Finite Element-Fictitious Boundary Methods (FEM-FBM) for time-dependent multiphase flow problems — Application to Sedimentation Benchmarks

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ABSTRACT

This contribution presents new numerical simulation techniques using a Finite Element approach coupled with the Fictitious Boundary Method (FEM-FBM) for non-stationary multiphase flow configurations in 3D. The fluid solution is computed by a Finite Element multigrid solver, which has been realized in the open source CFD package FEATFLOW, while complex dynamic or static geometrical features of the flow domain as well as solid particles, which interact with the surrounding fluid, are treated by the Fictitious Boundary Method. This approach allows the use of structured and unstructured computational meshes which can be static or adaptively aligned by dynamic grid deformation methods. Numerical results for this workshop's 'sphere sedimentation' test case are provided. The results show that the presented method can accurately handle the 3D particulate flow situations under consideration. Due to the high parallel efficiency of the FEATFLOW software the method can be used for large-scale problems.

In the field of Computational Fluid Dynamics one of the main research topics is the study of (rigid) particulate flows. The simulation and prediction of particulate flows has various important applications in mechanical, chemical or medical engineering. In the last few decades various basic techniques for the simulation of particulate fluid-solid flows have been developed [1], [2], [3]. The most distinctive feature of the techniques is the general approach to solving the fluid flow governed by the Navier-Stokes equations. The most common choices for particulate flows are the Finite Element Method [1] or the Lattice-Boltzmann Method [3], [4]. Our contribution uses the FEM with the FEATFLOW software package as solver [5]. The Finite Element based method can be further distinguished into Arbitrary Langrangian-Eulerian (ALE) and Eulerian approaches. In an ALE scheme both fluid and solid equations are combined in a single coupled variational equation which requires remeshing when the old computational mesh becomes too distorted and the flow field is then projection onto the new mesh. Thus the positions of the solids and the nodes of the mesh are updated explicitly while the velocities are implicitly determined. An Eulerian approach relies on the concept of a 'fictitious domain' [6] which is used to represent the solid phase inside of the fluid domain. An advantage of the Eulerian methods is that they allow for a fixed mesh being used so that the need for remeshing can be eliminated. The method presented in this work belongs to the Eulerian methods and is a variation of the Fictitious Domain method termed (Multigrid) Fictitious Boundary Method (FBM) [7]. In our FBM the knowledge of the fluid-solid boundary is of key importance, because it is used to calculate the hydrodynamic forces acting on the solid in a given time step using a volume integral formulation. The basic methods that have been developed several years ago have evolved over time and they are constantly improved with regard to the complexity of flow situations they can handle, the number of solids involved in the simulation and in terms of the computational efficiency of the solver. The multigrid FEM-FBM is no exception and since its early days it has been extended to 3D, adopted to handle arbitrary geometries and was efficiently mapped to parallel hardware which enables the method to utilize the potential of highly parallel architectures and to solve large-scale problems [8]. When a method is further developed care should be taken that not only the computational efficiency is improved, but also the accuracy of the method should at least retain its original quality or preferably improve as well. This is why standardized benchmarking is important and why we subject the current state of the FEM-FBM to the ‘sphere sedimentation’ benchmark defined by ten Cate et al. [9].

In the remainder of this work we present the underlying equations as well as the structure of our fluid-solid solver and we conclude by showing the numerical results of the ‘sphere sedimentation’ benchmark.

DESCRIPTION OF THE PHYSICAL MODEL

In our numerical studies of particle motion in a fluid, we assume that the fluids are immiscible and Newtonian and the particles are rigid bodies. We refer to the whole computational domain as $\Omega_T = \Omega_f \cup \Omega_p$, where Ω_f is the fluid domain and Ω_p the particle domain. The motion of an incompressible fluid with density ρ_f and viscosity v is governed by the Navier-Stokes equations in the domain Ω_f,

$$\rho_f \left(\frac{\partial u}{\partial t} + u \cdot \nabla u \right) - \nabla \cdot \sigma = 0, \quad \nabla \cdot u = 0 \quad \forall t \in (0, T) \tag{1}$$

where σ is the stress tensor of the fluid phase defined by:

$$\sigma = -pI + \mu_f \left(\nabla u + (\nabla u)^T \right). \tag{2}$$

The motion of N rigid particles in a fluid is described by the Newton-Euler equations with the translational velocity U_i and the angular velocity ω_i:

$$M_i \frac{\partial U_i}{\partial t} = (\Delta M_i) g + F_i + F_{col}, \; I_i \frac{\partial \omega_i}{\partial t} + \omega_i \times (I_i \omega_i) = T_i, \tag{3}$$

where M_i is the mass of the i-th particle; ΔM the mass difference between the fluid and solid occupying the same volume; I_i the moment of inertia tensor; F_i the hydrodynamic force and F_{col} the collision forces arising from particle-particle collisions; T_i is the torque about the center of gravity of the i-th particle.

