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Towards the numerical simulation of fluid/solid particles flow inside a pipe

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The modeling of moving solid particles in fluid flow has been the focus of many studies and has succeeded to attract sufficient attention by researchers. However, commonly used modeling approaches such as discrete element modeling (DEM) and direct numerical simulations (DNS) lack simplicity and have been computationally intensive [1]. The aim of this paper is to develop a new approach to simulate solid transport in an incompressible Newtonian fluid flow. This method is based on the Finite element method with penalization of the deformation tensor [2]. The fluid behavior is governed by the Navier-Stokes equations within the investigation domain. To take into account collisions, we present an algorithm which allows us to handle contacts between rigid particles [3, 4]. In this paper, 2D simulation fluid/particles flow is performed; some preliminary results are presented.

Keywords
Flow, Fluid/Particles, Contact handling

1 Mathematical formulation of the fluid-structure problem

We consider a connected, bounded and regular domain $\Omega \subset \mathbb{R}^2$ and we denote by $(B_i)_{i=1,\cdots,N}$ the rigid particles, strongly included in Ω. B denotes the whole rigid domain: $B = \cup_i B_i$. The domain $\Omega \setminus \overline{B}$ is filled with Newtonian fluid governed by the Navier-Stokes equations. We note μ the viscosity of the fluid, p the presure and $\mathrm{f_f}$ the external forces exerted on it. Since we consider a Newtonian fluid, the stress tensor $\underline{\underline{\sigma}}$ is given by the following relation (see Eq. (1)):

$$\underline{\underline{\sigma}} = 2\mu\mathbb{D}(\mathbf{u}) - p\mathbb{I}, \quad \text{where} \quad \mathbb{D}(\mathbf{u}) = \frac{\nabla(\mathbf{u}) + (\nabla(\mathbf{u}))^T}{2} \tag{1}$$

and p the presure. For the sake of simplicity we will consider homogeneous Dirichlet conditions on $\partial\Omega$. On the other hand, viscosity imposes a no-slip condition on the boundary ∂B

of the rigid domain.
At the initial time the particles with density ρ_i are distributed randomly over the fluid. The position of the center of the ith particle is denoted by x_i, by v_i and ω_i its translational and angular velocities. We denote by m_i and J_i the mass and the kinematic momentum about its center of mass:

$$m_i = \int_{B_i} \rho_i, \quad J_i = \int_{B_i} \rho_i \|x - x_i\|^2 \tag{2}$$

We have to find the velocity $\mathrm{u}(u_1, u_2)$ and the pressure field p defined in $\Omega \setminus \overline{B}$, as well as the velocities of the particles$\mathbf{V} := (\mathrm{v}_{\mathrm{i}=1,\ldots,\mathrm{N}}) \in \mathbb{R}^{2N}$ and $\omega := (\omega_{\mathrm{i}=1,\ldots,\mathrm{N}}) \in \mathbb{R}^N$ such that (see Eq. (3)):

$$\begin{cases} \rho_{\mathrm{f}}(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u}) - \mathrm{div}(\underline{\sigma}) = \mathbf{f}_{\mathrm{f}} & \text{in } \Omega \setminus \overline{B}, \\ \mathrm{div}(\mathbf{u}) = 0 & \text{in } \Omega \setminus \overline{B}, \\ \mathbf{u} = 0 & \text{on } \partial\Omega, \\ \mathbf{u} = \mathbf{v}_i + \omega_i (x - x_i)^{\perp} \text{ on } \partial B, \ \forall i \in \{1,\ldots,N\} \end{cases} \tag{3}$$

where ρ_{f} denotes the density of the fluid and $\mathbf{f}_{\mathrm{f}} = \rho_{\mathrm{f}} g e_y$ is the external force exerted on the fluid (gravity forces). The fluid exerts hydrodynamic forces on the particles. Newton's second law for these particles is written then as follows (see Eq. (4)):

$$\begin{cases} m_i \frac{dV_i}{dt} = \int_{B_i} \mathrm{f_i} - \int_{\partial B_i} \underline{\sigma} n, \\ \\ J_i \frac{d\omega_i}{dt} = \int_{B_i} (x - x_i)^{\perp}.\mathrm{f_i} - \int_{\partial B_i} (x - x_i)^{\perp}.\underline{\sigma} n, \end{cases} \tag{4}$$

