Application of the discrete element method (DEM) to particle laden multi-phase flows

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Abstract. The discrete element method (DEM) coupled with methods for computational fluid dynamics (CFD) is a very capable instrument to capture particle-laden multi-phase flows. While often the flow around individual particles is not resolved on the CFD-side particle interaction is captured in detail. More recently resolved flow simulations have gained in popularity which can be also based on the Lattice Boltzmann method (LBM). By coupling the latter with the DEM particle/fluid systems can even be studied in more detail. A brief review of both approaches is performed and possible applications are discussed.

Keywords: simulations, multi-phase flows, DEM-CFD, FVM, LBM, non-spherical particles.

Introduction

The discrete element method (DEM) has established itself as a powerful tool for modelling static or dynamic particle systems in the past 10 years. While in the beginning of the DEM dating back to Cundall and Strack in 1979 (Cundall & Strack, 1979) particles always were considered to be of spherical shape mostly due to runtime issues, they can for some time be non-spherical (comp. e.g. (Cleary, 2008; Markauskas, Kačianauskas, Džiugys, & Navakas, 2010; Höhner, Wirtz, Kruggel-Emden, & Scherer, 2011) which allows simulations in a wide range of engineering disciplines to capture real world processes and phenomena related to particle systems in a very precise manner. In recent years also coupled fluid/particle flows have shifted into the focus. Even in such flows the non-sphericity of particles has become an issue as it can have an influence on the overall behavior of the particle/fluid system (comp. e.g. (Hilton, Mason, & Cleary, 2010; Zhou, Pinson, Zou, & Yu, 2011; Ren et al., 2012; Kruggel-Emden & Oschmann, 2014; Oschmann, Hold, & Kruggel-Emden, 2014).

Research in the area of particle laden multi-phase flows is advancing fast. Simulations up to now have mostly been performed by coupling the DEM with computational fluid dynamics (CFD) not resolving the flow around individual particles. Thereby the CFD usually relies on the discretization of the Navier-Stokes equations based on the Finite Volume Method (FVM); however more recently other CFD approaches have also started to be more widespread used. At the moment resolved flow simulations have gained in popularity basing on the Lattice Boltzmann method (LBM) (see e.g. (Kravets, Rosemann, Reinecke, & Kruggel-Emden, 2019)) as they allow to dispense the use of empirical closures for momentum and possible heat as well as mass transfer between particles and the fluid phase. The two latter methods are briefly reviewed in the following and examples for their application given.

Particle unresolved DEM-FVM based CFD

In the coupled DEM-FVM based CFD method, the particle motion is modelled within a DEM-framework, while the fluid phase is represented by solving the volume averaged Navier-Stokes equations (Zhu, Zhou, Yang, & Yu, 2007). In the DEM the translational and rotational motion is obtained by integrating Newton's and Euler's equations of each particle given by

$$m_i \frac{d^2 \vec{x}_i}{dt^2} = \vec{F}_i^c + \vec{F}_i^{pf} + m_i \vec{g}; \quad (1)$$

$$\hat{I}_i \frac{d\vec{W}_i}{dt} + \vec{W}_i \times (\hat{I}_i \vec{W}_i) = \Lambda_i^{-1} (\vec{M}_i) = \Lambda_i^{-1} (\vec{M}_i^c + \vec{M}_i^{pf}), \quad (2)$$

with the particle mass m_i , particle acceleration $d^2 \vec{x}_i / dt^2$, contact force $\vec{F}_i^c$, particle/fluid force $\vec{F}_i^{pf}$, gravitational force $m_i \vec{g}$, angular acceleration $d\vec{W}_i / dt$, angular velocity $\vec{W}_i$, external moment $\vec{M}_i$ resulting out of contact $\vec{M}_i^c$ or particle/fluid forces $\vec{M}_i^{pf}$, the inertia tensor along the principal axis $\hat{I}_i$ and the rotation matrix converting a vector from the inertial into the body fixed frame Λ_i^{-1} with i the particle index.

