A SPH-DEM DISCRETIZATION FOR THE MODELLING OF COMPLEX MULTIPHASIC FREE SURFACE FLOWS

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Keywords: Smooth Particle Hydrodynamics, Discrete Element Method, Multi-phase, Free-surface, Meshless methods, Lagrangian approach

Abstract. Solid material advected by a fluid flow may contribute significantly to the momentum balance. Of special interest are free-surface flows that propagate as bores, which possess an enormous potential of incorporating solids. The motion of the solid mass may be difficult to predict due to the complexity of the modes of momentum transfer by the fluid motion and due to its interactions with other solids. A unified discretization of rigid solids and fluids that allows for detailed and resolved simulations of the fluid-solid phases is presented.

The model is based on the fundamental conservation laws of hydrodynamics, namely the continuity and Navier-Stokes equations, and the equation of conservation of momentum of solid bodies. The coupled numerical solution, based on Smoothed Particle Hydrodynamics (SPH) and Discrete Element Method (DEM) discretizations, resolves solid-solid and solid-fluid interactions in broad range of scales. Such entails details of momentum transfer at solid boundaries to large scales typical of engineering problems, such as transport of debris or hydrodynamic actions on structures.

A general overview of the methods and the coupling is addressed, and results for complex multiphasic flows are shown. Simple validations based on experimental work are discussed.
1 INTRODUCTION

The transport of solid material by a fluid flow is a common phenomena and, at the engineering scales, it may be associated with dramatic events such as inundations in urban scenarios. The importance of means to allow for risk analysis and consequent planning can not be overstated by the very nature of such events. They are usually unpredictable in frequency and magnitude and the destructive potential can be almost boundless, both in terms of property as in terms of human lives, as demonstrated by the inundation resulting from the tsunami that hit Japan March 2011.

The main difficulties with modelling such class of events arise from the characteristics of the phenomena and scale. The latter poses a problem even for the simplest models, since modelling even a single event can require remarkably large domains. This relates directly with the former, since the type of interaction and its relevant scales may require very high resolution adding to such large domains. The kind of non-linear and multiscale problem that is being addressed poses severe limitations to the usage of simple models [1]. Adequate closures for continuum models, for example, often require relevant simplifications from the rheological standpoint, greatly reducing their validity for generalized scenarios [2]. Furthermore, experimental validation of such models is remarkably complex and also relies on simplifications, both on the setup and on the analysis of the data [3, 4].

For many applications treating the flow as single phase, or as a continuum medium, is clearly insufficient. A model that can shed light into the mechanisms of these flows must attempt to characterize all relevant interactions at their proper scale. Within the meshless framework, efforts have been made on unifying solid and fluid modelling. Such is appealing since if the fluid phase is well discretized then most of such scales should be represented. [5] modelled a rigid body as a collection of Moving Particle Simulation (MPS) fluid particles, rigidified by default. This has become the standard approach due to its simplicity and good results. [6] modelled the effects of wave interaction on a caisson breakwater resorting to Smoothed Particle Hydrodynamics (SPH) and some special considerations for the particles that made up the solid body, effectively including a form of frictional behaviour. For normal interactions the continuum potential based forces of the form used in [6, 7] are not based in mechanics of contact of rigid bodies. Contact laws like the non-linear Hertzian models have been used extensively in the Discrete Element Method (DEM) literature [8], being regarded as one of the most, physically based, available class of contact laws. Further generalization allows for the inclusion and consideration of distinct materials in such interactions [9].

This work builds upon the DualSPHyics code (www.dual.sphysics.org), by introducing a model where inter particle forces of rigid body particles are taken from the contact law theories, therefore generalizing the shape possible for a typical DEM particle. The
very same particles are regarded by the fluid particles as SPH particles, possibly with a different density, allowing for a natural coupling between SPH and DEM. Buoyancy and other effects are naturally present when considering the floating rigid body as a cluster of SPH nodes, and so no other forces needed to be included in the discretization of the equations. The implementation has been already validated for interaction between fluid and fixed structures [10]. The DualSPHysics code enables simulation of million particles at a reasonable computation time by using GPU cards (Graphics Processing Units) as the execution devices. This allows to somewhat alleviate the previously expressed concerns about requirements of scale and resolution, since the computations are made up to two orders of magnitude faster than on normal CPU systems. Multi-GPU code is also being developed to further phase out the increased memory consumption by running high-resolution 3D models.

