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This documentation file is intended to provide only additional and updated material, beyond the other SPHERA GitHub repository files and the associated papers on International Journals (Sec.1).

# Description and references

SPHERA v.8.0 (RSE SpA) is free research software (FOSS) based on the SPH (“Smoothed Particle Hydrodynamics”) method, which represents a mesh-less Computational Fluid Dynamics technique for free surface and multi-phase flows.

So far, SPHERA has been applied to represent several types of floods (and landslides) with transport of solid bodies and bed-load transport, and sloshing tanks.

With Copyright 2005-2015 (RSE SpA - formerly ERSE SpA, formerly CESI RICERCA, formerly CESI-Ricerca di Sistema -), SPHERA has been developed for RSE SpA (hereafter RSE, unique owner of the patrimonial rights of SPHERA) by the following authors (SPHERA author list): Andrea Amicarelli, Antonio Di Monaco, Sauro Manenti, Elia Giuseppe Bon, Daria Gatti, Giordano Agate, Stefano Falappi, Barbara Flamini, Roberto Guandalini, David Zuccalà.

The main numerical developments featuring SPHERA (so far) are listed in chronological reverse order:

* 3D SPH numerical scheme for the transport of solid bodies in free surface flows. Reference: Amicarelli et al. (2015, CAF, [6]):

Amicarelli A., R. Albano, D. Mirauda, G. Agate, A. Sole, R. Guandalini; 2015; A Smoothed Particle Hydrodynamics model for 3D solid body transport in free surface flows; Computers & Fluids, 116:205–228, DOI 10.1016/j.compfluid.2015.04.018

* 3D SPH numerical scheme for a boundary treatment based on discrete surface and volume elements, and on a 1D Linearized Partial Riemann Solver coupled with a MUSCL (Monotonic Upstream-Centered Scheme for Conservation Laws) spatial reconstruction scheme. Reference: Amicarelli et al. (2013, IJNME, [5]):

Amicarelli A., G. Agate, R. Guandalini; 2013; A 3D Fully Lagrangian Smoothed Particle Hydrodynamics model with both volume and surface discrete elements; International Journal for Numerical Methods in Engineering, 95, 419–450, DOI: 10.1002/nme.4514.

* SPH numerical scheme for a 2D erosion criterion. Reference: Manenti et al. (2012, JHE, [98]):

Manenti S., S. Sibilla, M. Gallati, G. Agate, R. Guandalini; 2012; SPH Simulation of Sediment Flushing Induced by a Rapid Water Flow; Journal of Hydraulic Engineering ASCE 138(3): 227-311.

* 3D SPH numerical scheme for a boundary treatment based on volume integrals, which are numerically computed outside of the fluid domain (semi-analytic approach). Reference: Di Monaco et al. (2011, EACFM, [39]):

Di Monaco A., Manenti S., Gallati M., Sibilla S., Agate G., Guandalini R., 2011; SPH modeling of solid boundaries through a semi-analytic approach; Engineering Applications of Computational Fluid Mechanics, 5, 1, 1–15.

Other major numerical developments are available in SPHERA (i.e. 3D erosion criterion also with mixture-fixed bed interactions; bed-load transport), but they are preliminary at this stage.

Since its SPHERA v.7.0 branches SPHERA has being developed under a Git repository (GitHub web site). Its current version contains the folders of Table 1.1.

SPHERA is free software released under the GNU General Public License (Free Software Foundation).

The email address to contact the first author of SPHERA is: andrea.amicarelli@rse-web.it .

|  |  |
| --- | --- |
| **Folder** | **Description** |
| (main folder) | License file (GNU-GPL license). Documents on SPHERA registration at SIAE. |
| doc | Present documentation file. |
| src | SPHERA source code (with makefile) |
| bin | SPHERA executable files compiled with gfortran/ifort for run/debug executions |
| input | Input files for validated test cases (Sec.12). A template for the main input file with comments. |

Table 1.1 Folders in SPHERA Git repository.

# Warranties and responsabilities

SPHERA v.8.0 is released “as is” with no warranty. NEITHER RSE SPA, NOR ANY OF ITS REPRESENTATIVES (OR ANY CODE AUTHOR) MAKE ANY WARRANTY, EXPRESS OR IMPLIED, OR ASSUMES ANY LEGAL LIABILITY OR RESPONSIBILITY FOR THE ACCURACY, COMPLETENESS, EFFECTIVENESS, INTEGRITY, AVAILABILITY, OR USEFULNESS OF THE SOFTWARE, ANY INFORMATION PERTAINING TO THE SOFTWARE, OR REPRESENTS THAT ITS USE WOULD NOT INFRINGE PRIVATELY OWNED RIGHTS. No support service (for the code installation, use, teaching activities, …) is implied by or included in the software license. ”

# Citation of SPHERA v.8.0

All the published and unpublished items/products/documents of every kind (i.e. results, publications, software, projects, web pages, press and digital documents, teaching or technological devices, reports, dissemination tools/devices,…) related to SPHERA v.8.0 need the following citation: “SPHERA v.8.0 (RSE SpA)”.

Further proper citations may refer to SPHERA-related papers on International Peer-Reviewed Journals indexed by Scopus and Web of Science (Sec.1).

It is also mandatory to cite the use of SPHERA in all the related publications, reports and dissemination tools and media (also included press and digital products), by means of the following citation:

“SPHERA v.8.0 is realised by RSE SpA thanks to the funding “Fondo di Ricerca per il Sistema Elettrico” within the frame of a Program Agreement between RSE SpA and the Italian Ministry of Economic Development (Ministero dello Sviluppo Economico).”