Where, $\mathrm{f_i}$ denotes the external non-hydrodynamical forces exerted on the sphere, such as gravity : $\mathrm{f_i} = -\rho_i g e_y$. In order to avoid remeshing, we look for a weak formulation involving functions defined on the whole domain Ω.In this manner, it can be proven that this problem leads to the variational formulation (see Eq. (5)):

$$\begin{cases} Find\ (\mathbf{u}, p) \in \mathbf{K}_B \times \mathbf{L}^2_0(\Omega)\ such\ that \\ \\ \int_\Omega \tilde{\rho} \frac{D\mathbf{u}}{Dt}\mathbf{v} + 2\mu \int_\Omega \mathbb{D}(\mathbf{u}) : \mathbb{D}(\mathbf{v}) - \int_\Omega p \mathrm{div}(\mathbf{v}) = \int_\Omega \tilde{\mathrm{f}}.\mathbf{v}, \ \forall \mathbf{v} \in \mathbf{K}_B \\ \\ \int_\Omega q \mathrm{div}(\mathbf{u}) = 0, \ \forall q \in \mathbf{L}^2_0, \end{cases} \tag{5}$$

with $\tilde{\rho} := \rho_f \mathbf{1}_{\Omega\setminus\overline{B}} + \sum_{i=1}^N \rho_f \mathbf{1}_{B_i}$, $\quad \tilde{\mathrm{f}} := \mathrm{f}_f \mathbf{1}_{\Omega\setminus\overline{B}} + \sum_{i=1}^N \mathrm{f}_i \mathbf{1}_{B_i}\ and\ \mathbf{K}_B = \{\mathbf{u} \in H^1_0(\Omega) \mathbb{D}(\mathbf{u}) = 0\ in B\}$.
Using a penalty method, we will rather consider the following problem:

$$\begin{cases} Find\ (\mathbf{u}, p) \in \mathbf{H}^1_0(\Omega) \times \mathbf{L}^2(\Omega)\ such\ that \\ \\ \int_\Omega \tilde{\rho} \frac{D\mathbf{u}}{Dt}\mathbf{v} + 2\mu \int_\Omega \mathbb{D}(\mathbf{u}) : \mathbb{D}(\mathbf{v}) + \frac{2}{\varepsilon} \int_B \mathbb{D}(\mathbf{u}) : \mathbb{D}(\mathbf{v}) \\ \qquad - \int_\Omega p \mathrm{div}(\mathbf{v}) = \int_\Omega \tilde{\mathrm{f}}.\mathbf{v}, \ \forall \mathbf{v} \in \mathbf{H}^1_0(\Omega), \\ \\ \int_\Omega q \mathrm{div}(\mathbf{u}) = 0, \ \forall q \in \mathbf{L}^2(\Omega), \end{cases} \tag{6}$$

The time discretization is performed by using the method of characteristics.
The dynamics (translational and angular velocities) of the rigid spheres is gouverned by the following relations:

$$\dot{x_i} := \mathrm{v_i} := \frac{\displaystyle\int_{\partial B_i} \rho_i \mathbf{u} ds}{\displaystyle\int_{\partial B_i} \rho_i ds}, \qquad \dot{\theta}_i := \omega_i := \frac{\displaystyle\int_{\partial B_i} \rho_i \mathbf{u}.(x - x_i)^{\perp} ds}{\displaystyle\int_{\partial B_i} \rho_i \|x - x_i\|^2 ds}$$

2 Contact Handling Procedure

Let us detail the method in the case of spherical particles: we denote by $\mathbf{X}^n := (\mathrm{x_i^n})_{i=1,.....,N}$ the position of N particles (more precisely, the position of their gravity centre) at time t_n, by $\hat{\mathbf{V}}^n = (\hat{\mathrm{v}}_i)_{i=1,.....,N}$ the a priori translational velocity, by $\hat{\Omega}^n = (\hat{\omega}_i)_{i=1,.....,N}$ the a priori rotational velocity. As stated before, the a priori updated position of the particles, defined as:

$$\mathbf{X}^{n+1} = \mathbf{X}^n + \Delta t \hat{\mathbf{V}}^n + \frac{1}{2}\gamma^n \triangle t^2 \tag{7}$$

where γ the acceleration, calculated from the Newton's second law. Equation 7 may lead to non-admissible configuration, in the sense that the particles overlap. To avoid this, we project the velocities onto the following set:

$$K(X^n) = \{\mathrm{V} \in \mathbb{R}^{2N}, D_{ij}(\mathrm{X}^n) + \Delta t \mathrm{G}_{ij}(\mathrm{X}^n).\mathrm{V} + \frac{1}{2}\gamma^n \triangle t^2 \geqslant 0, \forall i < j\} \tag{8}$$

where D_{ij} is the distance between every two particles given as:

$$D_{ij}(\mathrm{X}^n) = \|\mathrm{x}_i^n - \mathrm{x}_j^n\| - (R_i - R_j) \tag{9}$$

