A collision model for DNS with ellipsoidal particles in viscous fluid

Authors : Ramandeep Jain, Silvio Tschisgale, Jochen Fröhlich

Reference : *A collision model for DNS with ellipsoidal particles in viscous fluid*, 2019.

Céline Van Landeghem
University of Strasbourg
Master 2 CSMI

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Introduction

Fluid-particle interaction : described by the semi-implicit Immersed Boundary Method.

Particle-particle interaction : characterized by three sub-models :

1. **Contact detection algorithm**
2. **Collision model :**
   - The particle surfaces are in direct contact.
   - Model based on the hard sphere approach.
   - Model without numerical parameters, and takes into account hydrodynamic forces.
3. **Lubrication model :**
   - Distance between particle surfaces very small.
   - Constant lubrication force.

Mathematical formulation

Hydrodynamic forces : described by the Navier-Stokes equations.

Particle dynamics : described by Newton's equations

$$m_p \frac{du_p}{dt} = \int_{dP} \tau \cdot n + V_p(\rho_p - \rho_f)(g + f_v) + f_c + f_{lub}$$

$$I_p \cdot \frac{d\Omega_p}{dt} + \Omega_p \times I_p \cdot \Omega_p = \int_{dP} R \times (T \cdot N) + M_c + M_{lub}$$

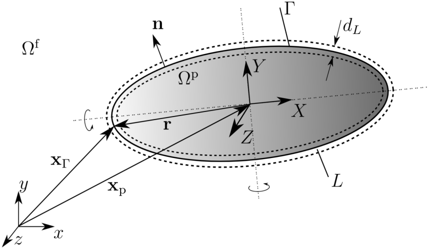
Fluid definitions :
$\rho_f \in \mathbb{R}^+$, density.
$\tau \in \mathbb{M}_{3,3}$, stress tensor.
$T \in \mathbb{M}_{3,3}$, stress tensor in local frame.

Particle definitions :
$P \in \mathbb{R}^3$, particle domain.
$m_p \in \mathbb{R}^+$, mass.
$V_p \in \mathbb{R}^+$, volume.

Particle definitions :
$\rho_p \in \mathbb{R}^+$, density.
$I_p \in \mathbb{R}^3$, moment of inertia.
$u_p \in \mathbb{R}^3$, translational velocity.
$\Omega_p \in \mathbb{R}^3$, angular velocity.
$R \in \mathbb{R}^3$, vector between mass center and surface point.

Forces definition :
$g \in \mathbb{R}^3$, gravity.
$f_v \in \mathbb{R}^3$, external forces on fluid.
$f_c \in \mathbb{R}^3$, collision force.
$f_{lub} \in \mathbb{R}^3$, lubrication force.
$M_c \in \mathbb{R}^3$, collision torque.
$M_{lub} \in \mathbb{R}^3$, lubrication torque.

Mathematical formulation



Discretized equation for translational velocity :

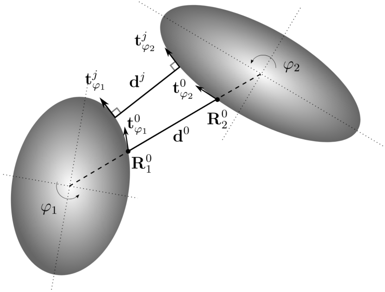
$$u_p^n - u_p^{n-1} = (m_p + m_L)^{-1} \Delta t \{ f_f + f_g + f_c + f_{lub} + f_v \}$$

Discretized equation for angular velocity :

$$\Omega_p^n - \Omega_p^{n-1} = -(I_p + I_L)^{-1} \{ \int_{n-1}^{n} \Omega_p \times I_p \cdot \Omega_p \} + \Delta t (I_p + I_L)^{-1} \cdot \{ M_f + M_c + M_{lub} \}$$

Silvio Tschisgale, Tobias Kempe, Jochen Fröhlich. *A general implicit direct forcing immersed boundary method for rigid particles*, 2018.

