PARTICLE CONTACT LAWS AND THEIR PROPERTIES FOR SIMULATION OF FLUID-SEDIMENT INTERACTION WITH COUPLED SPH-DEM MODEL

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Abstract. The transport of sediment due to the interaction of fluid and solids is a prevalent geophysical process. The detailed modelling of the interaction between the fluid and the sediment particles is still a challenging task. In the present study we model the fluid phase by smoothed particle hydrodynamics (SPH) using the classical approach where the fluid is assumed to be weakly compressible. The sediment, in terms of solid spheres made of granite, is modelled by the discrete element method (DEM). Both of them are meshfree particle methods but SPH is a continuum approach and DEM describes the motion and interaction of discrete solid objects. The interaction between SPH and DEM particles is modelled as particle-to-particle contact in combination with a boundary condition at the solid interface. Therefore, a contact law is used to capture the collision process and to ensure balancing of collision forces. In doing so, two contact types have to be modelled, i.e. sediment-sediment and fluid-sediment. The approach and properties these contact types are presented in detail. Advantages and drawbacks of the approaches are discussed based on examples.

1 INTRODUCTION

Sediment transport due to the interaction between fluid and sediment particles is a prevalent process in the environment as occurring in rivers for example. Common modelling approaches are mainly based on empirical closure conditions for the estimation of the transport rate. Numerical simulations for the investigation of the underlying processes in
detail are rather seldom [1]. This is mainly because of the difficulties that arise from the fluid-sediment interaction, especially when complex object geometries and moving boundaries have to be considered. For fluid-structure interaction, particle methods became a promising approach that may also be suitable for the simulation of sediment transport. The main advantage of meshfree particle methods is that there is no need for costly grid generation and interface tracing or capturing techniques. In the present study we model the fluid phase by smoothed particle hydrodynamics (SPH) using the classical approach where the fluid is assumed to be weakly compressible. The sediment, in terms of solid spheres made of granite, is modelled by the discrete element method (DEM). The interactions between the particles are modelled as particle-to-particle contacts, whereas three different contact types may be distinguished: sediment-sediment, fluid-sediment and fluid-fluid. The first is the basis of DEM, where contact laws are used to capture the collision process and to ensure balancing of collision forces. The latter corresponds to the SPH discretization. For the modelling of the fluid-sediment interaction, the combination of DEM and SPH is not straightforward, since SPH is a continuum approach and DEM is based on discrete force models. Thus, the interaction is considered as SPH-DEM particle contact in combination with a boundary condition for the SPH particle at the solid interface.

In this contribution the sediment-sediment and fluid-sediment interaction are presented in detail. The advantages and drawbacks of the approaches are discussed based on three examples: the collision of two sediment particles, the buoyancy force acting on a sediment particle and the settling of a sediment particle. It will be shown for the sediment-sediment interaction that the error of the interaction force strongly depends on time step size and material properties. For the fluid-sediment interaction the importance of an appropriate parametrisation of the contact law is pointed out.

2 MODELLING APPROACH

The governing equations used for modelling of the fluid flow are the Euler equations in Lagrangian form, whereas energy conservation is omitted (isothermal fluid). The simulation of the sediment particles is based on Newton’s second law and the dynamic Euler equations that describe the conservation of linear and angular momentum, respectively. For simplification purposes, the sediment particles are considered to be spherical.

3.1 Smoothed Particle Hydrodynamics

The idea behind SPH can be described as replacing the fluid by a set of points that follow the motion and carry information about the properties of the fluid. These points can be seen either as interpolation points for the discretization of the governing equations or as real material particles [2]. For the present work, the standard SPH method is used that is also termed “weakly compressible SPH”, where the computation of the pressure is based on an equation of state for water.