# SPHERA developers/authors

This section reports few and non-exhaustive notes, which may help potential authors of SPHERA or its derived codes.

If one receives a code with the GNU-GPL license, then she/he has to transmit the license rights unchanged. In particular, it can be useful to remind that GNU-GPL is viral. This also implies that a code, which contains just very few lines of a GNU-GPL code, becomes necessarily a GNU-GPL code in its entirety, when integrating those lines of a GNU-GPL code.

Every modifications of a code derived from a GNU-GPL code must underline every modifications with respect to the original GNU-GPL code.

# SPHERA official users

The information reported in this section only has an educational aim and does not modify the terms and conditions of SPHERA license.

SPHERA v.8.0 is available on GitHub ([151]). Potential developers or users may:

1. contribute to the development of SPHERA as code authors (by means of a free GitHub account; basic knowledge of Git is mandatory);
2. contribute to the validation of SPHERA as “official users” (by means of a free GitHub account; basic knowledge of Git is not mandatory);
3. use SPHERA independently (respecting the code license and citation terms);
4. independently introduce relevant modifications in SPHERA, thus obtaining a FOSS derived code (which has a different name from SPHERA and has to cite SPHERA as the original code) and redistribute it (bound to the GNU-GPL license and in the respect of SPHERA citation terms) or propose it to RSE for its integration in SPHERA;
5. to propose to RSE some program units (not belonging to SPHERA and developed with independent funds), which will be released with GNU-GPL license and integrated in SPHERA;
6. to propose to RSE some program units (of a code developed with independent funds -original code-), which will be released with GNU-LGPL license and integrated in SPHERA, without constraints for the authors to make their original code a FOSS (in its entirety).

The modifications of the source code and the new input files produced with independent funds by non-RSE authors could be proposed to RSE (with a non-RSE Copyright) to be integrated in SPHERA as FOSS program units and input files. In case of acceptance, these contributions will be kept updated by RSE in the following code versions, until RSE will consider them useful for SPHERA development and validation.

SPHERA authors and “official users” need to activate a free account on github.com and “fork” SPHERA, by clicking on the icon “fork” in the official SPHERA public repository ([151; Figure 5.1, Figure 5.2, Figure 5.3, Figure 5.4, Figure 5.5, Figure 5.6).

The basic knowledge of Git is mandatory only for SPHERA authors. In this context, the following links may be useful:

* https://git-scm.com/
* https://www.youtube.com/watch?v=U8GBXvdmHT4&index=3&list=PLg7s6cbtAD15Das5LK9mXt\_g59DLWxKUe

Anyone could be informed on the real-time code upgrades by means of automatic emails sent by GitHub. This free service is available by activating a free account at GitHub (https://github.com/join) and then clicking on the icon “watch” in the official public repository of SPHERA. When activating a GitHub account, it could be convenient to choose a user name, which included name, surname and affiliation. This will permit to get recognized and attend to SPHERA development/validation (the symbol “.” is not permitted within a GitHub user name).

Finally, SPHERA is indexed in the list of SPH codes of SPHERIC (SPH scientific Community; Figure 5.7).

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Figure 5.1. SPHERA on GitHub: master branch. Executable codes.

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Figure 5.2. SPHERA on GitHub: master branch. Documentation.

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Figure 5.3. SPHERA on GitHub. First FOSS release (SPHERA v.8.0).

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|  |

Figure 5.4. SPHERA on GitHub: master branch or trunk.

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Figure 5.5. SPHERA on GitHub: master branch. Input files.

|  |
| --- |
|  |

Figure 5.6. SPHERA on GitHub: master branch. Source code.



Figure 5.7. SPHERA indexed at SPHERIC web site (February 2016, extract from the list of the 13 SPH codes indexed at http://spheric-sph.org/sph-projects-and-codes ).

# The numerical model: transport of solid bodies in free surface flows and Semi-Analytic approach

Aftyer a brief introduction to Smoothed Particle Hydrodynamics (SPH), this section describes the balance equations for fluid (Sec.6.2) and body (Sec.6.3) dynamics and the 2-way interaction terms related to both fluid-body (Sec. 6.4) and solid-solid (Sec.6.5) interactions.

Please refer to SPHERA main references (Sec.1) for further details.

* 1. Smoothed Particle Hydrodynamics (SPH)

Smoothed Particle Hydrodynamics (SPH) represents a mesh-less CFD technique, whose computational nodes are represented by numerical fluid particles.

In the continuum, the functions and derivatives in the fluid dynamics balance equations are approximated by convolution integrals, which are weighted by interpolating (or smoothing functions), called kernel functions.

The integral SPH approximation (<>I) of a generic function (f) is defined as:

|  |  |
| --- | --- |
|  | (6.1) |

where W is the kernel function ([7]), x0 the position of a generic computational point and Vh the integration volume, which is called kernel support. This is represented by a sphere of radius 2h, possibly truncated by the frontiers of the fluid domain.

Any first derivative of a generic function, calculated along i-axis, can be computed as in (6.1), after replacing f with the targeted derivative. After integration by parts, one obtains:

|  |  |
| --- | --- |
|  | (6.2) |

The integration also involves the surface Ah of the kernel support. The associated surface integral is non-zero in case of a truncated kernel support. The representation of this term noticeably differentiates SPH codes (Adami et al., 2012, [1]; Hashemi et al., 2012, [64]; Macia et al., 2012, [97]; Mayrhofer et al., 2013, [105]; Ferrand et al., 2013, [49]; Amicarelli et al., 2013, [5]).

