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A collision strategy for particles in particulate flow simulations

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Abstract A novel collision strategy has been implemented for simulation of particulate flows using a Lagrange multiplier/fictitious domain method. In this Note, we present this new collision strategy that is based on Newton's principle of transfer of momentum. With this method, we have simulated motion of two discs under the influence of gravity in a viscous fluid, and the motion of 1008 discs under the effect of gravity. ***To cite this article: P. Parthasarathy, C. R. Mecanique 330 (2002) 77–81.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

fluid mechanics

Sur le traitement des collisions lors de la simulation numérique des écoulements particulaires

Résumé Dans cette Note on présente une nouvelle méthode pour le trai tment des collisions lors de la simulation numérique des écoulements particulaires. Cette méthode est basée sur le principe de Newton sur le transfert d es moments. Ce traitment des collisions a été combiné avec des méthodes de domaines fictifs avec multiplicateurs de Lagrange afin de simuler numérique ment des écoulement de mélanges de particules solides/fluides Newtoniens vis queux incompressibles. La méthodologie ci-dessus a été validée en simulant la sédimentation de deux disques rigides dans un fluide Newtonien visqueux incompressible, puis appliquée à la sédimentation de 1008 disques dans un fluide de même type. ***Pour citer cet article : P. Parthasarathy, C. R. Mecanique 330 (2002) 77–81.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

mécanique des fluides

1. Introduction

In [1] and [2] a distributed Lagrange multiplier/fictitious domain method was presented for simulation of the motion of rigid bodies in a Newtonian fluid. In this Note, we present results using this formulation for several discs moving due to gravity in a Newtonian fluid with a novel, more physical, collision strategy implementation. In our work, we use the principle of conservation of momentum to come up with impulses that originate due to collisions and use these impulses to accurately move the particles in the simulation. Results for the motion of two particles falling due to gravity in a fluid and the motion of 1008 discs falling under gravity are shown to highlight the accuracy and robustness of the algorithm have been presented in this Note.

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2. Combined formulation

Let $\Omega \subset \mathbb{R}^d$ (in our case $d = 2$; see Fig. 1) be a region filled with a Newtonian, viscous, incompressible fluid of density ρ_f and viscosity ν_f. Let there be N moving bodies $\{B_j\}_{j=1}^N$ in this fluid with density $\{\rho_j\}_{j=1}^N$. For this system, the flow of the fluid is described by the Navier–Stokes equations while the motion of rigid bodies is described by Newton–Euler's equations. To obtain a combined weak formulation for this problem, we define the following functional spaces $W_{g_0}(t) = \{\mathbf{v} \mid \mathbf{v} \in (H^1(\Omega))^d,\ \mathbf{v} = \mathbf{g}_0(t) \text{ on } \Gamma\}$, $L_0^2(\Omega) = \{q \mid q \in L^2(\Omega),\ \int_\Omega q \,\mathrm{d}x = 0\}$, and $\Lambda_j(t) = H^1(B_j(t)^d)$, $\forall j = 1, \ldots, N$.

With these spaces, we define the fictitious domain formulation with distributed Lagrange multipliers for our problem as:

$$\text{For } t > 0,\ \text{find } \mathbf{u}(t),\ p(t),\ \left\{\mathbf{V}_j(t), \mathbf{G}_j(t), \boldsymbol{\omega}_j(t),\ \boldsymbol{\lambda}_j(t)\right\}_{j=1}^N,\ \text{such that}$$

$$\mathbf{u}(t) \in W_{g_0}(t), \quad p(t) \in L_0^2(\Omega), \quad \left\{\mathbf{V}_j(t) \in \mathbb{R}^d,\ \mathbf{G}_j(t) \in \mathbb{R}^d,\ \boldsymbol{\omega}_j(t) \in \mathbb{R}^3,\ \boldsymbol{\lambda}_j(t) \in \Lambda_j(t)\right\}_{j=1}^N \tag{2.1}$$