For the discretization of the governing equations, the fluid continuum is approximated by particles, whereas any quantity or function \( A(\vec{r}) \) at location \( \vec{r} \) can be obtained by interpolation based on a kernel function \( W(r_{ab}, h) \), where \( r_{ab} = |\vec{r}_a - \vec{r}_b| \) is the distance between two particles \( a \) and \( b \), and \( h \) is the smoothing length. For the present work the Gaussian kernel with a cut-off at distance \( 2h \) is used.
Considering particles with mass \(m\), density \(\rho\) and position \(\vec{r}\) identified by indices \(a\) and \(b\), where \(a\) identifies the particle of interest and \(b\) the neighboring particles within cut-off distance with masses according to a volume element of the fluid \(m_b = \rho_b(\vec{r}_b) d\vec{r}_b\) and \(A_b = A_r(\vec{r}_b)\), the summation interpolant can be written as

\[
A_a(\vec{r}_a) = \sum_b m_b \frac{A_b}{\rho_b} W(r_{ab}, h) .
\]

The derivative of \(A_a\) can be obtained by ordinary differentiation of the kernel function. Consequently, the Euler equations can be discretized for particles according to this concept. The conservation of mass in its discretized form reads

\[
\frac{d\rho_a}{dt} = \rho_a \sum_b \frac{m_b}{\rho_b} (\vec{u}_a - \vec{u}_b) \cdot \nabla_a W_{ab} ,
\]

and the conservation of momentum reads

\[
\frac{d\vec{u}_a}{dt} = -\sum_b m_b \left( \frac{\rho_a}{\rho_a^2} + \frac{\rho_b}{\rho_b^2} + \Pi_{ab}(\alpha, \beta) \right) \nabla_a W_{ab} + \vec{f}_a ,
\]

where \(\Pi_{ab}(\alpha, \beta)\) is the artificial viscosity term [3], \(\vec{u}_a\) is the velocity, \(p_a\) is the pressure (similar for neighboring particles with index \(b\)). The particles are moved by

\[
\frac{d\vec{r}_a}{dt} = \vec{u}_a .
\]

The equation system is closed by an appropriate equation of state for the pressure \(p\):

\[
p_a = B \left( \frac{\rho_a}{\rho_f} \right)^{\gamma_p} - 1 , \quad B = \frac{c_s^2}{\gamma_p} ,
\]

where \(\rho_f\) is the reference density of the fluid and usually \(\gamma_p = 7\). The choice of \(B\) determines the speed of sound. Since the time-step size of the simulation may depend on the speed of sound \(c_s\), a rather small value compared to its effective value of \(~1500\) m/s is preferred to gain a faster simulation progress. In order to limit density variations to a maximum of 1%, the sound velocity is chosen so that the Mach number of the flow is 0.1 or less [3]; this yields \(c_s = 10u_{ref}\). The reference velocity \(u_{ref}\) depends on the problem, e.g. the wave propagation velocity in the case of free surface flow.

For time integration a predictor-corrector method based on the leapfrog scheme is used [4]. The size of the time step \(\Delta t\) is determined based on three characteristic time scales: the CFL-condition with \(u_{max} = \max(\vec{u}, c_s)\) and the maximum of acting internal as well as external forces, i.e. the viscous forces and the applied forces in terms of the maximum particle acceleration \(a_{max}\), whereas the former is only relevant for flows with low Reynolds numbers. For SPH, the relevant length scale is the smoothing length \(h\). According to these considerations, the size of a time step can be obtained by the assignment.
\[ \Delta t = \alpha_s \min \left( \frac{h}{u_{\text{max}}}, \frac{h^2}{\nu}, \sqrt{\frac{h}{a_{\text{max}}}} \right), \tag{6} \]

where \( \alpha_s \) is a safety factor in the range of 0.125 and 0.5 (see e.g. [5]). More recent and advanced considerations about the maximum time step are given in [6].