Far from boundaries, the SPH particle approximation of (6.2) reads:

|  |  |
| --- | --- |
|  | (6.3) |

where a summation on particle volumes (replaces the volume integral. The subscripts “0” and “b” refer to the computational particle and its “neighbouring particles” (fluid particles within the kernel support of the computational particle), respectively.

Usually, the approximation (6.3) is replaced by more complicated and accurate formulas. Further, the SPH technique can also approximate a generic n-th derivative, following the same approach of the cited equation.

SPH approximations can discretize the functions and derivatives in the fluid dynamics balance equations by means of a particle Lagrangian mesh-less technique.

SPH technique is characterized by several advantages: a direct estimation of the position of free surface and multi-phase interfaces; an effective representation of body dynamics transported in fluid flows; a direct estimation of Lagrangian derivatives (absence of non-linear terms on the Left-Hand Side of the balance equations); reliable simulations of fast transient phenomena; absence of a computational mesh (mesh-less); simple algorithms (for Weakly Compressible - SPH codes, possible convergence algorithms only refer to specific schemes and are little time consuming).

The main applications of SPH models refer to the following topics: floods (Vacondio et al., 2012, [168]; Amicarelli et al., 2015, [6]; Di Monaco et al., 2011, [39]); sloshing tanks (Souto-Iglesias et al., 2006, [155]; Delorme et al., 2009, [35]; Amicarelli et al., 2013, [5]); wave motion (e.g., Patel et al., 2009, [127]; Antuono et al., 2011, [11]; Liu et al., 2013, [94]; Omidvar et al., 2012a, [122]); hydraulic turbines (Marongiu et al., 2010, [100]); fast landslides (e.g., Kumar et al., 2013, [79]); erosion and bed-load transport (Manenti et al., 2012, [98]); liquid jets (e.g., Koukouvinis et al., 2013, [77]); pollutant dispersion; astrophysics (e.g., Price & Monaghan, 2007, [134]); magneto-fluid dynamics (e.g., Price, 2012, [132]); multi-phase and multi-fluid flows (e.g., Kajtar & Monaghan, 2012, [72]).

* 1. SPH approximation of the balance equations of fluid dynamics with a boundary treatment based on the semi-analytic approach of Di Monaco et al. (2011)

This section relies on [39] and [6], which are suggested for further details.

The numerical scheme for the main flow is a Weakly-Compressible (WC) SPH model, which takes benefit from a boundary treatment based on the semi-analytic approach of Vila (1999, [174]). Its basic features are deeply described in Di Monaco et al. (2011, [39]) and here briefly reported.

Consider Euler’s momentum and continuity equations, in the following forms:

|  |  |
| --- | --- |
|  | (6.4) |

where  is the velocity vector, p pressure,  fluid density, ij Kronecker’s delta, x position and t time. We need to compute (6.4) at each fluid particle position by using the SPH formalism and taking into account the boundary terms (fluid-frontier and fluid-body interactions), as described in the following.

Consider the discretization of (6.4), as provided by the SPH approximation of the first derivative of a generic function (f), according to the semi-analytic approach (“SA”; [174]):

|  |  |
| --- | --- |
|  | (6.5) |

The inner fluid domain here involved is filled with numerical particles. At boundaries, the kernel support is (formally) not truncated because it can partially lie outside the fluid domain. In other words, the summation in (6.5) is performed over all the fluid particles “b” (neighbouring particles with volume ) in the kernel support of the computational fluid particle (“0”). At the same time, the volume integral in (6.5) represents the boundary term, which is a convolution integral on the truncated portion of the kernel support. In this fictitious and outer volume (Vh’), one needs to define the generic function f (pressure, velocity or density alternatively).

The semi-analytic approach (“SA”) (the version of [39]) hypothesizes the following linearization and assumptions to compute f in Vh’:

|  |  |
| --- | --- |
|  | (6.6) |

The peculiar “SA” values of the functions and derivatives in Vh’ are assigned to represent a null normal gradient of reduced pressure at the frontier interface (while considering uniform density):

|  |  |
| --- | --- |
|  | (6.7) |

At the same time, the model sets free-slip conditions when estimating velocity at boundaries. The velocity vector is taken as uniform in the outer part of the kernel support. Here uSA is decomposed in the sum of a vector normal to boundary  and a tangential vector . The first is represented as a linear extrapolation from the computational fluid particle velocity. The latter is equal to its analogous vector of the same computational fluid particle (the subscript “w” refers to a generic frontier):

|  |  |
| --- | --- |
|  | (6.8) |

where n is the normal vector of the wall surface, as defined by its local orientation.

At this point, one can write the continuity equation for a Weakly Compressible SPH model (Einstein’s notation works for “j”), using the semi-analytic approach as a boundary treatment:

|  |  |
| --- | --- |
|  | (6.9) |

where Cs is introduced to represent a fluid-body interaction term.

On the other hand, we can analogously derive the approximation of the momentum equation (the notation indicates the SPH particle -discrete- approximation):

|  |  |
| --- | --- |
|  | (6.10) |

where as represents a new acceleration term due to the fluid-body interactions, M is the artificial viscosity (Monaghan, 2005, [111]), m the particle mass and r the relative distance between the neighbouring and the computational particle.

Finally, a barotropic equation of state (EOS) is linearized as follows:

|  |  |
| --- | --- |
|  | (6.11) |

The artificial sound speed c is 10 times higher than the maximum fluid velocity (WC approach) and “ref” stands for a reference state.