Contact detection algorithm



Boundary point $R = (R_X, R_Y, R_Z)$ **:**

$$\begin{cases} R_X = a\cos(\phi)\sin(\varphi), \\ R_Y = b\sin(\phi)\sin(\varphi), \\ R_Z = c\cos(\varphi), \end{cases}$$

where a, b, c axis and ϕ, φ azimuthal and polar angle.

Algorithm properties :

- **Iterative method :**

$$\varphi^{j+1} = \varphi^j + \frac{D_{eq}}{a}\frac{d^j \cdot t^j_\varphi}{|d^j||t^j_\varphi|},$$

$$\phi^{j+1} = \phi^j + \frac{D_{eq}}{a}\frac{d^j \cdot t^j_\phi}{|d^j||t^j_\phi|},$$

where $t_{\phi^j}, t_{\varphi^j}$ vectors located at R^j, tangential to boundary. d^j distance between R^j of particles and D_{eq} equivalent diameter.

- **Stopping criterion :**

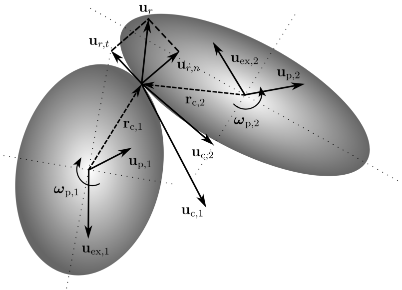
$$d^j \cdot t^j_\phi < \delta \quad d^j \cdot t^j_\varphi < \delta$$

- **Criterion of use :**

$$|x_{p,1} - x_{p,2}| \leq a_1 + a_2 + d_{lub}$$

- **Fast convergence.**
- **No additional parameters.**

Collision model



Starting point of collision model : Time level t^{n-1} representing first contact.
Hard-sphere approach : Collision time is small, so that at time level t^{n-1} only the particle velocities change, while their position and orientation remain unchanged.
-> Collision force f_c can be approximated by a constant value over the time interval Δt.

Aim : Approximate f_c to get particle velocities after collision at time level t^n.
Step 1 : Considering particle velocities at contact point at time level t^n :

$$u_c^n = u_p^n + \omega_p^n \times r_c,$$
$$\Rightarrow u_c^n = u_c^{n-1} + u_{ex} + (m_p + m_L)^{-1} p_c + (i_p + i_L)^{-1} \cdot l_c \times r_c,$$

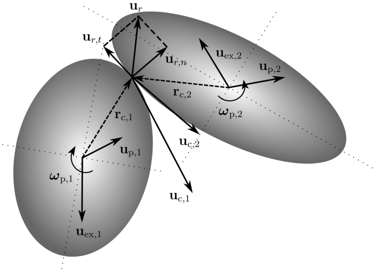
where u_{ex} known velocity due to external forces, $p_c = \Delta t f_c$ and $l_c = \Delta t m_c = r_c \times p_c$ linear an angular momentum due to collision.

Collision model

Step 2 : Determining the value of p_c :
The relationship between p_c and I_c allows writing :

$$u_c^n = u_c^{n-1} + u_{ex} + K \cdot p_c,$$

where K a symmetric system matrix. p_c has same magnitude for both particles, but is directed in opposite direction :



$$u_{c,1}^n = u_{c,1}^{n-1} + u_{ex,1} - K_1 \cdot p_c,$$
$$u_{c,2}^n = u_{c,2}^{n-1} + u_{ex,2} + K_2 \cdot p_c.$$

The difference gives :

$$p_c = (K_1 + K_2)^{-1} \cdot (u_r^n - u_r^{n-1} - u_{ex,r}),$$

$u_r^n = u_{c,2}^n - u_{c,1}^n$ the relative velocity at contact point.

Collision model

Step 3 : Determining the unknown $u_r^n = u_{r,n}^n + u_{r,t}^n$ using Poisson hypothesis :

$$u_{r,n}^n = -e_{d,n} u_{r,n}^{n-1} = -e_{d,n}(u_r^{n-1} \cdot n)n$$
$$u_{r,t}^n = -e_{d,t} u_{r,t}^{n-1} = -e_{d,t}(u_r^{n-1} \cdot t)t$$

Where $e_{d,n}, e_{d,t}$ dry and tangential coefficient of restitution.