and

$$\begin{cases} \rho_f \displaystyle\int_\Omega \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\nabla\mathbf{u}\right) \cdot \mathbf{v}\,\mathrm{d}x + 2\nu_f \int_\Omega \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v})\,\mathrm{d}x - \sum_{j=1}^N \left\langle \boldsymbol{\lambda}_j, \mathbf{v} - \mathbf{Y}_j - \boldsymbol{\theta}_j \times \overrightarrow{\mathbf{G}_j\mathbf{x}} \right\rangle_j \\ \quad - \displaystyle\int_\Omega p\nabla \cdot \mathbf{v}\,\mathrm{d}x + \sum_{j=1}^N \left(1 - \frac{\rho_f}{\rho_j}\right)\left[M_j \frac{\mathrm{d}\mathbf{V}_j}{\mathrm{d}t} \cdot \mathbf{Y} + \left(\mathbf{I}_j \frac{\mathrm{d}\boldsymbol{\omega}_j}{\mathrm{d}t} + \boldsymbol{\omega}_j \times \mathbf{I}_j \boldsymbol{\omega}_j\right) \cdot \boldsymbol{\theta}_j\right] \\ \quad = \displaystyle\sum_{j=1}^N \left(1 - \frac{\rho_f}{\rho_j}\right) M_j \mathbf{g} \cdot \mathbf{Y}_j, \quad \forall \mathbf{v} \in \left(H_0^1(\Omega)\right)^d,\ \forall \mathbf{Y}_j \in \mathbb{R}^d,\ \forall \boldsymbol{\theta}_j \in \mathbb{R}^3 \end{cases} \tag{2.2}$$

$$\int_\Omega q\nabla \cdot \mathbf{u}(t)\,\mathrm{d}x = 0, \quad \forall q \in L^2(\Omega) \tag{2.3}$$

$$\frac{\mathrm{d}\mathbf{G}_j}{\mathrm{d}t} = \mathbf{V}_j, \quad \forall j = 1, \ldots, N \tag{2.4}$$

$$\left\langle \boldsymbol{\mu}_j, \mathbf{u}(t) - \mathbf{V}_j(t) - \boldsymbol{\omega}_j(t) \times \overrightarrow{\mathbf{G}_j(t)\mathbf{x}} \right\rangle_j = 0, \quad \forall \boldsymbol{\mu}_j \in \Lambda_j(t),\ \forall j = 1, \ldots, N \tag{2.5}$$

$$\mathbf{V}_j(0) = \mathbf{V}_j^0, \quad \boldsymbol{\omega}_j(0) = \boldsymbol{\omega}_j^0, \quad \mathbf{G}_j(0) = \mathbf{G}_j^0, \quad \forall j = 1, \ldots, N \tag{2.6}$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega \setminus \bigcup_{j=1}^N \overline{B_j(0)} \quad \text{and} \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{V}_j^0 + \boldsymbol{\omega}_j^0 \times \overrightarrow{\mathbf{G}_j^0\mathbf{x}}, \quad \forall \mathbf{x} \in \overline{B_j(0)} \tag{2.7}$$

In Eqs. (2.1)–(2.7), $\mathbf{u}$ $(= \{u_i\}_{i=1}^d)$ and p are the velocity and pressure of the fluid. $\mathbf{V}_j$, $\boldsymbol{\omega}_j$, M_j, $\mathbf{I}_j$, $\mathbf{G}_j$ are the translational velocity, rotational velocity, mass, moment of inertia (about $\mathbf{G}_j$) and center of mass of the jth particle respectively. $\{\boldsymbol{\lambda}_j\}_{j=1}^N$ is a family of Lagrange multipliers, $\mathbf{D}(\mathbf{v}) = (\nabla\mathbf{v} + \nabla\mathbf{v}^t)/2$ is the strain-rate tensor, and $\mathbf{g}$ is the acceleration due to gravity.

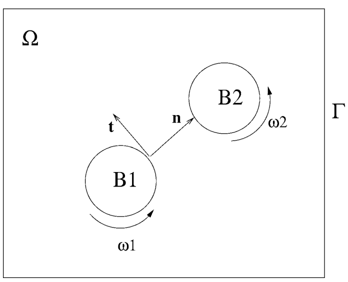


Figure 1. Example of a two-dimenional flow region with two discs.

