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Original Research Paper

A modified direct method for void fraction calculation in CFD–DEM simulations

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ABSTRACT

The void fraction of computational cells in numerical simulations of particulate flows using computational fluid dynamics–discrete element method (CFD–DEM) is often directly (or crudely) calculated assuming that the entire body of a particle lies in the cell at which the particle centroid resides. This direct method is most inexpensive but inaccurate and may lead to simulation instabilities. In this study, a modified version of the direct method has been proposed. In this method, referred to as the particle meshing method (PMM), the particle is meshed and the solid volume in a fluid cell is calculated by adding up the particle mesh volume with the basic working principle being the same as that of the direct method. As a result, the PMM inherits the simplicity and hence the computational advantage from the direct method, whilst allowing for duplicating the particle shape and accurate accounting of particle volume in each fluid cell. The numerical simulation characteristics of PMM including numerical stability, minimum particle grid number, prediction accuracy, and computational efficiency have been examined. The results showed that for a specific cell-to-particle size ratio, there was a minimum particle grid number required to reach the stable simulation. A formula of estimating the minimum particle grid number was derived and discussed. Typically, a particle grid number of about 5 times the minimum number was suggested to achieve the best computational efficiency, which was comparable or even higher than that of simulations using the analytical approach. PMM also exhibited the potential to be applied for complex computational domain geometries and irregular shaped particles.

1. Introduction

Computational fluid dynamics–discrete element method (CFD–DEM) simulation of particulate flows prevailing in industrial processes has become increasingly popular in the past few decades [see e.g., 1,2–5]. Generally, the CFD–DEM method has been proved to be effective in capturing the majority of macro- and micro-scale characteristics of the fluid–solid two-phase flow, whilst providing insight into the underlying science specifically at the particle scale. The quality of prediction results of the CFD–DEM simulation however is found to be strongly relying on the accurate account of the presence of particles in the two-phase flow.

The presence of solid particles in CFD–DEM simulations of the two-phase flow is considered by incorporating the volume fraction of the solid phase in computational fluid cells into the governing equations. The solid volume fraction is commonly calculated by a direct or crude method assuming that the entire body of the particle lies in the fluid cell at which the particle centroid resides [1,2]. This direct method is computationally inexpensive as it only involves searching of the particle centroid host cell. However, the direct method may lead to large errors when the particle centroid is near the fluid cell boundaries. Such large errors might yield a significant fluctuation in the value of cell void fraction when the particle centroid moves in and out of the fluid cell leading to simulation instabilities and unrealistic particulate flow behaviours.

Attempts have been made towards the accurate calculation of cell void fraction. Chen et al. [6] analytically calculated the void fraction in a one dimensional (1D) CFD–DEM simulation to solve classical soil mechanics problems. The 1D implementation of the analytical approach is quite straightforward. Li [7] analytically calculated the void fraction on two-dimensional (2D) structured meshes in the CFD–DEM simulation of flow structure formation and evolution in dense gas–solid flows. Freireich et al. [8] and Peng et al. [5] detailed the three-dimensional (3D) analytical solution of void fraction in structured rectangular cells. Wu et al. [9] derived a

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Nomenclature

A	factor (–)
$\mathbf{A}$	face area factor
d	diameter (m)
$\mathbf{f}_c$	collision contact forces acting on the particle (N)
$\mathbf{f}_f$	total fluid forces acting on the particle (N)
$\mathbf{f}_d$	drag force (N)
$\mathbf{f}_{sg}$	local mean particle-fluid interaction forces (N)
g	acceleration of gravity (m/s^2)
I	particle inertia (kg m^2)
l_0, l_1, l_2	domain dimension (m)
m	particle mass (kg)
N_p	particle number inside a cell
$N_{c,b}$	total number of computational cells that cover the fluidised bed of particles
p	pressure (Pa)
r	radius (m)
S_c	equivalent cell size (m)
T	torque acting on the particle (N m)
U_{sf}	gas superficial velocity (m/s)
$\mathbf{u}$	fluid velocity vector (m/s)
V	volume (m^3)
V_e	volume of particle grid (m^3)
$\mathbf{v}$	particle velocity vector (m/s)
$\mathbf{x}$	coordinates of a point (m)