### 3.2 Discrete Element Method

The original concept of the DEM [7] is to allow for a usually small but non-physical interpenetration of colliding rigid bodies. The interpenetration is regarded to be an equivalent for the surface deformation and contact forces are related to the displacement or the amount of interpenetration \( \delta \) in general. With regard to a pair of colliding particles, the penetration continues until the forces exerted by the particles are balanced by the contact force, i.e. when maximum penetration is reached. This can be modelled by a spring-damper system (Figure 1), where the collision force is expressed as the sum of a penalty and a damping force:

\[ \vec{F}_c = \vec{F}_n (k(\delta)) + \vec{F}_d. \tag{7} \]

The penalty force \( \vec{F}_n (k(\delta)) \) acts in the direction of the surface normal and is discussed in the next section. A simple approach for modelling dissipation is the application of a viscous damper that depends on the collision velocity \( \vec{v} = |\vec{v}_i - \vec{v}_j| \) in the direction of the spring-damper system axis. The damping force is \( \vec{F}_d = -d \vec{\dot{\delta}} \vec{c}_{sd} \) where \( d \) is the viscous damping coefficient. With the depicted spring-damper system tangential forces such as fiction may be considered. For a general formulation of a nonlinear spring-damper model see [8].

**Figure 1**: Spring-damper system for the modelling of penalty forces due to overlapping including friction.

The time dependent motion of sediment particles is simulated according to Newton’s second law that describes the conservation of linear momentum (here for constant mass)
\[ m \frac{d\vec{v}}{dt} = \vec{F}_a, \]  
\[ \mathbf{I} \cdot \frac{d\mathbf{\omega}}{dt} + \mathbf{\omega} \times (\mathbf{I} \cdot \mathbf{\omega}) = \vec{M}_a \]  

where \( \vec{v} \) is the velocity and \( m \) is the mass of the particle, and the solution of the dynamic Euler equations for the conservation the angular momentum

where \( \mathbf{I} = \mathbf{I}^T \) is the tensor of moment of inertia in the fixed principal frame of the particle and \( \mathbf{\omega} \) the angular velocity. For the solution of equation (9) using quaternions see e.g. [9]. The applied force \( \vec{F}_a \) acting on a particle is the sum of contact forces \( \vec{F}_c \) and external forces, i.e. due to gravity. Consequently, the applied torque \( \vec{M}_a \) is the sum of torque due to contact- and external forces.

For the time integration of a dissipative DEM the Newmark-\( \beta \) schemes are appropriate [9]. However, in combination with SPH the same scheme with identical parameters is also used for the DEM to avoid asynchronism. The size of a time step can be obtained by similar conditions as for the SPH method. The relevant length scale is the radius of the smallest sphere \( r_{\text{min}} \). Furthermore, the maximum velocity \( u_{\text{max}} \) and maximum acceleration \( a_{\text{max}} \) are taken into account. Including a safety factor \( \alpha_s \), this leads to the following conditions for the time-step size

\[ \Delta t = \alpha_s \min \left( \frac{r_{\text{min}}}{u_{\text{max}}}, \sqrt[3]{\frac{r_{\text{min}}}{a_{\text{max}}}} \right). \]  

3 CONTACT LAWS

According to the previously introduced spring-damper system, the contact forces act either in normal or tangential direction. In normal direction the penalty force \( F_n(k(\delta)) \) can be determined using different approaches, either linear or nonlinear depending on \( k(\delta) \), i.e. material properties. In tangential direction different kinds of friction may be considered but in the current scope only the friction between fluid and sediment particles is discussed (see section 3.2).

3.1 Sediment-sediment interaction

Linear Force Model

Considering a perfectly elastic spring with stiffness \( c \) [N/m], the force to obtain a displacement \( \delta \) [m] in the direction of the spring-damper system axis \( \vec{e}_{sd} \) is

\[ \vec{F}_s(\delta) = -c\delta \vec{e}_{ij} = \vec{F}_n(k(\delta)) \], i.e. \( k(\delta) = c\delta \).
Hertz Force Model