* 1. SPH balance equations for rigid body transport

This section relies on [6], which is suggested for further details.

Body dynamics is ruled by Euler-Newton equations, whose discretization takes advantage from the SPH formalism and the coupling terms derived in the following sections:

|  |  |
| --- | --- |
|  | (6.12) |

Here the subscript “B” refers to a generic computational body and “CM” to its centre of mass.

The first two formulas of (6.12) represent the balance equations for the momentum and the time law for the position of the body barycentre (FTOT is the global/resultant force acting on the solid). The last two formulas of (6.12) express the balance equation of the angular momentum ( denotes the angular velocity of the generic body) and the time evolution of the solid orientation ( is the vector of the angles lying between the body axis and the global reference system). MTOT represents the associated torque acting on the body and the matrix of the moment of inertia of the computational body (Einstein’s notation works for the subscript “l”):

|  |  |
| --- | --- |
|  | (6.13) |

In this sub-section, r implicitly represents the relative distance from the body centre of mass.

In order to solve the system (6.12), we need to model the global force and torque, as described in the following. The resultant force is composed of several terms:

|  |  |
| --- | --- |
|  | (6.14) |

G represents the gravity force, while PF and TF the vector sums of the pressure and shear forces provided by the fluid. Analogously, PS and TS are the vector sums of the normal and the shear forces provided by other bodies or boundaries (solid-solid interactions). As this study focuses on inertial and quasi-inertial fluid flows, we do not implement neither turbulence scheme nor tangential stresses (simplifying hypothesis). Future works are needed to extend the formulation to a wider category of fluid flows.

The fluid-solid interaction is expressed by the following pressure force:

|  |  |
| --- | --- |
|  | (6.15) |

The computational body is numerically represented by solid volume elements, here called (solid) “body particles” (“s”). Some of them describe the body surface and are referred to as “surface body particles”. These particular elements are also characterized by an area and a vector n of norm 1. This is perpendicular to the body face of the particle (it belongs to) and points outward the fluid domain (inward the solid body).

The pressure of a body particle is computed by means of the boundary treatment of Adami et al. (2012, [1]), here implemented and adapted as described in Sec.6.3. Further, the solid-solid interaction term (Ps) is presented in Sec.6.4.

On the other hand, the torque in (6.12) is discretized as the summation of each vector product between the relative position rs, of a surface body particle with respect to the body centre of mass, and the corresponding total particle force:

|  |  |
| --- | --- |
|  | (6.16) |

Time integration of the equations in (6.12) is performed using a Leapfrog scheme synchronized with the fluid dynamics balance equations. This means that the body particle pressure is computed simultaneously to fluid pressure, so that this parameter is staggered of around dt/2 with respect to all the other body particle parameters.

After time integration, the model obtains the velocity of a body particle as the sum of the velocity of the corresponding body barycentre and the relative velocity:

|  |  |
| --- | --- |
|  | (6.17) |

Finally, the model updates the body particle normal vectors and absolute positions, according to the following kinematics formulas (is the increment in the body rotation angle during the on-going time step and Rij the body rotation matrix):

|  |  |
| --- | --- |
| ,, | (6.18) |

* 1. Fluid-body interaction terms

This section relies on [6], which is suggested for further details.

The fluid-body interaction terms rely on the boundary technique introduced by Adami et al. (2012, [1]), here implemented and adapted for free-slip conditions. If boundary is fixed, this method can be interpreted as a discretization of the semi-analytic approach used to treat fluid-boundary interactions (Sec.6.2). The outer domain of (6.5) is here represented by all the body particles inside the kernel support of the computational fluid particle. Further, Adami et al. (2012, [1]) introduce a new term, related to the acceleration of the fluid-solid interface, which influences the estimation of body particle pressure. The implementation and our modifications of this technique is hereafter described.

The fluid-body interaction term in the continuity equation represents a discrete approximation of the analogous term in (6.9), used to treat solid frontiers (free-slip conditions):

|  |  |
| --- | --- |
|  | (6.19) |

Analogously, the fluid-body interaction term in the momentum equation (6.10) assumes the form:

|  |  |
| --- | --- |
|  | (6.20) |

The pressure value of the generic neighbouring surface body particle “s” is derived as follows.

Consider a generic point at a generic fluid-body interface. In case of free-slip conditions, the normal projection of the acceleration on the fluid side (“f”) and on the solid side (“w”) are equal (in-built motion in the direction normal to the interface):

|  |  |
| --- | --- |
|  | (6.21) |

The “wall” acceleration at the position of a generic body particle can then be derived by linearizing (6.21). This depends on the particular computational fluid particle “0” we are considering, so that we can refer to the interaction subscript “s,0”:

|  |  |
| --- | --- |
|  | (6.22) |

One may apply a SPH interpolation over all the pressure values estimated according to (6.22) to derive a unique pressure value for a body particle:

|  |  |
| --- | --- |
|  | (6.23) |

This pressure value is finally used in (6.21). The formulation provided by (6.19), (6.21) and (6.13) differs from Adami et al. (2012, [1]) because of the presence of ns in (6.23), necessary to represent free-slip conditions.

Only a minority of the body particles represents the body surface, but we also need many inner body particles to estimate ps. Thus, the model defines the normal vectors for the neighbouring body particles lying inside the bodies, as described by the following algorithm.