Greek symbols

α	fraction of particle volume divided by a fluid cell (–)
β	momentum exchanging coefficient (–)
γ	scaling factor (–)
δ	contact overlapping (m)
ε	local void fraction
Δt	time step (s)
λ	size magnification factor from template particle to real particle (–)
μ	shear viscosity (kg/(m s))
ρ	density (kg/m^3)
τ	viscous stress tensor
ψ	normalised net mass flow rate
Λ	mass flow rate through cell faces (kg/s)
φ	cell-to-particle size ratio
ΔV_c	computational cell volume (m^3)
χ	operator sign (–)
Θ	granular temperature (m^2/s^2)
$\boldsymbol{\omega}$	particle angular velocity (rad/s)
ϑ	average deviation in the calculation of cell void fraction by PMM

General subscripts

d	drag
f	face
g	gas phase
i, j, k	particle index
min	minimum
max	maximum
p	particle phase
pg	particle grid
r	relative
x, y, z	direction

set of equations to analytically solve the cell void fraction on both 2D and 3D unstructured meshes. The analytical solution is computationally very expensive as evaluations of trigonometric functions need to be conducted at every time step [10].

Various non-analytical approaches have also been reported in the literature for the calculation of cell void fraction. For example, Link et al. [11] and Khawaja et al. [12] represented a particle as a porous cube. The size of the cube depended on the particle diameter and a constant scaling factor. Using the fictitious porous cube, the presence of particles was weakly felt by the fluid flow. As such, grid refinement did not lead to local extremes in the void fraction field, and hence the solution was grid independent. Lim et al. [13] calculated the void fraction for a fluid cell grouped together with its surrounding cells via the direct method. This method added stability by calculating the cell void fraction for a larger virtual cell that comprised several real fluid cells. However, this technique also added greater spatial smoothing to the averaging procedure since quantities such as velocity and pressure were calculated for the real fluid cells, but void fraction was calculated on a larger volume scale. Moreover, this method may lead to large errors if the local cell void fraction is vastly different from that of the larger virtual volume, e.g., in bubbly fluidised beds. Following the approach used in the local averaging of granular materials, Kuang et al. [14] proposed a more general method in this regard using virtual spherical cells containing local points of interest. The porosity and the source terms due to particle–fluid interactions were calculated for the virtual spherical cells and then mapped into CFD cells. Sun et al. [15] and Xiao and Sun [16] assumed that each computational cell accepts contributions from all of the particles in the system. Based on the assumption, the local cell void fraction was calculated through a statistically averaging approach using a weighting function that is similar to the estimation of probability density function from discrete points. Inevitable statistical error exists in this approach and strongly depends on the form of the weighting functions and the parameters (e.g. bandwidth). Moreover, the implementation of this approach has a computational complexity of the order of $O(N_pN_c)$, as all particles and cells need to be visited and examined at each time step. Gui et al. [17], Hilton et al. [18] and Hobbs [19] used regular squares or cubes to subdivide the particles. Apparently, the regular squares or cubes cannot provide a smooth representation of particle boundaries and thus unavoidably introduces error. Hilton et al. [18] minimised the error by linearly approximating the particle boundary, but the method is limited to spherical or regular non-spherical particles (e.g. ellipsoids and cuboids) and simple geometries (only in which the recursive approach and the linear approximation can be implemented). Boyce et al. [10] proposed a square-grid method, in which the distribution of particle volume on a square grid was calculated and then mapped on to the computational fluid cells that can be of arbitrarily complex shape. The method has an obvious source of inaccuracy as it is very likely that a fraction of the particle volume can be registered as being in a fluid cell in which the particle is not located, considering the squared cell is larger and contains several fluid cells.

As a whole, the simplistic nature of the current non-analytical approaches can compromise the accuracy of the calculation for the flexibility to cope with complex domain geometries. However, as repeatedly indicated in the literature [see e.g., 4,5], the accurate calculation of cell void fraction is a must in CFD–DEM simulations to ensure the numerical stability and the reliability of prediction results. Moreover, in most of practical problems the simulation needs to deal with complex geometries and/or irregularly shaped particles. The implementation of the analytical approach becomes extremely difficult and very computationally demanding.