A more physically motivated approach for modelling the interaction of two perfectly elastic spheres with frictionless surfaces is based on the contact theory of Hertz [10]. The nonlinear force law is written as

\[ \vec{F}_n(k(\delta)) = -K \delta^n \vec{e}_{ij} , \]  

i.e. \( k(\delta) = K \delta^n \), (12)

where \( K \) is the generalised stiffness constant and \( n = 1.5 \) [10]. For two colliding spheres \( i \) and \( j \), the stiffness parameter depends on the radii and the material properties,

\[ K = \frac{4}{3(\sigma_i + \sigma_j)} \left[ \frac{r_i r_j}{r_i + r_j} \right]^{\frac{1}{2}}, \]  

with material parameters \( \sigma_i \) and \( \sigma_j \):

\[ \sigma_k = \frac{1 - \nu_k^2}{E_k}, \]  

(14)

where \( \nu_k \) is Poisson’s ratio and \( E_k \) is Young’s modulus. An in-depth description of the Hertz contact theory is given by [11], for example.

3.2 Fluid-sediment interaction

Introduction

Universal and robust boundary conditions for the simulation of fluid-structure interaction with SPH are still an unsolved problem and part of ongoing research, see e.g. [12-14]. There are different solutions that include the creation of virtual boundary particles to avoid incomplete SPH interpolants: ghost particles, repulsive particles and dynamic particles [15]. The approach applied in this work is a combination of the first two concepts; thereby the main goal is to avoid penetration of the solid boundary by fluid particles.

Modified Lennard-Jones Potential

The use of a Lennard-Jones (LJ) potential allows modelling of the interaction of fluid particles with a rigid body in a similar manner as molecular interaction. Other than the original LJ potential that leads to an infinitely large force for a particle distance towards zero, [16] propose a force law with a finite value \( k \) of the force at the boundary (\( \vec{F}_n(r_{ij}) = 0 \) where \( r_{ij} \) is the distance between two particles). The maximum force value \( k \) at the boundary may be also denoted as stiffness of the boundary. Furthermore, the influence of the potential is limited to a given distance \( R \), i.e. \( \vec{F}_n(r_{ij}) = 0 \) for \( r_{ij} \geq R \). The point where the force changes from repulsion to attraction can be set equal to \( r_0 \). For the investigation of wall bounded flows, an approach depending on the particle distance to the boundary \( \delta_w \) is preferable.
For the interaction of a fluid particle with a sphere of radius \( r_s \), the following definitions are introduced:

\[
\delta_w := r_{ij} - r_s, \quad \delta_{w0} := r_0 - r_s, \quad D_w := R - r_s.
\]

Consequently, the force exerted by the modified Lennard-Jones (MLJ) potential within a maximum distance to the solid surface is

\[
\vec{F}_n(\delta_w) = \begin{cases} 
  k \left( \frac{\delta_w - D_w}{D_w + r_s} \right)^2 \left( \frac{\delta_w - 2D_w + \delta_w}{\delta_w - D_w} \right) \cdot e_{ij}, & \text{if } \delta_w < D_w, \\
  0, & \text{otherwise}.
\end{cases}
\]

Considering only repulsive forces (Figure 2), i.e. \( D_w = \delta_{w0} \), equation (16) becomes

\[
\vec{F}_n(\delta_w) = k \left\{ \frac{\delta_{w0} - \delta_w}{\delta_{w0} + r_s} \right\}^4 \cdot e_{ij}, \quad \delta_w \leq \delta_{w0}.
\]

To balance a given external force of amount \( F \) the equilibrium distance to the wall is

\[
\delta_{weq} = \delta_{w0} - \left( \delta_{w0} + r_s \right) \left( \frac{F}{k} \right)^{1/4}
\]

If a certain equilibrium distance to the wall is preferred, the appropriate stiffness could be obtained by rearranging equation (18),

\[
k = F \left( \frac{\delta_{w0} + r_s}{\delta_{w0} - \delta_{weq}} \right)^4.
\]
**Ghost particle**

For an SPH particle in contact with a sediment particle, an incomplete interpolant at the boundary has to be avoided. This is rudimentary done by creation of a ghost particle $P'_i$ with the same properties as the original particle $P_i$ (Figure 2). Indeed, this leads to slip conditions at the boundary. Thus, a fiction law has to be introduced to consider wall effects.