For any fluid-body particle interaction, each fluid particle searches for the most representative surface body particle to define ns in (6.23) -“s0” interaction-. If the on-going body particle “s” belongs to the body surface, then it is immediately considered as representative. Otherwise, the fluid particle “0” isolates its visible neighbouring surface body particles. Visibility is assessed considering the sign of the projection of the inter-particle distance on the body particle normal. The visible neighbour, which is the closest to the joining segment of particles “0” and “s”, is then selected. This particle provides the normal “ns” for the fluid-solid particle interaction “s0” in (6.23).

The assumption (6.21) relies on the fact that all the involved variables are differentiable in time. This means that this equation cannot properly deal with impulses (infinite accelerations). However, the numerical accelerations of our model are always finite and the solid particle accelerations can be easily used in (6.23). Nevertheless, we prefer defining a maximum threshold for |as|, here equal to 10g.

* 1. Modelling the solid-solid interaction terms

This section relies on [6], which is suggested for further details.

The solid-solid interaction term in (6.14) -Ps- represents body-body and body-boundary (full elastic) impingement forces, whose time and spatial evolution, in the continuum, is theoretically proportional to Dirac’s delta. The numerical model needs to discretize Ps, as explained hereafter.

The “boundary force particle” method of Monaghan (2005, [111]) defines repulsive forces to represent a conservative full elastic impingement between two SPH interacting particles (of any medium). In particular, the acceleration  of particle “j”, due to the impingement with particle “k”, is aligned with the inter-particle distance r and inversely proportional to its absolute value r:

|  |  |
| --- | --- |
|  | (6.24) |

The analytic function fbfp is symmetric with respect to the impact point. The dependence of (6.24) on the particle masses allows conserving both global momentum  and kinetic energy (one may notice that  and ). The formulation works for inter-particle high velocity impacts.

This formulation is here implemented and extended to whole solid bodies (not only particle impingements), even at low velocities, as well as body-frontier interactions.

Consider the overall force Ps, which represents the impingements between a generic computational body (“B”) and all its neighbouring bodies (“K”) and frontiers (“K\*”).

Ps is decomposed in elementary 2-body (PBK) and body-frontier (PBK\*) interactions:

|  |  |
| --- | --- |
|  | (6.25) |

Adopting the same principles of the boundary force particle method, PBK involves interactions between all the body particles “j” of the computational body “B” and their neighbour body particles “k”, belonging to the neighbouring body “K”:

|  |  |
| --- | --- |
|  | (6.26) |

The components of the inter-particle relative distance, rpar and rper, are parallel and perpendicular to the neighbour normal, respectively. The term within brackets in (6.26) deforms the kernel support of the body particles “j”, so that it mainly develops along the direction aligned with the normal of the neighbouring particle (dxs is the size of the body particles). The weighting function  is expressed according to Monaghan (2005, [111]) and depends on q= rjk/h:

|  |  |
| --- | --- |
|  | (6.27) |

The present model introduces two modifications for body-body interactions, with respect to the original formulation of the boundary force particles. The first one concerns the impact velocity , which replaces the term “0.1c” in the formulation of Monaghan (2005, [111]) and properly deals with low velocity impacts. It avoids too strong or too weak impingement forces. For each body-body interaction, the impact velocity has a unique value for all the particle-particle interactions during the on-going time step. This velocity is computed as the maximum of the absolute values of the inter-particle relative velocity (projected over the normal of the neighbouring particle). For this purpose, the model considers all the inter-particle interactions recorded while the 2 bodies are approaching. The expression for the impact velocity reads:

|  |  |
| --- | --- |
|  | (6.28) |

where t0 refers to the beginning of the approaching phase. When other forces (e.g. pressure and gravity forces) are taken into account, the impact velocity can eventually increase in the inter-body impact zone, causing a potential and partial penetration of a solid into another body. In this case, and only during the approaching phase, (6.28) allows increasing the magnitude of the impingement force, depending on the actual impact velocity (instead of the undisturbed impact velocity). This modification avoids mass penetrations in case of complex impingements.

Further, (6.26) introduces the coefficient I. This normalizing parameter corrects discretization errors and better preserves the global momentum and kinetic energy of the body-body system during the impingement. If one omitted I, (6.26) would drastically under-estimate the impingement forces if the whole mass of the bodies did not lie within the impact zone (of depth 2h). To avoid this shortcoming, a formulation for I is presented hereafter. Consider the absolute value of the impingement force Ps as a function of the global parameters of the bodies, instead of the particle values. This second formulation for PBK is denoted as follows:

|  |  |
| --- | --- |
| , | (6.29) |

The inter-body velocity impact is now defined as the highest among the particle impact velocities, while the relative inter-body distance is considered as the minimum among the corresponding inter-particle distances. In practise, can be roughly, but more efficiently, estimated as the sum of the absolute values of the two body particles, whose interaction shows the highest relative velocity in the system.

One may now derive a proper definition for I, by equalling PBK to PBK’:

|  |  |
| --- | --- |
|  | (6.30) |

In practise, the model prefers using the following approximated formulation to speed-up the simulations:

|  |  |
| --- | --- |
|  | (6.31) |

This is equivalent to considering the body impact velocity as a weighted average of the particle impact velocities.

At a first approximation, the normalizing factor I roughly represents the inverse of the fraction of the system mass which lies into the impingement zone. This mass should numerically represent the 2-body system during the impact. On the other hand, one cannot use (6.30) to model a body-body impact. In this case, for example, a definition for the direction of Ps’ is required, but the direction of the relative distance between the two bodies does not avoid mass penetration. This would happen, for example, if two cubic bodies, very close to each other and with null barycentre velocities, began to rotate.