A flexible approach to model complex shaped particles in the discrete element method is the representation by polyhedrons. In this method a triangular surface mesh is applied to represent the desired particle shape and a common plane algorithm is used for contact detection (Höhner et al., 2011). Contact force laws are applied similarly as used for spherical particles (Kruggel-Emden, Simsek, Rickelt, Wirtz, & Scherer, 2007a; Kruggel-Emden, Wirtz, & Scherer, 2007b). The normal component of the contact forces is obtained from a linear spring damper model

$$\vec{F}^n = k^n \delta \vec{n} + \gamma^n \vec{v}_{rel}^n, \quad (3)$$

where: k^n is the spring stiffness, δ the virtual overlap, $\vec{n}$ a normal vector, γ^n a damping coefficient and $\vec{v}_{rel}^n$ the normal velocity in the contact point. Both k^n and γ^n determine the coefficient of normal restitution between particles e_{pp}^n as well as particles and walls e_{pw}^n . For the calculation of the tangential forces a linear spring limited by the Coulomb condition is used

$$\vec{F}^t = \min(k^t |\vec{\xi}^t|, \mu_C |\vec{F}^n|) \vec{t}, \quad (4)$$

where: k^t is the stiffness of a linear spring, μ_C is the friction coefficient, $\vec{\xi}^t$ is the relative tangential displacement and $\vec{t}$ is the tangential unit vector. Rolling friction can additionally be considered.

The fluid phase is described with Computational Fluid Dynamics (CFD) in an Eulerian framework. The fluid velocity is considered as a spatially averaged quantity on the cell level. The CFD-framework passes the fluid properties and the velocity of the fluid to the DEM. The equation of continuity (5) and the equation of momentum (6) are solved

$$\frac{\partial(\varepsilon_f \rho_f)}{\partial t} + \nabla(\varepsilon_f \rho_f \vec{u}_f) = 0; \quad (5)$$

$$\frac{\partial(\varepsilon_f \rho_f \vec{u}_f)}{\partial t} + \nabla(\varepsilon_f \rho_f \vec{u}_f \vec{u}_f) = -\varepsilon_f \nabla p + \nabla(\overline{\varepsilon_f \tau}) + \varepsilon_f \rho_f \vec{g} + \vec{f}_{int}, \quad (6)$$

where $\vec{u}_f$, ρ_f and p are the physical fluid velocity, density and pressure. $\vec{f}_{int}$ is the volumetric particle/fluid interaction momentum source applied in each CFD cell, ε_f is the local fluid porosity and τ is the fluid viscous stress tensor $\tau = \eta_e \left[(\nabla \vec{u}_f) + (\nabla \vec{u}_f)^T \right]$ with η_e the effective viscosity determined from a possible turbulent model. The particle/fluid interaction $\vec{f}_{int}$ is given component wise as $f_{int,j} = \bar{\beta}_j (u_{f,j} - \bar{v}_j)$, where $\bar{v}_j$ is the fluid cell averaged particle velocity, and $\bar{\beta}_j$ is the fluid cell averaged particle/fluid friction coefficient with $j = x, y, z$.

The particle/fluid force $\vec{F}_i^{pf}$ consists of all individual particle/fluid forces such as drag force $\vec{F}_i^d$ and pressure gradient force $\vec{F}_i^{\nabla p}$ acting on a particle i written as $\vec{F}_i^{pf} = \vec{F}_i^d + \vec{F}_i^{\nabla p}$. Both can be combined to $\vec{F}_i^d + \vec{F}_i^{\nabla p} = \bar{\beta}_j V_i (\vec{u}_f - \bar{v}_j) / (\varepsilon_f (1 - \varepsilon_f))$, where V_i is the particle volume of particle i and $j = x, y, z$. For the calculation of the drag force $\vec{F}_i^d$ and the combined drag and pressure gradient force $\vec{F}_i^d + \vec{F}_i^{\nabla p}$ various models are available. Very popular and widely used for spherical particles and also applicable for non-spherical particles is the approach by Di Felice (Di Felice, 1994), where the force for an isolated spherical particle is calculated and altered by the influence of surrounding particles. The respective force reads

$$\vec{F}_i^{pf} = \vec{F}_i^d + \vec{F}_i^{\nabla p} = \frac{1}{2} \rho_f |\vec{u}_f - \bar{v}_i| C_D A_\perp \varepsilon_f^{1-\chi} (\vec{u}_f - \bar{v}_i), \quad (7)$$

where C_D is the drag coefficient, $A_\perp$ is the cross-sectional area perpendicular to the flow and χ a correction factor. Eq. (7) can be rewritten in terms of the particle/fluid friction coefficient as

$$\bar{\beta}_i = \frac{1}{2} \rho_f C_D A_\perp \varepsilon_f |\vec{u}_f - \bar{v}_i| (1 - \varepsilon_f) \frac{1}{V_i} \varepsilon_f^{(1-\chi)}. \quad (8)$$