The hydrodynamic force F_i and the torque T_i can be calculated using a surface integral formulation which has the following form:

$$F_i = -\int_{\partial \Omega_i} \sigma \cdot n_i \, d\Gamma_i, \quad T_i = -\int_{\partial \Omega_i} (X - X_i) \times (\sigma \cdot n_i) \, d\Gamma_i \tag{4}$$

In the FEM-FBM a single grid is used to cover the whole domain Ω_T, the particles are defined on the grid by using an indicator function $\alpha_i(x)$. This indicator function allows performing the fluid calculation on the whole domain.

$$\alpha_i(x) = \begin{cases} 1 & for\ x \in \Omega_i, \\ 0 & for\ x \in \Omega_T \setminus \Omega_i \end{cases} \tag{5}$$

A two-way coupling between fluid and solid phase is achieved by applying the forces F_i and T_i to the particles and by imposing the resulting particle velocity as a velocity boundary condition on the fluid:

$$\begin{cases} \nabla \cdot u = 0 & for\ x \in \Omega_T, \\ \rho_f \left(\frac{\partial u}{\partial t} + u \cdot \nabla u \right) - \nabla \cdot \sigma = 0 & for\ x \in \Omega_f, \\ u(x) = U_i + \omega_i \times (x - x_i) & for\ x \in \overline{\Omega}_i,\ i = 1, \ldots, N. \end{cases} \tag{6}$$

The evaluation of the forces F_i and T_i by the surface integral in (4) has the disadvantages that an explicit reconstruction of the surface from the information stored in the computational grid is a time-consuming task and more importantly such an approach would be of first order only. The alternative is to use a volume integral formulation. The key aspect that leads to this formulation is to notice that the gradient of the indicator function is non-zero only on the cells of the mesh that are located directly on the particle-fluid boundary. Furthermore, the gradient is equal to the normal vector n_i of the particle on the particular cell of the grid i.e., $n_i \approx \nabla\alpha_i$. The volume integral formulation can thus be stated as:

$$F_i = -\int_{\Omega_T} \sigma \cdot \nabla \alpha_i \, d\Omega, \quad T_i = -\int_{\Omega_T} (x - x_i) \times (\sigma \cdot \nabla \alpha_i) \, d\Omega \tag{7}$$

It is important to realize that although this volume integral is defined on the whole domain Ω_T, the gradient $\nabla\alpha_i$ is non-zero only on the cells that intersect the surface of the particle. Thus, it is sufficient to only perform the numerical evaluation of the formula on the cells intersecting the particles which greatly increases the computational efficiency.

NUMERICAL SOLUTION

The numerical solution scheme of the multigrid FEM fictitious boundary method can be summarized as follows:

- Solve the fluid equations (6) on the fluid domain using the positions and velocities of the particles as fictitious boundary conditions
- Calculate the corresponding hydrodynamic forces from the fluid solution using equation (7)
- Solve equations (3) to get the translational and angular velocities of the particles to obtain the updated positions and velocities of the particles.
- Update the fictitious boundary conditions

DEFINITION OF THE TEST CASE

The 'sphere sedimentation' benchmark of ten Cate et al. [9] is a well-known test configuration for Liquid-Solid solvers. We used the FEM-FBM to simulate this configuration and present the results in this section. At first we briefly summarize the configuration of the benchmark. The computational domain for this test case is a boxed-shaped container with the following dimensions *depth* × *width* × *height* = 100 × 100 × 160 *mm*. In this domain a spherical particle is placed with the initial position of its center located at (50, 50, 127.5). The diameter of the spherical particle is d_p = 15 *mm* and the density is ρ_p=1120 kg/m^3. The physical properties of the fluid such as the fluid density ρ_f and viscosity ν_f are varied in order to test the solver at different Reynolds numbers. The experiments performed by ten Cate focus on four main test cases which are referred to as E1-E4. The corresponding simulations are called S1-S4. In table (Tab. 1) the different configurations are summarized, where u_∞ denotes the maximum sedimentation velocity in a container of infinite height and *Re* refers to the Reynolds number, calculated as $Re = d_p u_\infty \rho_f / \nu_f$.