Finally, the model represents body-boundary interactions. A generic boundary is modelled as a body with infinite mass and discretization tending to zero (the semi-analytic approach, used to model frontiers, is an integral method). The interaction force assumes the following expression (here the subscript “K\*” refers to a generic neighbouring frontier):

|  |  |
| --- | --- |
|  | (6.32) |

# The numerical model: bed-load transport

This section describes a preliminary model for bed-load transport (Amicarelli & Agate, 2014, [4]; Sec.7.1) and its possible speed-up by means of a 2-interface 3D erosion scheme (Amicarelli & Agate, 2014, [4], Sec.7.2), which extends the main (1-interface) 2D erosion scheme of Manenti et al. (2012, [98], Sec.7.2).

This bed-load transport model is a SPH adaptation of the approximated model of Chauchat & Médale (2010, [30]) and is not consistent with the “packing limit” of the Kinetic Theory of Granular Flow (KTGF). A corrected and upgraded version of this preliminary model will be released with the following versions of SPHERA.

In this code version, the bed-load transport model can only be associated with the boundary treatment of the Semi-Analytic approach (SASPH).

* 1. Preliminary model for bed-load transport

The preliminary model for bed-load transport represents the dynamics of a mixture of pure liquid and (solid) granular material. In particular, mixture viscosity does not need any calibration.

The mixture density is defined as:

|  |  |
| --- | --- |
|  | (7.1) |

where  represents the phase volume fraction and the subscripts “f” and “s” refers the fluid and solid phases, respectively. The volume equation reads:

|  |  |
| --- | --- |
|  | (7.2) |

Molecular diffusion is not represented as the model deals with suspensions (not solutions) and the relative velocity of phases is null by hypothesis.

The Weakly-Compressible approach (“WC”) makes the mixture density to slightly vary. This allows estimating pressure depending on the density displacement from its reference value (barotropic equation of state).

The continuity equation assumes the following form:

|  |  |
| --- | --- |
|  | (7.3) |

Provided the boundary treatment of (Di Monaco et al., 2011, [39]), the SPH approximation of (7.3) reads:

|  |  |
| --- | --- |
|  | (7.4) |

The velocity vector in the virtual region beyond the frontier is defined as in Di Monaco et al. (2011, [39]):

|  |  |
| --- | --- |
|  | (7.5) |

Consider Einstein dilute viscosity:

|  |  |
| --- | --- |
|  | (7.6) |

The norm of the deviatoric (shear) stress tensor of the solid phase (in the bed-load transport layer) follows a generalized Mohr-Coulomb friction model:

|  |  |
| --- | --- |
|  | (7.7) |

where  is the internal friction angle and ’ is the vertical effective stress.

The norm of the mixture shear stresses assumes the following form:

|  |  |
| --- | --- |
|  | (7.8) |

once provided the strain-rate tensor:

|  |  |
| --- | --- |
|  | (7.9) |

Every SPH particle represents a volume of pure fluid (“fluid SPH particles”, s=0) or a mixture of saturated granular material (“mixture SPH particles”).

In case porosity is unknown, the following values are adopted:

|  |  |
| --- | --- |
|  | (7.10) |

where the extreme values for uniform soils are derived from 3D analytic formulas.

Consider the definition of the apparent viscosity for a Bingham fluid ():

|  |  |
| --- | --- |
|  | (7.11) |

where is the critical shear stress, k consistency and n a characteristic exponent of the medium. After combining the above equations, one obtains the following expression for the apparent viscosity of the mixture:

|  |  |
| --- | --- |
|  | (7.12) |

which is regularized by Chauchat & Médale (2010, [30]) as follows:

|  |  |
| --- | --- |
|  | (7.13) |

Bn is Bingham number, a characteristic constant, Hs and Us the scale height and velocity, respectively. Eq. (7.13) can be approximated by assuming . This allows reducing the computational costs and does not introduce any appreciable difference in the test cases investigated in Amicarelli & Agate (2014, SPHERIC, [4]).

The momentum equation for the mixture reads:

|  |  |
| --- | --- |
|  | (7.14) |

The mixture (total) pressure is composed of the fluid pressure and the effective stress, whose formulation is very approximated:

|  |  |
| --- | --- |
|  | (7.15) |

The subscript “blt-top” represents the top of the bed-load transport layer.

The second invariant of the strain-rate tensor (free divergence flows) reads:

|  |  |
| --- | --- |
|  | (7.16) |

Provided the boundary treatment of (Di Monaco et al., 2011, [39]), the SPH approximation of (7.14) reads:

|  |  |
| --- | --- |
|  | (7.17) |

The artificial viscosity is always activated, both for approaching and separating particles (the latter configuration was not considered in Di Monaco et al., 2011, [39]):

|  |  |
| --- | --- |
|  | (7.18) |

Renormalization (Randles & Libertsky, 1996, [137]) applies to the velocity derivatives in (7.16), only for 2D simulations:

|  |  |
| --- | --- |
|  | (7.19) |

A barotropic equation of state (WC approach) for the mixture is linearized around the reference state (“ref”):

|  |  |
| --- | --- |
|  | (7.20) |

The sound speed (cref) should be at least 10 times higher than the maximum velocity in the fluid (WC approach). It is sufficient to define a unique speed of sound for both mixture and pure water, as the maximum value resulting from considering all the numerical particles. The sound speed is computed by providing the bulk modulus as an input parameter for each medium:

|  |  |
| --- | --- |
|  | (7.21) |

The stability conditions for time integration are:

|  |  |
| --- | --- |
|  | (7.22) |

where CFL is the Courant-Friedrichs-Lewy number.