χ is calculated as a function of the Reynolds-number $Re = \varepsilon_f \rho_f d_e |\vec{u}_f - \vec{v}_i| / \eta_f$ as

$$\chi = 3.7 - 0.65 \exp\left(-\left(1.5 - \log(Re)\right)^2 / 2\right), \quad (9)$$

with d_e the diameter of a volume equivalent spherical particle and η_f the fluid viscosity. The drag coefficient C_D of a single particle (spherical or non-spherical) can be derived from correlations such as Hölzer und Sommerfeld (Hölzer and Sommerfeld, 2008) which can be written as

$$C_D = \frac{8}{Re} \frac{1}{\sqrt{\phi_\perp}} + \frac{16}{Re} \frac{1}{\sqrt{\phi}} + \frac{3}{\sqrt{Re}} \frac{1}{\phi^{3/4}} + 0.42 \times 10^{0.4(-\log(\phi))^{0.2}} \frac{1}{\phi_\perp}, \quad (10)$$

where $\phi_\perp$ is the crosswise sphericity which is the ratio between the cross-sectional area of the volume equivalent sphere and the projected cross-sectional area of the considered particle perpendicular to the flow.

The porosity ε_f can be calculated based on a subgrid cell approach (Oschmann et al., 2014). A finer resolved grid is examined and it is checked if a particular subgrid cell center lies within a part of a particle. If this is the case the respective subcell is considered as fully filled with solid. Based on the obtained ratio the local fluid porosity is calculated (Oschmann et al., 2014)..

Particle resolved DEM-LBM based CFD

In order to perform particle resolved DEM-CFD simulations, the Lattice Boltzmann method (LBM) as CFD approach has gained increasing popularity, due to its simplicity as well as its good scalability (Succi, 2008, 2015; He, Liu, Li, & Tao, 2019). As a direct numerical method (DNS), the LBM is able to resolve the flow around individual particles providing a detailed understanding of the interaction between the particle and fluid phase. For hydrodynamic problems, the Lattice Boltzmann method recovers the solution of the incompressible Navier-Stokes equation. Lattice Boltzmann models require the definition of a collision operator describing the interaction of distribution functions within the fluid domain.

The collision of density distribution functions f_i in a node located at $r = (x, y, z)^T$ in the fluid domain and the subsequent streaming in one time step Δt along the lattice velocity e_i to the neighboring node at $r + e_i \Delta t$ can be written as

$$f_i(r + e_i \Delta t, t + \Delta t) = f_i(r, t) - \Omega_i(f), \quad i = 1, 2, \dots, n, \quad (11)$$

where the collision is described by the collision operator $\Omega_i(f)$ which is described later. The D3Q19 lattice ($n = 19$) which is often adopted includes the discrete velocities

$$e_i = \begin{cases} (0, 0, 0), & i = 1, \\ (\pm 1, 0, 0)c, (0, \pm 1, 0)c, (0, 0, \pm 1)c, & i = 2 - 7, \\ (0, \pm 1, \pm 1)c, (\pm 1, 0, \pm 1)c, (\pm 1, \pm 1, 0)c, & i = 8 - 19, \end{cases} \quad (12)$$

where $c = \Delta x / \Delta t$ is the lattice speed which is often set to 1 for convenience.