Case number	ρ_f [kg/m³]	ν_f [Ns/m²]	u_∞ [m/s]	*Re* [-]
E1	970.0	0.373	0.038	1.5
E2	965.0	0.212	0.060	4.1
E3	962.0	0.113	0.091	11.6
E4	960.0	0.058	0.128	31.9

Tab. 1 Fluid properties for the different test cases

The simulations S1-S4 are carried out over a total simulation time of 5.0 seconds. We store various data for each case. Most importantly we store the velocity of the particle u_p, the height of the particle *h*, the kinetic energy of the fluid domain $E_{kin,f}$ and the kinetic energy of the spherical particle $E_{kin,p}$. To calculate $E_{kin,p}$ we use the standard kinetic energy equation for rigid bodies:

$$E_{kin,p} = \frac{1}{2} m u^2 \qquad (8)$$

The kinetic energy of the fluid is defined as:

$$E_{kin,f} = \int_\Omega \rho_f u^2 d\Omega \qquad (9)$$

In a finite element framework this can be efficiently evaluated as:

$$E_{kin,f} = U^T M_\rho U \qquad (10)$$

Where *U* is the velocity solution in the degrees of freedoms and M_ρ is the mass matrix.

NUMERICAL RESULTS

In this section we present the results of the simulations S1-S4 using the multigrid FEM-FBM. The computational domain was discretized using an unstructured mesh T with different levels of refinement. The coarse grid T_1 consists of 2100 vertices and 1216 hexahedral elements, we computed the results on refinement level 4 which corresponds to grid T_4 with 1075200 vertices 622592 elements. The simulations were run for a total simulation time of 5.0 seconds using a time step size $\Delta t = 0.001$. At first we examine the sedimentation velocity observed in the simulations S1-S4 and then compare this data to the experimental and simulation data provided by ten Cate. The sedimentation velocity is shown in figure (Fig. 1) on the maximum mesh resolution level T_4. To compare the simulation data to the data obtained in the experiment ten Cate used the ratio of the maximum velocity measured in the experiment to the theoretically determined maximum sedimentation velocity and the ratio of the maximum velocity in the simulation to the theoretical maximum. We computed these values and summarized the comparison of our values to those of the experiment and simulation by ten Cate in table (Tab. 2).

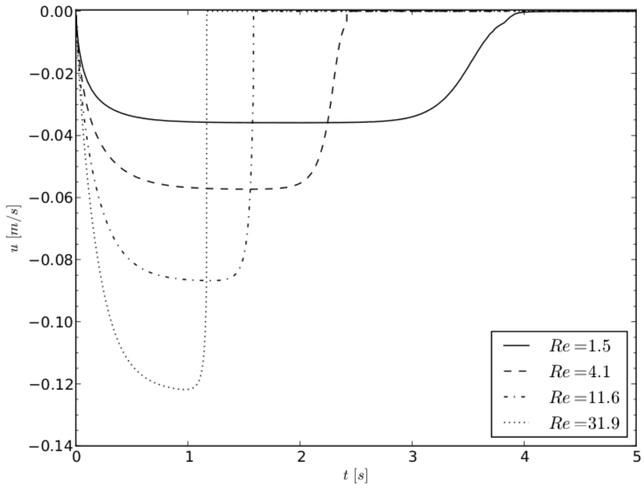

Fig. 1 Sedimentation velocity for different Reynolds number

Re	u_{max}/u_∞	u_{max}/u_∞ *ten Cate*	u_{max}/u_∞ *exp*
1.5	0.945	0.894	0.947
4.1	0.955	0.950	0.953
11.6	0.953	0.955	0.959
31.9	0.951	0.947	0.955

Tab. 2 Comparison of the u_{max}/u_∞ ratios between the FEM-FBM, ten Cate's simulation and ten Cate's experiment