* 1. 2-interface 3D erosion criterion

A 2-interface 3D erosion criterion is implemented to speed-up the computational velocity of the model for bed-load transport (Sec.7.1), if the erosion is the only cause of mobilization of the solid grains. The erosion criterion aims to select those mixture particles, which needs the bed-load transport model to be applied.

The main erosion scheme is the 1-interface (“pure fluid - fixed bed”) 2D erosion criterion of Manenti et al. (2012, [98]), based on the formulation of Shields - van Rijn. Two modifications to this scheme are integrated: the extension to the third dimension and the treatment of a second interface (“bed-load transport layer - fixed bed”).

The erosion criterion refers to the interaction of a generic fixed mixture particle and the fluid flow above (pure fluid or mixture). Its reference parameters are represented by the closest mobile particle (of mixture or pure fluid) above the fixed particle. In any case, the interactions with the pure fluid are privileged, if available.

The formulation of van Rijn (1993, [172]) reads:

|  |  |
| --- | --- |
|  | (7.23) |

where c is Shields parameter and Re\* is the grain Reynolds number:

|  |  |
| --- | --- |
|  | (7.24) |

The assessment of the friction velocity (u\*) follows the procedure below.

If the reference height of the fluid (z) belongs to the Surface Neutral Boundary Layer (SNBL), the model computes the roughness coefficient z0, according to the formula of Manenti et al. (2012, [98]) and those associated to the similarity theory or the SNBL:

|  |  |
| --- | --- |
| , | (7.25) |

where kv is von Karman constant and U is the flow velocity at the reference height.

If z refers to the SNBL, the model considers the velocity profile of the Sub-Viscous Layer, with a direct estimation of the friction velocity:

|  |  |
| --- | --- |
|  | (7.26) |

In this case, U can be smaller than u\*. This usually happens at the lower interface (“bed-load transport layer - fixed bed”).

In synthesis, the model estimates u\* (by means of an iterative procedure if z refers to the SNBL -u\* depends on z0, which is in turn function of u\*-), then Re\* and c. Shield parameter is computed:

|  |  |
| --- | --- |
|  | (7.27) |

and compared with c. The erosion criterion is satisfied if

In practise, Shields criterion is derived under 1D stationary and uniform conditions, and does not explicitly depend on the friction angle. This is explicitly taken into account to quantify the effects of the fixed bed slope, as explained in the following.

The 2D erosion criterion for horizontal beds can be extended to 3D generic slopes, by means of the coefficient k, which is defined as follows:

|  |  |
| --- | --- |
|  | (7.28) |

kis always non-negative and smaller than (or equal to) its 2D value k. In fact, if the slope angle transversal to the main flow direction () is not null, erosion is enhanced. Further, in the presence of a bed with a locally ascendant slope (<0), k can be higher than the unity. In this case, (7.28) can possibly provide a second non-physical solution, with k, which is not taken into account because it corresponds to a flow with an inverted direction.

The normal at the interface “bed-load transport - fixed bed” is defined by a means of a normalized SPH approximation of the relative distance between the mobile sub-domain and the generic SPH particle of the fixed bed:

|  |  |
| --- | --- |
|  | (7.29) |

In the absence of a free surface, the normal is aligned with gravity, by definition.

The main slope angle quantifies the slope of the fixed bed in the direction of the main flow. Assuming that, close to the interface, the mixture velocity is parallel to the fixed bed, only depends on the direction of the velocity vector of the closest particle (3D definition):

|  |  |
| --- | --- |
|  | (7.30) |

In 2D, one could alternatively define  as function of the velocity direction or the interface normal. The latter assumption reduces the model errors and is used in 2D:

|  |  |
| --- | --- |
|  | (7.31) |

The transversal slope angle  is defined as:

|  |  |
| --- | --- |
|  | (7.32) |

The unity vector n2 represents the bi-normal to the fluid particle trajectory and is independent on the sign of .

The value of k is a solution of the quadratic equation of Seminara et al. (2002, [144]):

|  |  |
| --- | --- |
|  | (7.33) |

In the presence of two admissible roots, the model chooses the closest to k, provided ; in the absence of roots, the model assumes k=k

The drag coefficient CD is approximated by the formula of Morrison (2013, [116]) for a fluid flow around a sphere:

|  |  |
| --- | --- |
|  | (7.34) |

with CD varying between 0.1 and 1. Reynolds number is here defined as follows:

|  |  |
| --- | --- |
|  | (7.35) |

with equal to the absolute value of velocity at the closest particle and d50 representing the 50-th percentile of the particle-size distribution of the soil.

In this context, the lift is assumes the form:

|  |  |
| --- | --- |
|  | (7.36) |

where zint is the interface height. A formula for the lift coefficient is derived, by interpolating the experimental data of Seminara et al. (2002, [144]):

|  |  |
| --- | --- |
|  | (7.37) |

with CL varying between 0.07 and 0.5.

The mixture pressure of a generic fixed SPH particle is computed, after assuming hydrostatic conditions within the fixed bed:

|  |  |
| --- | --- |
|  | (7.38) |

Provided the absence of a fixed bed along the vertical and the simultaneous presence of fixed particles (or frontiers) within the kernel support, the mixture SPH particle is held fixed.