**Friction**

The tangential force $\vec{F}_t(\delta_w)$ that acts on a fluid particle in contact with a sediment particle is actually a viscous shear force $\vec{F}_v(\delta_w)$ plus effects due to the character of the surface. The tangential force can be written as

$$\vec{F}_t(\delta_w) = \begin{cases} \vec{F}_v(\delta_w) \tanh \{ \eta \{ v_t \} \} \vec{e}_t, & \text{if } \delta_w < D_{\text{visc}}, \\ 0, & \text{otherwise,} \end{cases}$$

where $\{ v_t \}$ is the value of relative tangential velocity $v_t$ and $D_{\text{visc}}$ is the influence distance of the force with respect to the surface. The viscous shear force can be expressed as $\vec{F}_v(\delta_w) = \mu_v (\Delta s)^2 \vec{v}_t / \delta_w$, where $\Delta s$ is the initial spacing of SPH particles and $\mu_v$ is a coefficient that is related to the viscosity of the fluid and the surface roughness. To prevent numerical instabilities, the hyperbolic tangent of the relative tangential velocity is used, i.e. $\eta \{ v_t \}$, where $\eta$ is the friction slope.

### 4 Examples

#### 4.1 Role of Material Properties

The parameters of the Hertz law, i.e. Poisson’s ratio $\nu_k$ and Young’s modulus $E_k$, are material properties commonly used in engineering practice. However, this connection to real materials has to be used with care, since the used approaches for the interaction forces are approximations that balance momentum but they do not render the contact of real material in detail. Although, the Hertz law is a reasonable model for the latter, the size of the time step would be very small already for moderate accuracy when it comes to very stiff materials such as granite. Thus, use of modified material properties which allow for larger time steps while still maintaining the accuracy requirements seems to be a useful approach. However, in such a case a larger penetration, i.e. a larger displacement of the sphere, has to be accepted. To illustrate this, consider the collision of two identical spheres with opposite velocity. The Hertz force model is applied as contact law. For varying Young’s modulus $E$ the maximum penetration depth $\delta_{\text{max}}$ can be estimated based on the conservation of energy [17] and thus the correct penalty force is known. The ratio of $\delta_{\text{max}}$ and the sphere radius $r_s$, $a = \delta_{\text{max}} / r_s$, can be used as a measure of displacement. For the present example, $a$ is varied between 0.09% ($E = 6.0 \times 10^{10}$ N/m$^2$) and 5% ($E = 3.44 \times 10^6$ N/m$^2$). In Figure 3 the standard deviation of the penalty force against the size of the time step is depicted. For the present example it is shown, that for the same level of accuracy, an approximately five times larger penetration has to be accepted to gain a magnitude in time-step size. For fluid-sediment simulations this aspect might be relevant, because the time-step size of SPH is usually larger than that of the DEM.
4.2 Buoyancy

Improper representation of the buoyancy force may lead to an incorrect weight of the submerged body. Thus, the resistance of the body against acting fluid dynamic forces may be misleading as well. To illustrate the influence of the contact law parameters, a simple experiment is carried out, where a sediment particle with radius \( r_s = 0.015 \text{ m} \) is initially located in the middle of a small tank of water at height \( z_s = 0.5 h_f \), with \( h_f = 0.1 \text{ m} \).

The interaction of the fluid particles with the sphere is modelled by the MLJ potential. The distance to the sphere surface where the penalty force is zero is set equal to the smoothing length, i.e. \( \delta_{w0} = h \), which corresponds to an active penalty force as soon as interaction takes place. The stiffness of the potential is obtained by evaluating a slightly modified form of equation (19), namely

\[
\Psi_{eq} = \frac{\delta_{weq}}{h} \quad \text{and} \quad k = F \left( \frac{h + r}{h (1 - \Psi_{eq})} \right)^4,
\]