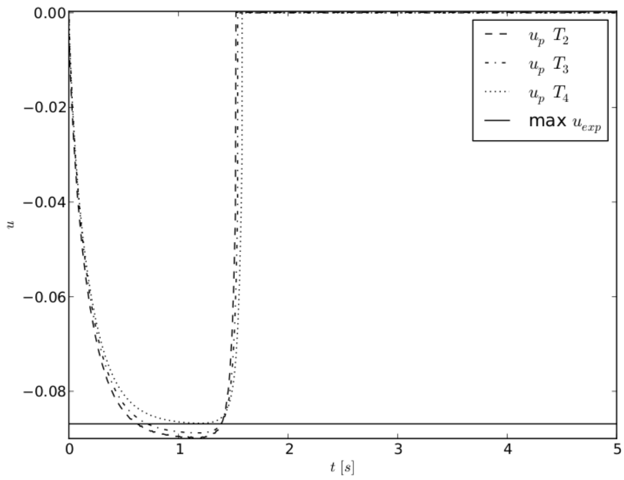

Fig. 2 S3 test case calculated on 3 mesh levels

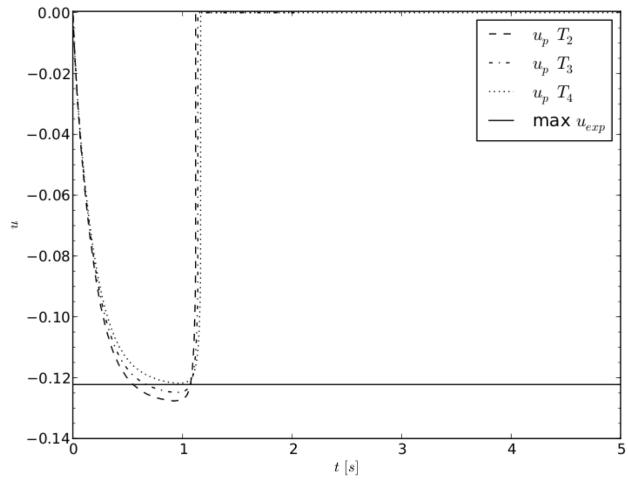

Fig. 3 S4 test case calculated on different mesh levels

To demonstrate the validity of our multigrid framework, we computed the S3 and S4 cases on different levels of mesh refinement. The underlying assumption is that the accuracy of the results should improve in case that the mesh refinement level is increased. Figures (Fig. 2) and (Fig. 3) display the sedimentation velocity computed on different refinement levels. In order to evaluate the result a line indicating the maximum velocity measured in the experiment is inserted. We can observe that as the mesh refinement increases the maximum velocity reached in the simulation gets closer to that of the experiment in both of the analysed cases. Additionally, the shape of the curves seems to get closer to those published by ten Cate. This behaviour is a strong indication that the underlying multigrid framework is working as expected.

The particle trajectories, represented by the dimensionless height of the gap between the particle and the bottom wall of the domain h/d_p, are shown in figure (Fig. 4).

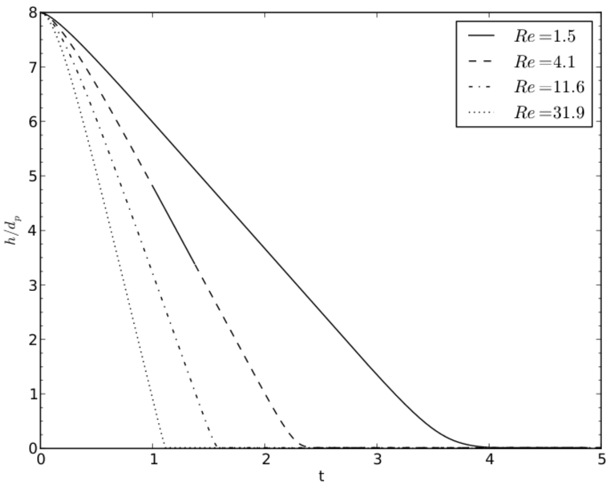

Fig. 4 Trajectories of the particle for different Reynolds numbers

The results for the kinetic energy of the fluid and particle for test cases S1-S4 are displayed in figures (Fig. 5 - Fig. 8).