At each time step, $\mathrm{V} \in \mathbb{R}^{2N}$ is an admissible vector if the particles with velocity $\{\mathrm{V}$ do not overlap at the next time step:

$$E(X^n) = \{\mathrm{V} \in \mathbb{R}^{2N}, D_{ij}(\mathrm{X}^n + \Delta t \mathrm{V}^n + \frac{1}{2}\gamma^n \triangle t^2) \geqslant 0, \forall i < j\} \tag{10}$$

We not that equation 8 is the linearized form of equation 10 and, furthermore, it can be shown that $K(X^n) \subset E(X^n)$. It means in particular that particles with admissible velocities at time t_n do not overlap at time t_{n+1}.
The constrained problem is formulated as a saddle-point problem, by using the introduction of Lagrange multipliers:

$$\begin{cases} Find(\mathrm{V}^n, \Lambda^n) \in \mathbb{R}^{2N} \times \mathbb{R}_+^{N(N-1)/2} \quad such\, that \\ \mathcal{J}(\mathrm{V}^n, \lambda) \leqslant \mathcal{J}(\mathrm{V}^n, \Lambda^n) \leqslant \mathcal{J}(\mathrm{V}, \Lambda^n), \quad \forall (\mathrm{V}^n, \lambda) \in \mathbb{R}^{2N} \times \mathbb{R}_+^{N(N-1)/2} \end{cases} \tag{11}$$

with the following functional:

$$\mathcal{J}(\mathrm{V}, \lambda) = \frac{1}{2} \mid \mathrm{V} - \hat{\mathbf{V}}^n \mid^2 - \sum_{1 \leqslant i \leqslant j \leqslant N} \lambda_{ij}(D_{ij}(\mathrm{X}^n) + \Delta t \mathrm{G}_{ij}(\mathrm{X}^n).\mathrm{V}) + \frac{1}{2}\gamma^n \triangle t^2 \tag{12}$$

Where $\mathrm{G}_{ij}(\mathrm{X}^n) \in \mathbb{R}^{2N}$ is the gradient of distance D_{ij}. The number of Lagrange multipliers (λ_{ij}) corresponds to the number of possible contacts.
This problem is solved by an Uzawa algorithm.

3 case test

In this section, we present the simulation of the flow of an incompressible fluid, with a density of $\rho_f = 1000kg/m^3$ and a dynamic viscosity $\mu = 0.001Pa.s$, involving 100 particles, of density $\rho_p = 2250kg/m^3$ randomly distributed in the pipe. The radius and length of the pipe are respectively $r \times L = 0.12m \times 1.4m$.
In this case, particles with $0.015m$ are subjected to a Poiseuille flow, and a parabolic profile is imposed at the inlet. The configurations obtained at different time steps are presented (figure 1).

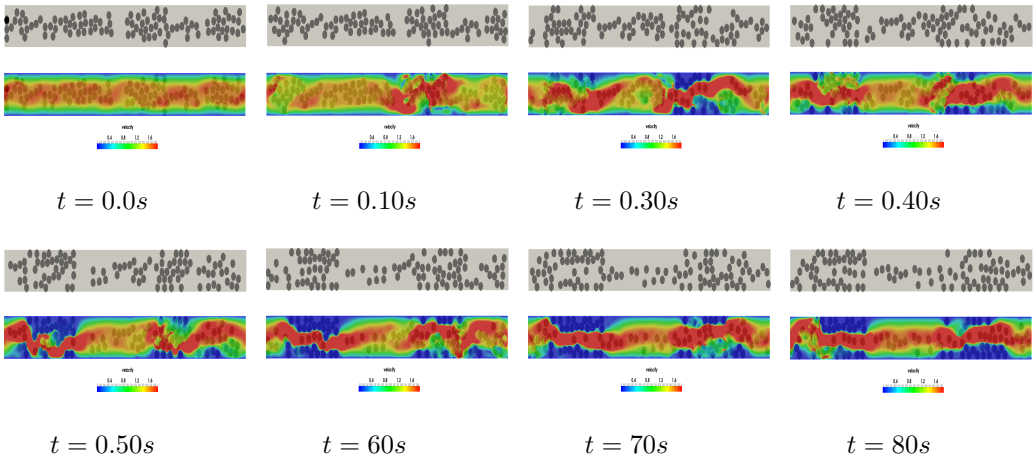

Figure 1: Fluid/solid particles flow: Configuration at different time steps.

The test cases presented make it possible to verify and validate the consideration of the rigid movement by the penalty method. In horizontal pipe, the effect of gravity, normal to the pipe axis, makes the flow pattern richer and higher.

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