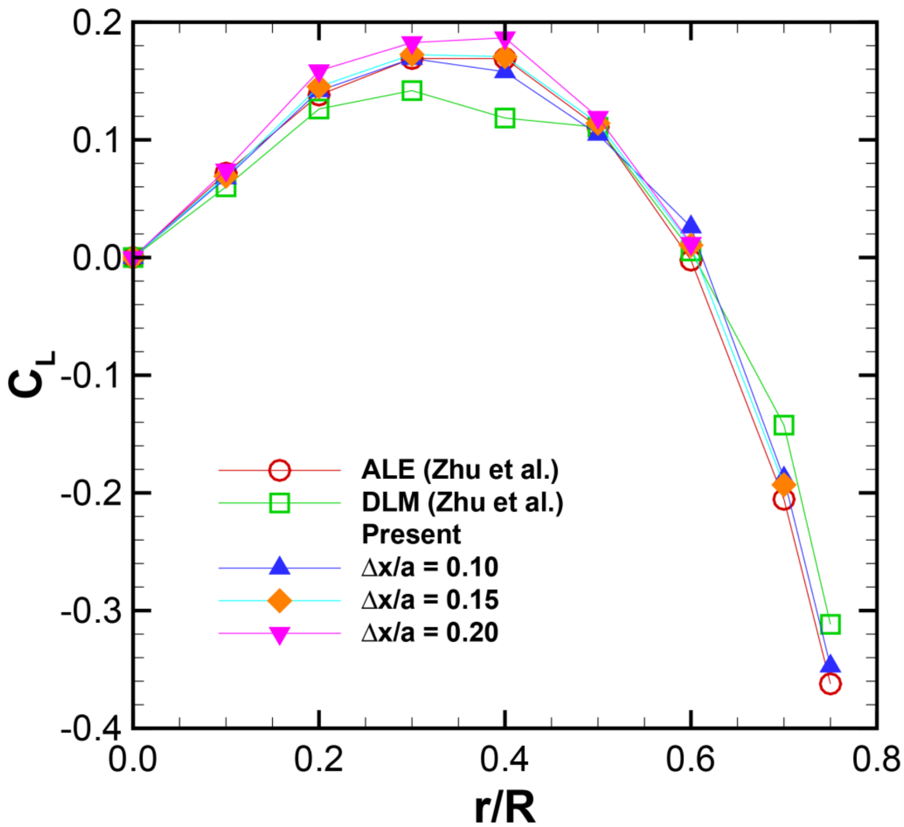

Fig. S1 The nondimensional lift coefficients of a sphere with $\kappa = 0.15$ at various radial positions of a tube at $\mathrm{Re} = 100$. The results from ALE (open circles), DLM (open squares) codes by Zhu *et al.*[5] and our results (solid marks) are in good agreement.