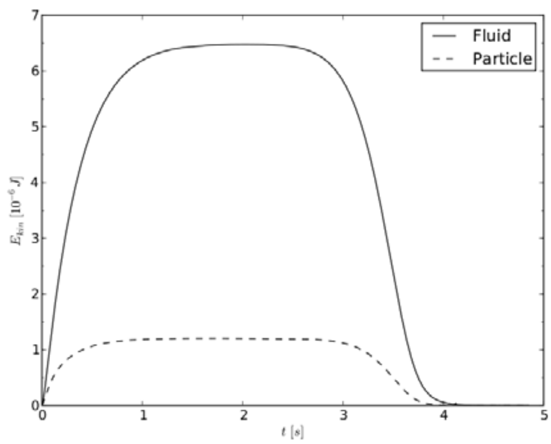

Fig. 5 Kinetic energy of the fluid and the sphere (S1)

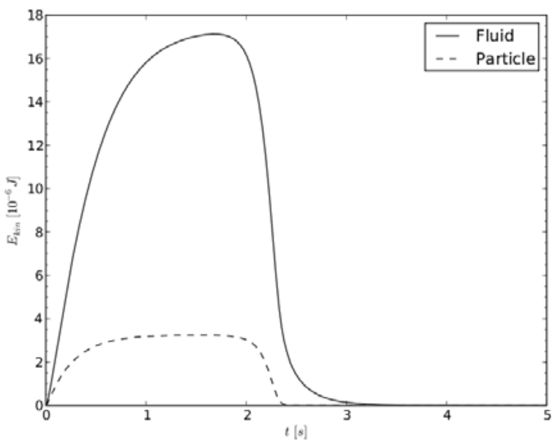

Fig. 6 Kinetic energy of the fluid and the sphere (S2)

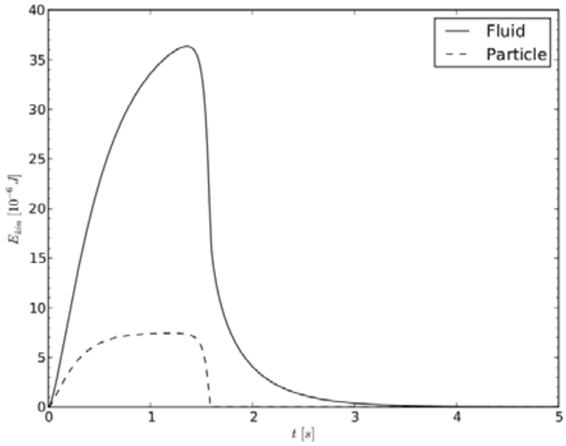

Fig. 7 Kinetic energy of the fluid and the sphere (S3)

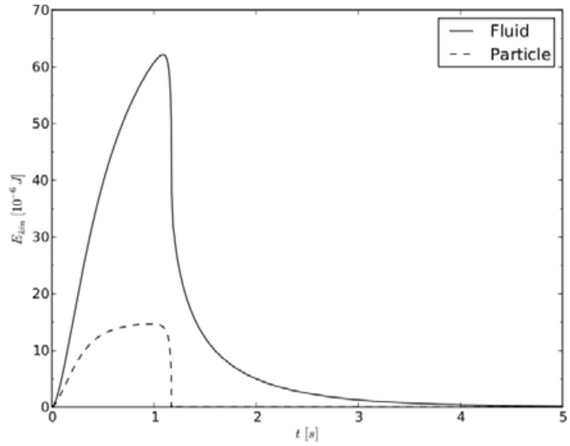

Fig. 8 Kinetic energy of the fluid and the sphere (S4)

CONCLUSIONS

The values obtained for the sedimentation velocity and particle trajectories compare very well to those of the experiment and the simulations of ten Cate in all of test cases S1-S4. Characteristic features of the particle behaviour like the velocity plateau that is reached in the S1 case or the relatively abrupt deceleration of the particle in the S4 case are clearly visible. Furthermore, the method is able to capture flow features like the deceleration phase of the particle in cases S1-S3 when it close to the bottom wall of the domain without the introduction of additional forces on a sub-mesh level. We attribute this to the high mesh resolution that the method able to handle efficiently. The data calculated for the kinetic energy of the fluid and the particle also closely matches the experimental data and the simulations of ten Cate. The results lead us to the conclusion that the FEM-FBM is able to efficiently and accurately predict particle motion in fluid at different Reynolds numbers and to resolve the associated flow features precisely.

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