An experimental campaign portraying sets of rigid bodies subjected to a dam-break wave is used to validate model. Comparisons are made by direct visual comparison of the behaviour of the system.

2 METHOD FORMULATION

In SPH, the fluid domain is represented by a set of nodal points where physical properties such as mass, velocity, pressure and vorticity are known. These points move with the fluid in a Lagrangian manner and their properties change with time due to the interactions with neighbouring particles. The therm Smoothed Particle Hydrodynamics arises from the fact that the nodes, for all intended means, carry the mass of a portion of the medium, hence being easily labelled as Particles, and their individual angular velocity is disregarded, hence the Smooth. The method relies heavily on integral interpolant theory [11], that can be resumed to the exactness of

\[ A(r) = \int_{\Omega} A(r') \delta(r - r') \, dr', \]

for any continuous function \( A(r) \) defined in \( r' \), where \( \delta \) is the Dirac delta function and \( r \) is a distance. The nature of the Dirac delta function renders this identity useless however, and an approximation at \( r \) can be obtained by replacing it with a suitable weight function \( W \), called a kernel function. \( W \) should be an even function, defined on a compact support, i.e. if the radius is \( \epsilon h \) then \( W(r - r', h) = 0 \) if \( |r - r'| \geq \epsilon h \), with \( \lim_{h \to 0} W = \delta \) and \( \int_{\Omega} W(r', h) \, dr' = 1 \), where \( h \) is the smoothing length and defines the size of the kernel support. This leads to

\[ A(r) = \int_{\Omega'} A(r') \, W(r - r', h) \, dr', \quad \Omega' : |r - r'| \leq \epsilon h, \]
known as the integral interpolant. An approximation to discrete Lagrangian points can be made, by a proper discretization of the kernel function

$$A_i \approx \sum_j A_j V_j W(r_{ij}, h),$$

(3)
called the summation interpolant, extended to all particles $j$, $|r_{ij}| = |r_i - r_j| \leq \epsilon h$, where $V_j$ is the volume of particle $j$ and $A_i$ is the approximated variable at particle $i$. The cost of such approximation is that particle first order consistency, i.e., the ability of the kernel approximation to reproduce exactly a first order polynomial function, may not be assured by the summation interpolant, since

$$\sum_j V_j W(r_{ij}, h) \approx 1,$$

(4)
which is specially understandable in situations were the kernel function does not verify compact support, for example near the free surface or other open boundaries. Forcing the summation to equal 1 is called the Shepard correction

$$A_i = \frac{\sum_j A_j V_j W(r_{ij}, h)}{\sum_j V_j W(r_{ij}, h)},$$

(5)
restoring up to 1st order consistency, for non-uniform distributions and incomplete support. A spatial first order derivative can be written as

$$\nabla A_i(r) = \int_{\Omega'} \nabla_{r'} A(r') W(r - r') dr' \Rightarrow \nabla A_i \approx \sum_j A_j V_j \nabla W(r_{ij}, h),$$

(6)
but it is also subject to corrections in order to ensure consistency up to the desired precision [11].

3 DISCRETIZATION OF GOVERNING EQUATIONS

3.1 Equations of Motion in SPH

The nature of the classical SPH formulation renders an incompressible system difficult to model [12], and as a result most studies rely on the discretization of the compressible Navier-Stokes system

$$\frac{d\mathbf{v}}{dt} = -\frac{\nabla p}{\rho} + \nabla \tau + \mathbf{g}$$

(7)
$$\frac{d\rho}{dt} = -\rho \nabla \mathbf{v},$$

(8)
where $\mathbf{v}$ is the velocity field, $p$ is the pressure, $\rho$ is the density and $\tau$ and $\mathbf{g}$ are the stress tensor and body forces, respectively. The continuity equation is traditionaly discretized
by employing the notion that $\rho \nabla \mathbf{v} = \nabla (\rho \mathbf{v}) - \mathbf{v} \nabla \rho$, rendering equation (8)

$$\frac{d\rho_i}{dt} = -\rho_i \sum_j m_j (\mathbf{v}_i - \mathbf{v}_j) \nabla W(r_{ij}, h)$$

(9)

This produces a zero divergence field for a $\mathbf{v} = k$ field. A similar approach is taken with the momentum equation (7), with the pressure gradient being written as

$$\frac{\nabla p}{\rho} = \frac{\nabla p}{\rho} + \frac{p_j}{\rho^2} \nabla \rho,$$

(10)

the SPH discretization is given by

$$\frac{\nabla p}{\rho} \approx \sum_j m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \nabla W(r_{ij}, h),$$

(11)

a symmetrical, balanced form of the pressure term that respects the action reaction principle.