Based on the distribution functions the local density ρ , the momentum j and the velocity $u = (u, v, w)^T$ can be obtained by

$$\rho = \sum_{i=1}^n f_i \quad \text{and} \quad j = \rho_0 u = \sum_{i=1}^n f_i e_i. \quad (13)$$

In the MRT model by d'Humières (d'Humières, 2002), distribution functions are transformed into the moment space m via

$$m(r, t) = M f(r, t), \quad (14)$$

with the transformation matrix M defined as

$$M = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \\ 0 & 2 & 2 & -1 & -1 & -1 & -1 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -4 & -4 & 2 & 2 & 2 & 2 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 \\ -30 & -11 & -11 & -11 & -11 & -11 & -11 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 \\ 12 & -4 & -4 & -4 & -4 & -4 & -4 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -4 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & -4 & 4 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -4 & 4 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & -2 & 2 & 2 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \end{bmatrix}. \quad (15)$$

The collision operator for the MRT model can be written as

$$\Omega(f) = M^{-1}S[m - m^{eq}]. \quad (16)$$

The macroscopic moments are

$$m = (\rho, j_x, j_y, j_z, 3p_{xx}, 3\pi_{xx}, p_{ww}, p_{yz}, p_{xz}, p_{xy}, e, \varepsilon, q_x, q_y, q_z, \pi_{ww}, m_x, m_y, m_z)^T, \quad (17)$$

where the first four hydrodynamic moments for density and momentum are conserved and the other variables are non-conserved kinetic moments. The equilibrium moments only depend on the conserved moments and can be computed as

$$m^{eq} = \left(\rho, j_x, j_y, j_z, \frac{1}{\rho_0}(2j_x^2 - j_y^2 - j_z^2), 0, \frac{1}{\rho_0}(j_y^2 - j_z^2), \frac{j_y j_z}{\rho_0}, \frac{j_x j_z}{\rho_0}, \frac{j_x j_y}{\rho_0}, -11\rho + \frac{19}{\rho_0}j \cdot j, -\frac{475}{63\rho_0}j \cdot j, -\frac{2}{3}j_x, -\frac{2}{3}j_y, -\frac{2}{3}j_z, 0, 0, 0, 0 \right)^T, \quad (18)$$

where the system's mean density ρ_0 is often used to reduce compressibility effects (d'Humières, 2002). The advantage of the MRT model is that the individual moments can be relaxed towards their equilibrium with different rates s_i which are defined in the matrix

$$S = \text{diag}(0, 0, 0, 0, s_v, s_\pi, s_v, s_v, s_v, s_v, s_e, s_\varepsilon, s_q, s_q, s_q, s_\pi, s_m, s_m, s_m). \quad (19)$$

The relaxation rate s_v is connected to the model's kinematic viscosity

$$\nu = c_s^2 \left(\tau_v - \frac{1}{2} \right) \Delta t = c_s^2 \left(\frac{1}{s_v} - \frac{1}{2} \right) \Delta t, \quad (20)$$

where τ_v denotes the relaxation time. The other relaxation rates are free parameters which can be used to optimize the performance of the MRT model. Often $s_\pi = s_\varepsilon = 1.4$, $s_e = 1.19$ and $s_m = 1.98$ to improve the stability as suggested by d'Humières (d'Humières, 2002). Furthermore, following Verhaeghe et al. (Verhaeghe, Luo, & Blanpain, 2009) $s_q = 8(2 - s_v)/(8 - s_v)$ in order to remove the viscosity-dependence in parts.

Besides inflow and outflow boundary conditions a popular way to satisfy the no-slip boundary condition on particle surfaces or walls is the application of bounce-back schemes, the simplest of which is the halfway bounce-back

$$f_i(r_f, t + \Delta t) = \tilde{f}_i(x_f, t) + 2\omega_i \rho_0 \frac{u_b \cdot e_i^-}{c_s^2}, \quad (21)$$

where the post-collision distribution $\tilde{f}_i(x_f, t)$ is reflected at the boundary during the streaming to get the missing pre-collision distribution $f_i(r_f, t + \Delta t)$. Due to the boundary's motion with velocity u_b , a portion of mass is covered or uncovered by the particle which is added to the reflected distribution. The local boundary velocity $u_b = u_p + \omega_p \times r_b$

at the boundary position r_b takes into account the particle's translational velocity u_p as well as the rotational velocity ω_p .