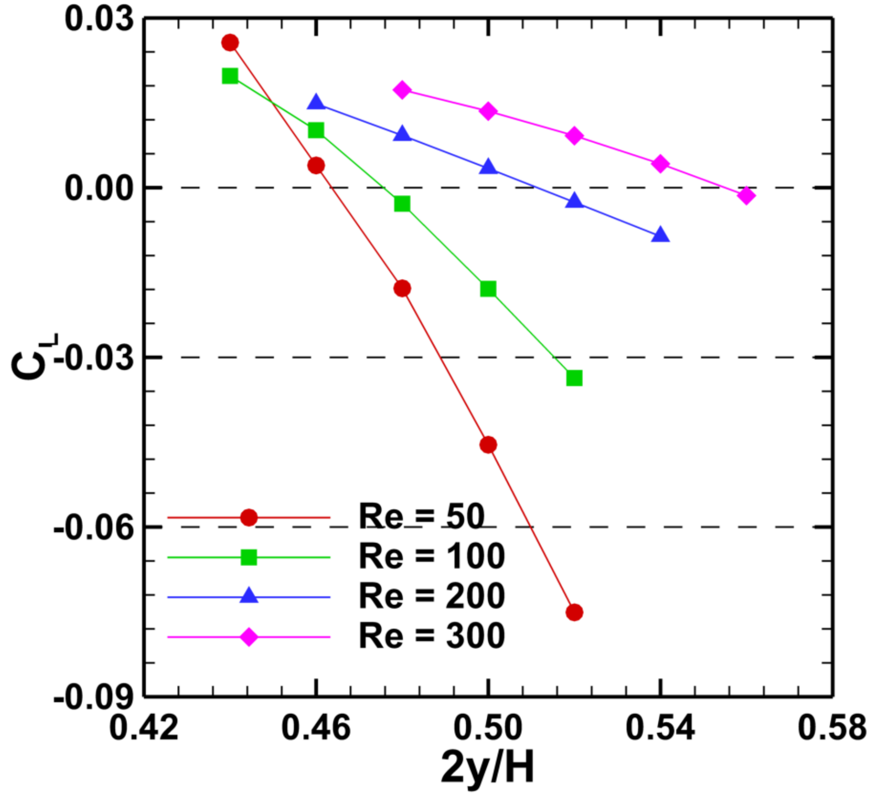

Fig. S2 The 2y/H for the curves shown in Fig. 6 are determined as 0.46, 0.48, 0.52 and 0.55 for Re = 50, 100, 200 and 300, respectively.

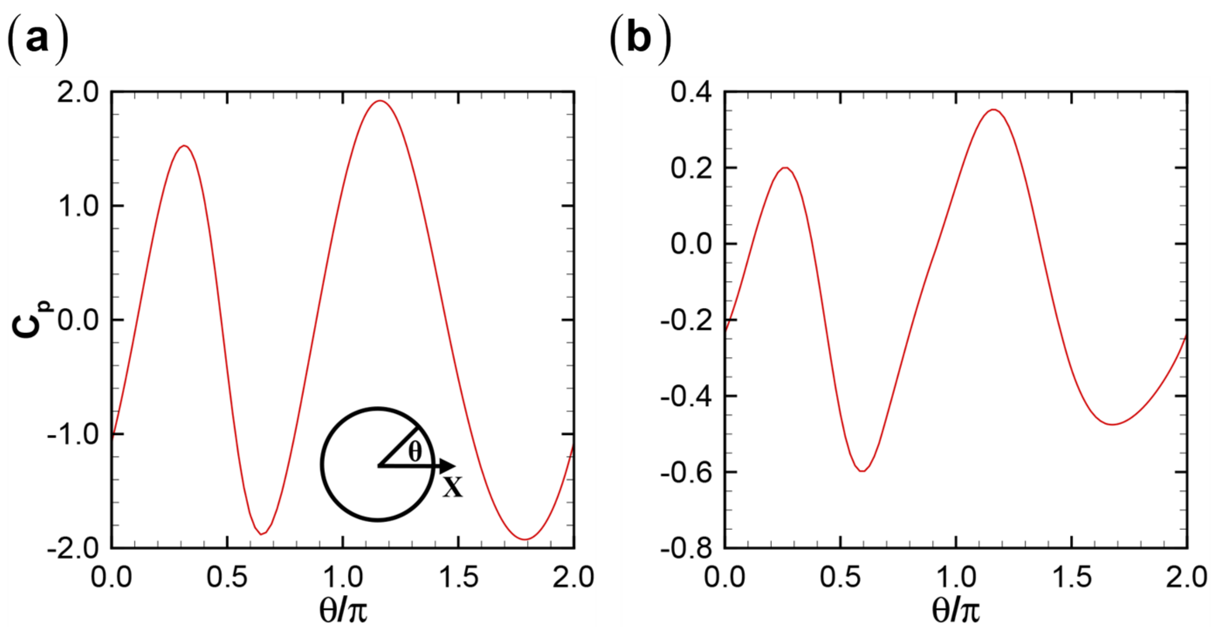

Fig. S3 The distribution of nondimensional pressure coefficient on the sphere with $\kappa = 0.3$ in the $2y/H = 0.55$ plane for (a) $\mathrm{Re} = 50$ and (b) $\mathrm{Re} = 300$. The angle θ donates the angle between the radial vector and the x-axis (main flow direction).

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