The deviatoric stress tensor is not usually computed by the second derivative since it is too sensitive to particle disorder and limits the choice of the kernel functions. However, numerical viscosity mitigates problems due to instabilities arising in the system coming from the unstructured behaviour of the particles. Different viscosity treatments have been developed, and the simplest is the artificial viscosity [11], used in this work, designed to treat shock-tube problems. It is written as

$$\Pi_{ij} = \begin{cases} \frac{-\alpha \bar{c}_{ij} \mu_{ij}}{\rho_{ij}} & \mathbf{v}_{ij} \cdot \mathbf{r}_{ij} < 0 \\ 0 & \mathbf{v}_{ij} \cdot \mathbf{r}_{ij} \geq 0 \end{cases} \quad \text{with} \quad \mu_{ij} = \frac{h v_{ij} r_{ij}}{r_{ij}^2 + 0.01 h^2},$$

(12)

where $c$ is the sound celerity and $\alpha$ is a parameter subject to calibration. Although it has been demonstrated that it models the $\mu \nabla^2 \mathbf{v}$ term [13], it is considered dissipative regarding shear and vorticity. The momentum equation (7) can now be written

$$\frac{d\mathbf{v}_i}{dt} = -\sum_j m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) \nabla W(r_{ij}, h) + \mathbf{g}$$

(13)

where $\Pi_{ij}$ represents the stress term.

Newton’s equations for rigid body dynamics are discretized as

$$M_I \frac{d\mathbf{V}_I}{dt} = \sum_{k \in I} m_k \mathbf{f}_k$$

(14)
\[
I_I \frac{d\Omega_I}{dt} = \sum_{k \in I} m_k (r_k - R_I) \times f_k,
\]

where body possesses a mass \(M_I\), velocity \(V_I\), angular velocity \(\Omega_I\) and center of gravity \(R_I\). \(f_k\) is the force by unit mass applied to particle \(k\), belonging to body \(I\). This force encompasses body forces, fluid resultants as well as the result of any rigid contact that might occur.

### 3.2 Rigid contact considerations for DEM particles

The contact force \(F^T_i\) acting on particle \(i\) resulting from collision with particle \(j\) is decomposed into \(F_n\) and \(F_t\), normal and tangential components respectively. Both of these forces are further decomposed into a repulsion force, \(F^r\), that takes into account the deformation of the particle, and a damping force, \(F^d\), for the dissipation of energy during the deformation.

In the current work, the normal forces are given by a modified, non-linear, Hertzian model \[9\]

\[
F_{n,ij} = F^r_{n} + F^d_{n} = k_{n,ij} \delta_{ij}^{3/4} e_{ij} - \gamma_{n,ij} \delta_{ij}^{1/4} \dot{e}_{ij},
\]

where \(k_{n,ij}\) is the stiffness constant of pair \(ij\), \(\delta_{ij} = \max(0, (d_i + d_j)/2 - |r_{ij}|)\) is the particle overlap, \(e_{ij}\) is the unit vector between the two mass centres and \(\gamma_{n,ij}\) is the damping constant. The stiffness and damping constants are given by \[9\]

\[
k_{n,ij} = \frac{4}{3} E^* \sqrt{R^*}; \quad \gamma_{n,ij} = C_n \sqrt{6 M^* E^* \sqrt{R^*}},
\]

with \(C_n\) of the order of \(10^{-5}\). The other parameters are given by

\[
\frac{1}{E^*} = \frac{1 - \nu_i^2}{E_i} + \frac{1 - \nu_j^2}{E_j}; \quad R^* = \frac{r_i r_j}{r_i + r_j}; \quad M^* = \frac{m_i m_j}{m_i + m_j},
\]

where \(E\) is the Young modulus, \(\nu\) is the Poisson ratio and \(m\) is the mass of the body.