3. Collision model

To time-discretize the system we employ the Marchuk–Yanenko splitting (more details on this particular implementation of the M–Y scheme can be found in [1] and [2]). In our implementation, the velocity of particles and their positional change are computed at different steps and hence, there needs to be a good model for detecting collisions so that the particles do not overlap each other's boundary. We use the principle of conservation of momentum applied on inelastic collision as shown here.

Consider discs 1 and 2 that are about to collide as in Fig. 1. Let their pre-collisional velocities in the normal and tangential directions be V_{n1}, V_{n2}, V_{t1}, V_{t2}. Let ω_1 and ω_2 be the pre-collisional rotational velocities and r_1 and r_2 be their radii. The relative velocities are given by

$$V_{rn} = V_{n1} - V_{n2}, \qquad V_{rt} = V_{t1} - V_{t2} + r_1\Omega_1 - r_2\Omega_2 \tag{3.1}$$

At the time of collision, impulses are generated both in the normal and tangential direction and let these be represented by J_n and J_t respectively. The impulses are given by,

$$J_n = -\overline{m}(1 + e_n)V_{rn} \quad \text{and} \quad J_t = e_t V_{rt} \tag{3.2}$$

where

$$\overline{m} = \frac{m_1 m_2}{m_1 + m_2}, \qquad e_n = -\frac{v_{n1} - v_{n2}}{V_{n1} - V_{n2}}$$

m_1 and m_2 are the respective masses of the particles, and e_n is the coefficient of restitution that takes into account inelasticity in collisions. e_t is given by,

$$e_t = \mu_k \frac{J_n}{|V_{rt}|}, \quad \text{if } |J_{tmax}| > \mu_s |J_n|, \quad \text{else } e_t = -\frac{1}{3}\overline{m} \tag{3.3}$$

where $J_{tmax} = -2\overline{m}V_{rt}$, and μ_s and μ_k are the coefficients of static and kinetic frictions respectively. The "else" part in (3.3) signifies the occurence of zero post-collisional tangential relative velocity. Now the new velocities are given by,

$$\begin{aligned} v_{n1} &= V_{n1} + \frac{J_n}{m_1}, \qquad v_{t1} = V_{t1} + \frac{J_t}{m_1}, \qquad \omega_1 = \omega_1 + \frac{J_t}{I_1} \\ v_{n2} &= V_{n2} - \frac{J_n}{m_2}, \qquad v_{t2} = V_{t2} - \frac{J_t}{m_2}, \qquad \omega_2 = \omega_2 + \frac{J_t}{I_2} \end{aligned} \tag{3.4}$$

where I_1 and I_2 are the moments of inertia of the two bodies and the lower case symbols indicate velocities after collision. A 3-dimensional variant of this method can be found in [3]. Extension of this method to wall-particle collisions is straightforward.

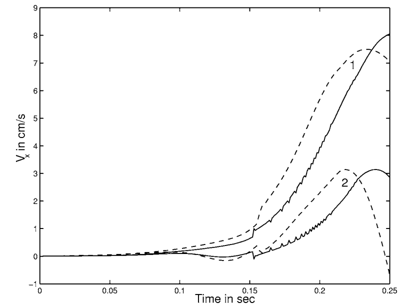
This model has been implemented in such a way that each collision in a time step Δt is tracked and the collisions proceed from the earliest to the last, taking into account the changes in the system due to each collision. This is achieved by detecting the first collision, moving all particles to the time instan t of that particular collision and applying the collision model to the particles involved. This process of detecting the first collision and applying the collision model is repeated until all collisions within Δt have been detected.