where \( \Psi_{eq} = \delta_{weq}/h \) and the amount of the force is equal to the median pressure acting on the sphere, i.e. at the middle of the sphere \( F = (h_f - z_s) \rho_f g \Delta s^{-1} \), where \( \sigma \) is the dimension of the problem and \( g \) the gravitational acceleration. The parameter \( \Psi_{eq} \) actually determines the characteristics of the potential and thus the gradient of the repulsive force. For the given case with almost no fluid motion other force laws would also work, but they may not be able to prevent particle penetration with the estimated parameters when it comes to dynamic problems with larger flow velocities.
For this example, different resolution of fluid particles in terms of the initial particle distance $\Delta s = [0.01, 0.005, 0.0025]$ m, hereafter referred to as particle resolution, are considered and the parameter $\psi_{eq}$ is varied until the difference of the exact and simulated submerged weight is within a few per cent. According to equation (21) the force law depends on the parameter $\psi_{eq}$ which actually defines the equilibrium distance between the fluid particles and the sphere by $\delta_{weq} = h \psi_{eq}$. Thus, the parameter $\psi_{eq}$ indirectly controls the amount of displaced fluid and, consequently, the buoyancy force. Furthermore, the mass of the fluid particles is set according to $m_s = \rho_0 (\Delta s)^3$ wherein the term $(\Delta s)^3$ corresponds to a finite volume of fluid and $\rho_0$ to the initial density. Hence, it could be expected that $\delta_{weq}$ converges to $\Delta s/2$ for decreasing values of $\Delta s$ and $\psi_{eq} \rightarrow 1/3$ for the present case with $h = 1.5\Delta s$. This tendency was quite well reproduced by the experiments.

4.3 Settling of sphere

The influence of the scaling of the contact law on the terminal settling velocity of a sphere in a water tank with water depth $h_f$ is exemplified here. The force law is scaled by varying $d_{w0}$. Besides the standard configuration with $d_{w0} = h$, three different setups are studied: $d_{w0} = 2h$ and $d_{w0} = 3h$, resulting in a boundary condition with a smaller maximum repulsive force and slower increase for decreasing particle distance, and $d_{w0} = 0.5h$, which has the opposite effect.

The reference for the MLJ is assumed to be equal to the maximum dynamic pressure $F = 0.5 \rho_f w_s^2 \Delta s^{\sigma - 1}$, where $w_s$ is an estimate for the terminal settling velocity. However, the total pressure acting on the sphere is actually larger, because the a priori unknown ambient pressure is not considered.

For the case with the standard configuration, $d_{w0} = h$, and the case with $d_{w0} = 0.5h$, the difference of the reference force and the total effective pressure is less important, since the deviation is compensated by the force law in terms of a slightly smaller wall distance than the supposed equilibrium distance. For this configuration, the majority of the fluid particles do not penetrate the sphere surface, as depicted in Figure 4. In the two cases where $d_{w0} > h$, the increase of the repulsive force is slower than for the standard configuration and the deviation...
The combination of two meshfree particle methods, namely SPH and DEM, are considered for the simulation of fluid flow and sediment transport. Thereby, the sediment-sediment and fluid-sediment interaction is modelled by contact laws.

For the sediment-sediment interaction the Hertz force law is used that relates material properties to a repulsive contact force depending on penetration. It is shown by the example of two colliding spheres, that the accuracy of the contact force is strongly related to the material properties and the time-step size. Maintaining the level of accuracy, the time-step can be increased while reducing the stiffness of the material. However, the displacement of the particles also increases. This may become an issue (damping) in the case of simulations where small variations play a role, e.g. motion and forces due to turbulence quantities.

The proposed contact law for fluid-sediment interaction is computationally efficient, easy to implement for arbitrary geometries and allows for the creation of multiscale models. However, the choice of model parameters is not straightforward, since the reference force for the contact law may not be known a priori. Furthermore, physical properties of the sediment particles are affected by the contact law such as the buoyancy. For the used approach, this implies that the contact law depends on the particle resolution and the problem at hand. For this the adjustment of the repulsive force according to local fluid dynamic properties, e.g. the local flow depth [18], may be an improvement. However, this approach is limited to situations where flow conditions are more or less steady.

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