Regarding tangential contacts, the complex mechanism of friction is modelled by a linear dash-pot bounded above by the Coulomb friction law. The Coulomb law is modified with a sigmoidal function in order to make it continuous around the origin regarding the tangential velocity \[14\]. One can write

\[
F_{t,ij} = \min(\mu_{IJ} F_{n,ij} \tanh(8 \delta_{ij}^t) e_{ij}^t; \quad F^r_t + F^d_t),
\]

where

\[
F^r_t + F^d_t = k_{t,ij} \delta_{ij}^t e_{ij}^t - \gamma_{t,ij} \dot{e}_{ij}^t
\]
The friction coefficient at the contact of $I$ and $J$, should be expressed as a function of the two friction coefficients of the distinct materials. The stiffness and damping constants are derived to be $k_{t,ij} = 2/7 k_{n,ij}$ and $\gamma_{t,ij} = 2/7 \gamma_{n,ij}$ [15], as to insure internal consistency of the time scales required for stability. This mechanism models the static and dynamic friction mechanisms by a penalty method. The body does not statically stick at the point of contact, but is constrained by the spring-damper system.

### 3.3 Pressure Field Recovery, Stability Region and Particle Movement

The presented compressible formulation of SPH for the Navier-Stokes employs an equation of state to determine the pressure field, in order not to solve an additional partial differential equation, that relies on the correct tracking of a free surface, such as the Poisson equation [16]. Following [11], the commonly used estimate relationship between pressure and density is Tait’s equation

$$ p_i = \frac{\rho_0 c_0^2}{\gamma} \left[ \left( \frac{\rho_i}{\rho_0} \right)^\gamma - 1 \right] $$

(21)

where $\rho_0$ is a reference density, $c_0$ is a numerical sound celerity and $\gamma = 7$ for a fluid like water. According to equation 21, the compressibility of the fluid depends on $c_0$, in such a way that for a high enough sound celerity the fluid is virtually incompressible. However the value of $c_0$ in the model should not be the actual speed of sound since this value is present in the definition of the stability region of the scheme. The stability region must be modified to accommodate another restriction, the DEM compatible time-step. The CFL condition can be written as

$$ \Delta t = C \min \left[ \min_i \left( \sqrt{\frac{h|f_i|}{f_i}} \right) ; \min_i \left( \frac{h}{c_0 + \max_j \left| \frac{h v_{ij} r_{ij}}{r_{ij}} \right|} \right) ; \min_i \left( \pi/C50 \sqrt{\frac{k_{n,ij}}{m_{ij}}} \right) \right], $$

(22)

where $C$ is the CFL constant of the order of $10^{-1}$ determined in accordance with the case. The first term results from the consideration of force magnitudes, the second is a combination of the CFL condition for numerical information celerities and a restriction arising from the viscous terms [12] and the third term takes into account a theoretical solution for the DEM stability constraints, that disregards the CFL. If the sound celerity in the simulation is too high, it will render $\Delta t$ very small and the computation more expensive. Following [11], $c_0$ is kept to an artificial value of around 10 times the maximum flow speed, restricting the relative density fluctuations at less than 1%. As a consequence, the estimated pressure field by equation (21) usually shows some instabilities and may be subject to scattered distributions. The diffusive terms introduced in [17], designed to smooth the oscillations in the pressure field are used in equation (8). These terms do not allow a hydrostatic solution since a net force is developed near the free surface, but the
test cases in this work represent a very unsteady flow, for which such terms are acceptable. Some complex formulations incur on much more expensive computations [18].

Particle positions are updated every time-step, but instead of integrating \( \frac{dr_i}{dt} = v_i \), the XSPH smoothed velocity variant [11] is used.

\[
\frac{dr_i}{dt} = v_i + \epsilon \sum_j \frac{m_j v_{ji}}{\rho_{ij}} W(r_{ij}, h),
\]

where \( \epsilon \approx 0.5 \), resulting in a locally smoother velocity field, while preserving linear and angular momentum. The particles are moved more orderly and no dissipation but dispersion is introduced.