For the coupling of the LBM with the DEM it is essential to evaluate the particle-fluid forces in particulate flows, which can be efficiently done in LB simulations through the momentum exchange method (MEM). The main idea of this method is to sum up the momentum change over all boundary links of a particle. In the case of moving particles, the formulation of the MEM has a great impact on accuracy and stability (Peng, Teng, Hwang, Guo, & Wang, 2016; Tao, Hu, & Guo, 2016). Often the force evaluation for the particle-fluid force F_{pf} by Wen et al. (Wen, Zhang, Tu, Wang, & Fang, 2014) is adopted, where the boundary velocity is explicitly taken into account to obtain stable results:

$$\vec{F}_{pf} = \frac{\Delta x^3}{\Delta t} \sum_{r_i \in i_{bl}} [\tilde{f}_i(r_i, t)(c_i - u_b) - \tilde{f}_i(r_i, t + \Delta t)(c_i - u_b)]. \quad (22)$$

The moment can be computed along with the force as follows:

$$\vec{M}_{pf} = \frac{\Delta x^3}{\Delta t} \sum_{r_i \in i_{bl}} (r_b - r_p) [\tilde{f}_i(r_i, t)(c_i - u_b) - \tilde{f}_i(r_i, t + \Delta t)(c_i - u_b)], \quad (23)$$

where r_p is the position of the particle centre. Both $\vec{F}_{pf}$ and $\vec{M}_{pf}$ can be introduced into Eqs. (1) and (2) resembling the particle resolved DEM-LBM based CFD.

Possible applications of particle unresolved DEM-FVM and resolved DEM-LBM

Particle unresolved DEM-FVM approaches have been applied to a variety of applications so far. As they are computationally less demanding than particle resolved approaches basing on the DEM-LBM they can be applied to the modelling of whole apparatuses or technical processes. Some examples for applications are given in Figure 1.

Figure 1. (a) Particle velocities of spherical particles (left) and plate shaped particles (right) in a bend being part of a pneumatic conveying system; (b) experimental setup to perform pressure drop investigations in a packed bed; (c) pressure drop of $d = 7$ mm spherical particles and (d) pressure drop of $6 \text{ mm} \times 6 \text{ mm}$ cylinders

One application of unresolved DEM-FVM are pneumatic conveying systems which comprise of vertical and horizontal sections which are often interconnected by bends. In such systems (comp. Figure 1a) a variety of bulk solids is transported in industrial applications. The particle shape of the bulk solids has an influence on the acceleration behavior at the entry of pneumatic conveying systems as well as the particle/fluid behavior after bends, where the particles form ropes which disperse thereafter. The particle shape thereby directly effects the dispersion kinetics (see Figure 1a) and thereby the overall pressure drop, but also the stressing of the pipe walls which in consequence leads to possible erosion as well as attrition on the particle side. DEM-FVM simulations have advanced to the point that they can help optimize the transport of bulk solids in pneumatic conveying systems.

A second application are fluidized and packed beds (Figure 1b). Results for the pressure drop obtained experimentally for packings of both spherical and non-spherical particles match well with simulation results obtained by DEM-FVM (see Figures 1c and 1d). Currently for many particle shapes no correlations for pressure drop are available. Here DEM-FVM can contribute towards the prediction and optimization of pressure drop in much more complicated systems than shown in Figure 1b.

Particle resolved DEM-LBM based CFD is computationally much more demanding, however is not dependent on closures such as Eqs. (7)–(10). Static packing of particles (Figure 2a) can be investigated by particle resolved DEM-LBM to obtain improved closures for momentum but also heat transfer (see e.g. (Kravets et al., 2019)). On the other hand, particle resolved DEM-LBM simulations allow a detailed insight into the dynamics of particle-fluid systems as all relevant interactions are resolved (Figure 2b). Such level of detail is required in several applications like e.g. micro fluidic devices.

Figure 2. (a) Fluid velocities in a packing of spherical particles and (b) setup of moving particles modelled as part of the particle resolved DEM-LBM

Conclusions

A review of two state of the art methods to couple the DEM with computational fluid dynamics was made. Relevant aspects of the approaches were addressed in terms of the underlying framework of equations. Current applications were given. It is concluded that as computationally resources are still enhancing the number of possible applications of the discussed approaches is expected to grow significantly in the future making their improvement a relevant emerging field.

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