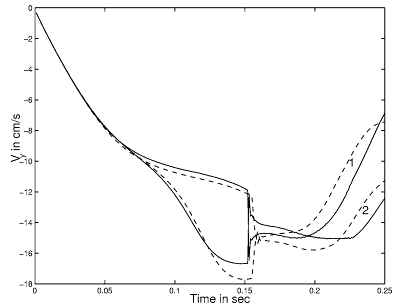
4. Numerical experiments

We simulated the well documented case of two discs, one on top of another separated by a small distance, falling under the effect of gravity. It has been seen that the top disc accelerates due to lower drag and the *drafting, kissing and tumbling* phenomenon occurs. We have compared our results with the results of [1]. For this simulation, we used a uniform grid of gridlength $\Delta h = 1/192$ and timestep $\Delta t = 0.001$. Discs of density $\rho_j = 1.5$ and diameter $D = 0.25$ were dropped in a fluid of density $\rho_f = 1.0$ and viscosity $\nu_f = 0.01$ contained in a domain $\Omega = (0, 2) \times (0, 6)$.

The comparison shown in Fig. 2 shows a very different behaviour after the discs collide while the pre-collisional development is very similar. Since in our collision scheme we take into account friction between the discs during collision, angular velocity increases rapidly after collision. Due to the conversion some part of the energy from translational to rotational, we see that translational velocity reduces in our simulation in comparison to [1]. The maximum Reynolds number (based on particle diameter $\mathrm{Re} = Du/\nu_f$) reached was 418.

To test the robustness of our algorithm, we simulated the sedimentation of 1008 discs. With the fluid properties remaining the same as in the previous experiment, we used the following parameters, $\rho_j = 1.5$





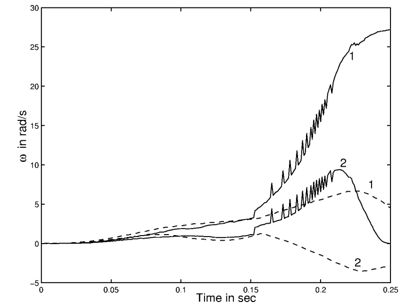


Figure 2. Velocity versus time plots of two particles. From left to right: (1) velocity in the direction perpendicular to gravity (2) velocity in the direction of gravity and (3) rotational velocity (solid lines indicate present work and dashed lines (- -) indicate results from [1]).

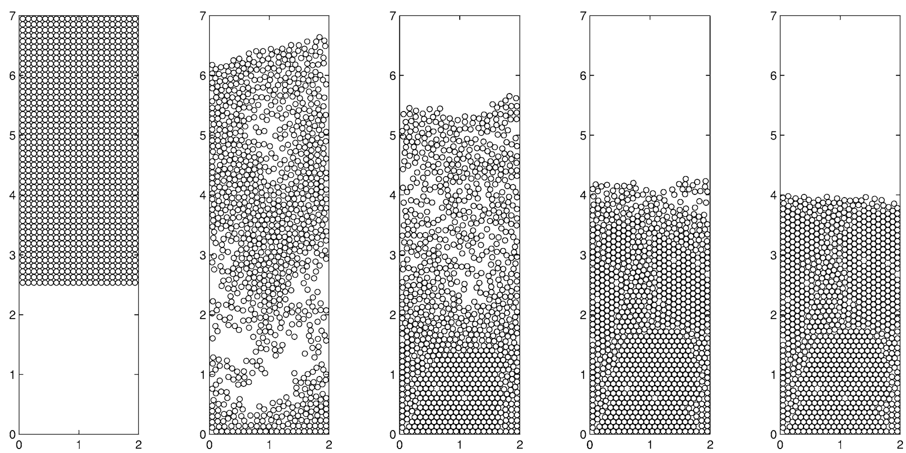


Figure 3. Evolution of motion of 1008 particles of specific gravity 1.5 sedimenting in a viscous fluid under the effect of gravity. From left to right, evolution traced at $t = 0$, $t = 1.0$, $t = 2.0$, $t = 3.0$ and $t = 3.28$ time units.

for all particles, $D = 0.09$, $\Delta h = 1/128$, $\Delta t = 0.001$ and $\Omega = (0, 2) \times (0, 7)$. Fig. 3 shows the progress of the sedimentation. The algorithm was able to handle effectively a large number of collisions, in the order of tens of thousands in one time step. The advantage of our algorithm is that there is no possibility of two discs overlapping each other at any point and no checks have to be introduced for this. The collision parameters used in all our experiments are $e_n = 0.95$, $\mu_k = 0.2$ and $\mu_s = 0.2$.

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