4 RESULTS

The experimental campaign took place in the Wave Channel of the Hydraulics laboratory (LHIST) of the Civil Engineering Department at Instituto Superior Técnico, Lisbon, Portugal. The flume was sectioned at 8.0 m long and is 0.70 m wide, with glass side walls in order to grant optical access to the flow. The material can be considered very smooth both in the walls and the bed. The installed gate provides an 'instantaneous' removal for the dam-break, with an opening time of 0.21 s, lesser than the required theoretical limit for a dam-break \( t_o(h_0 = 0.40) = \sqrt{\frac{2h_0}{g}} \approx 0.29 \). The objects were 0.15 m side PVC cubes, filled with a material that resulted in a final relative density 0.8. The instrumentation consisted of three synchronized video cameras pointing from the upstream, top and downstream directions, as well as a high-speed camera on the side, normal to the flume wall.

The simulations were ran with a \( CFL = 0.2 \), \( \alpha = 0.05 \), XSPH \( \epsilon = 0.5 \), initial \( dx = 0.01 \) m and a Wendland kernel with \( h = 0.87\sqrt{3dx^2} \). This resolution results in approximately \( 10^6 \) particles, using 1300 mb of the 1450 available in the GPU. The used integration scheme was a predictor corrector Sympletic. For the rigid contact formulation, \( E = 3 \times 10^3 \) kNm\(^{-2}\), \( \nu = 0.23 \) and \( \mu = 0.45 \). These values do not necessarily reflect the material characteristics alone but also take into account numerical considerations to ensure accuracy. These values are typically dependant on the used integrator scheme and are, therefore, subject of fine tuning in order to reproduce correctly the desired behaviours [9].

Visualization is performed using an interpolation using the same kernel as for the simulation in order to generate a free surface as a mass isosurface. The objects are represented as polygons that track the underlying particles used for the computation.

Two tests are presented: Test 1 consists of a column of 3 cubes, aligned with the longitudinal axis of the flume at 90; Test 2 consists of a cube wall made of 6 cubes, with 3 vertical levels. Such configurations provide added complexity to the system, since several contacts are resolved, each with its two modes of interaction. Figures 1 to 3 show a top-view. The results from Test 1 reveal some of the mechanisms of collapse of the structure. The bottom cube is quickly mobilized by the fluid force, from the pressure rise
upstream and it slides between the bed and the upper cubes. A small amount of moment is transferred by friction to the top cubes, and these eventually rotate around the edge of the bottom cube, finally interacting with the fluid and the flume bed. Discrepancies in the fluid motion are noticeable, beyond the artefacts introduced by the surface reconstruction algorithm. These seem to arise from the resolution requirements to effectively model every relevant scale of the experiment. The Reynolds number for the objects is of the order of $4 \times 10^5$, many orders of magnitude higher than the initial $0.010$ m discretization allows to resolve gracefully. This is clearly responsible for most of these discrepancies, such as the dry bed downstream of the objects, angle of the flow separation upon impact and structure of the wave front. It is hypothesized that it is also responsible for most of
the mismatch in the motion of the objects: important scales of the moment transferring mechanisms are not be fully resolved.

Test 2 represents an even greater challenge. 0.05 m intervals are left between the objects and from the observation of the experiments, these seem to contribute greatly to the mode of collapse of the wall. Figures 4 to 6 represent the experimental and simulated instants. Again, the failure of the group of cubes seems to be reproduced fairly, considering

the limitations stated previously and the complexity of the configuration. Most of the object motion is captured to a satisfying degree, with translations and rotations virtually identical prior to extended contact with the fluid. This seems to indicate that the rigid discretization is sound and the chosen parameters are adequate.
5 CONCLUSIONS AND FUTURE WORK

The purpose of the work is to present a generalized DEM model and a straightforward coupling to a standard Smoothed-Particle-Hydrodynamics model. The simple validation presented serves as a benchmark for the model, demonstrating it copes well with the difficulties of modelling complex scenarios even if under-resolved. The model is expected to give more accurate results with the much needed increased resolution, more robust boundary conditions and a more detailed treatment of the viscous terms and sub-particle turbulent stresses, leading to lesser dissipation and a more consistent description of the near bed flow structures and the ones forming at the impact locus. The largest difficulty in increasing resolution is machine memory, since there is a large number of particles in
the flume reservoir upstream that need to be modelled. Works with multi-GPU paralelization are being carried, with very promising results in bypassing such limitations, making possible more definite validations and eventually the production of highly resolved data of real scale flows with incorporated solid material.

Acknowledgements

This research was partially supported by project PTDC/ECM/117660/2010, funded by the Portuguese Foundation for Science and Technology (FCT). First author acknowledges FCT for his PhD grant, SFRH/BD/75478/2010.

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