Step 4 : Determining particle behavior after contact [3] :
Assuming that particles stick fully after contact, $e_{d,t} = 0$, the change in relative velocity and linear momentum get :

$$\Delta u = u_r^{n-1} - u_r^n = u_r^{n-1} + e_{d,n}(u_r^{n-1} \cdot n)n$$
$$p_c = -(K_1 + K_2)^{-1} \cdot \Delta u - (K_1 + K_2)^{-1} \cdot u_{ex,r}$$

Particles stick after contact :

$|p_c \cdot t| \leq \mu_s |p_c \cdot n|$, μ_s static coefficient of friction.
$\Rightarrow p_c$ good approximation of collision response.

Particles slide after contact :

Redefinition of p_c using Coulomb law of friction :

$$p_c = p_n(n + \mu_k t),\ p_n = -\frac{\Delta u \cdot n + u_{ex,r} \cdot n}{(K_1 + K_2) \cdot (n + \mu_k t) \cdot n},$$

μ_k kinetic coefficient of friction.

Lubrication model

Lubrication model with constant force f_{lub} :

- Ensures that hydrodynamic forces are resolved short time before and after direct contact, for distances smaller than d_{lub}.
- Constant force avoids uncontrolled variations of f_{lub}.

Model for spherical particles :

$$f_{lub} = \begin{cases} 0\,, & d > d_{lub}, \\ -k(St_r)\frac{\mu_f u_{r,n}}{d_{lub}}\left(\frac{r_1 r_2}{r_1+r_2}\right)^2\,, & d \leq d_{lub}, \end{cases}$$

depending on particles radii, distance d_{lub}, fluid viscosity, normal relative velocity at contact point and relative Stokes number :

$$St_r = \frac{\rho_p}{9\rho_f}\frac{|u_{r,n}|}{\nu_f}\left(\frac{r_1 r_2}{(r_1+r_2)/2}\right)$$

Gauss function [4] :

$$k(St_r) = 125\exp\left\{-\frac{1}{20000}St_r^2\right\}$$

Model for arbitrary particles :
Particle surfaces are approximated by a sphere of same curvature using Gaussian curvature at contact point R [1] :

$$G = \frac{1}{a^2 b^2 c^2\left[\frac{R_X^2}{a^4} + \frac{R_Y^2}{b^4} + \frac{R_Z^2}{c^4}\right]^2}$$

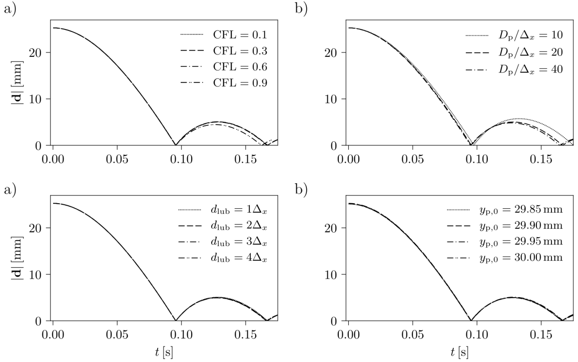
Radius of Gaussian curvature :

$$R_G = \frac{1}{\sqrt{G}}$$

used to replace the particles radii.

Sensitivity analysis

Sensitivity of the model to different quantities for a particle-wall collision :



CFL :
- Rebound trajectories are damped for larger time steps.
- No differences for CFL ≤ 0.6.

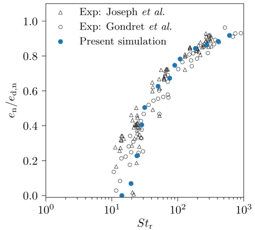
Distance d_{lub} :
- No visible differences.

Spatial resolution :
- Trajectory before and after collision differs from reference for larger mesh sizes.
- Fluid forces are only marginally captured.

Initial height :
- No visible differences.

Validation

Normal collision of a spherical particle with a wall [5] [4]



The relative Stokes number is varied to analyze its influence on the restitution coefficient for normal collision :

$$e_n = -\frac{|u_{p,n,out}|}{|u_{p,n,in}|},$$

$u_{p,n,in}$, $u_{p,n,out}$ the particle normal velocities before and after the lubrication zone.

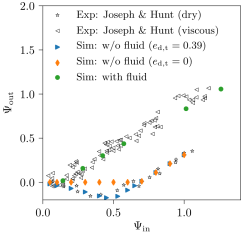
Oblique collision of a spherical particle with a wall [6]

Particles are driven by the acceleration :

$g = (g\sin(\phi_{in}), -g\cos(\phi_{in}), 0)^T$, ϕ_{in} incidence angle.

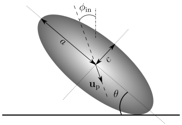
Comparison of the rebound angle Ψ_{out} to the impact angle Ψ_{in} :

$$\Psi_{in} = \frac{|u_{c,t,in}|}{|u_{c,n,in}|} \quad , \Psi_{out} = \frac{|u_{c,t,out}|}{|u_{c,n,in}|}$$



Results

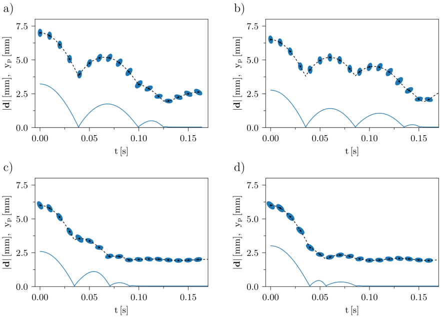
Oblique collision of ellipsoidal particles



For ellipsoidal particles the rebound trajectory does not only depend on the relative Stokes number but also on the particle axis a, b, c, the particle orientation θ and angular velocity.

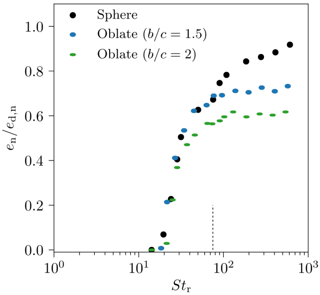
Rebound trajectories for different θ for oblate ellipsoids, $a = b$, $\frac{b}{c} = 2$:

a) $\theta = \frac{\pi}{2}$
b) $\theta = \frac{4\pi}{9}$
c) $\theta = \frac{\pi}{3}$
d) $\theta = \frac{\pi}{4}$



Results

Normal collision of oblate particles with a wall



Investigation on the dependency of the restitution coefficient as a function of the relative Stokes number, considering different ratio of particles axis, $\frac{b}{c}$:

- Maximum value for normalized restitution coefficient decreases with increasing ratio $\frac{b}{c}$.
- Lubrication forces become larger with increasing flatness of particles ; increasing radius of curvature.

References for collision models

- Soft sphere collision model :

M.N.Ardekani, P.Costa, W.P.Breugem, L.Brandt. *Numerical study of the sedimentation of spherical particles*, 2016.

E.Biegert, B.Vowinckel,E.Meiburg. *A collision model for grain-resolving simulations of flows over dense, mobile, polydisperse granular sediment beds*, 2017.

- Collision model for complex shaped particles :

S.Fukuoka, T.Fukuda, T.Uchida. *Effects of sizes and shapes of gravel particles on sediment transports and bed variations in a numerical movable-bed channel*, 2014.

R.Sun, H.Xiao, H.Sun. *Realistic representation of grain shapes in CFD-DEM simulations of sediment transport with a bonded-sphere approach*, 2017.

- Hertzian contact theory :

S.Ray, T.Kempe, J.Fröhlich. *Efficient modelling of particle collisions using a non-linear viscoelastic contact force*, 2015.

References for collision models

- Adaptive collision model :

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- Multi-collision model :

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