# The numerical model: DB-SPH method for boundary treatment

This section describes the “Discrete Boundary” (DB) - SPH method for boundary treatment (Amicarelli et al., 2013, [69]). Consider that the activation of the DB-SPH method also alters the balance equations in the internal domain (Sec.6.2), as described in the following sub-sections.

* 1. DB-SPH particle approximation and modifications of the balance equations

According to the DB-SPH method, the first derivative of a generic function (f) is approximated by means of the following SPH particle approximation:

|  |  |
| --- | --- |
|  | (8.1) |

In (8.1), the volume integral in (6.2) is replaced with a summation over the fluid particles within the kernel support. The surface integral of the same equation is replaced with a summation over the wall surface elements “a” intercepted by the kernel support volume (Vh). (8.1) is normalized by the integral Shepard coefficient () to obtain this further definition:

|  |  |
| --- | --- |
|  | (8.2) |

 varies as function of the involved computational particle “0”. Provided fixed time and position, represents a constant for a particle equation system because it does not depend on the neighbouring particles. Thus, the normalization of the kernel derivative is simply obtained dividing by . This normalization allows considering the truncated kernel support as if it were entire (in the continuum), but with non-spherical shape.

Eq. (8.2) is used to approximate the pressure gradient term of Euler momentum equation (Sec.6.2). In the absence of the semi-particles, defined by Ferrand et al. (2013, [49]) in 2D, the boundary terms of (8.2) seem too modest to avoid the penetration of fluid particles trough the solid frontiers, once (8.2) is applied to the fluid dynamics balance equations. This limit seems due to the characteristics of the kernel function and its derivative (SPH truncation errors). Thus, the present model adopt semi-particles, whose 3D definition is slightly different from the edge particles (semi-particles) of Ferrand et al. (2013, [49]).

The “semi-particles” represent special fluid particles, which are smallest than the (inner) fluid particles. Each semi-particle is associated to a surface wall element. Semi-particle positions are formally located at the solid frontiers of the fluid domain, but the volumes of the semi-particles completely lie in the inner domain and touch the solid boundaries. The union of the semi-particle volumes represents a thin film of fluid, which is a buffer zone between the inner domain (filled with computational particles) and the wall frontiers. The film depth is smaller than the characteristic length of the fluid particles (dx).

Surface elements and semi-particles share the same values of their parameters. Every surface element is defined by its position, velocity, area (length in 2D) and normal vector. Semi-particles additionally require the mass.

Every discrete surface element represents a portion of frontier with area  (3D) or length (in 2D). At the same position, a fluid semi-particle is located. The semi-particle volumes are smaller than the fluid particle volumes not to alter the spatial resolution. The semi-particle position is located on one side of the physical volume of the semi-particle. However, this position should be representative of the entire semi-particle volume. This implies that the maximum distance between any edge of the semi-particle and its position should be smaller than . Provided this constraint, the semi-particle depth coefficient should be high enough to improve the model accuracy.

Normally, SPH models do not consider the free surface as a frontier of the fluid domain as the atmospheric pressure is usually null in the gaseous sub-domain and on the free surface itself. Here, the DB-SPH approximation (8.2) introduces the parameter p0(≠0) in the surface terms of the momentum equation. Formally, one should explicitly model the free surface by means of surface elements over which summing the pressure gradient boundary terms of (8.2). In any case, this complication does not seem necessary if pressure gradients keep small enough at the free surface. This shortcoming is common in SPH mono-phase modelling (using other boundary treatments), and its effects are normally considered negligible (even because pressure gradients are generally zero at the very free surface).

When activating the DB-SPH boundary treatment, density in the inner domain is estimated by means of a SPH particle approximation, which replaces the continuity equation (Ferrand et al., 2013, [49]):

|  |  |
| --- | --- |
|  | (8.3) |

where the kernel is normalized by a corrected estimation of the integral Shepard coefficient.

The following correction of  avoids excessive SPH truncation errors at the free surface:

|  |  |
| --- | --- |
|  | (8.4) |

The integral Shepard coefficient is replaced with the discrete Shepard coefficient at the free surface, which is numerically defined where .  can be set equal to 0.05 or chosen as an input parameter to better detect the free surface, depending on the test case and the spatial resolution.

A direct estimation of  would imply the expensive estimation of 3D analytical integrals. Instead, the present model follows the procedure of Ferrand et al. (2013, [49]), as synthesized by (8.5) and (8.6). Consider the Lagrangian derivative of :

|  |  |
| --- | --- |
|  | (8.5) |

The initial values of  are approximately provided by the associated values of , as the model exactly assigned the initial values of the fluid particle volumes:

|  |  |
| --- | --- |
|  | (8.6) |

The integral Shepard coefficient  is initialized, according to the following procedure.

1. Some fictitious fluid particles are inserted in the computational domain to cover all the truncated parts of the kernel supports in the fluid domain (e.g., the gaseous sub-domain in mono-phase simulations of free surface flows). The density of the fictitious particles is negligible with respect to the computed fluid densities. The fictitious particles are neighbours of the computational particles, close to the free surface. The “fictitious neighbouring particles” define several air volumes, which are provided as input “fictitious fluid volumes”.
2. The model computes the initial values of  by means of the approximated values provided by the estimation of the discrete Shepard coefficient. Thanks to the fictitious particles (having the same characteristic length of the computational particles), the estimation of  (and then of ) is sufficiently accurate, as the kernel supports are never truncated by the free surface.
3. The “fictitious air particles” can be removed at the end of initialization.
   1. 1D Linearized Partial Riemann Solver

At boundaries, the fluid velocity component, which is perpendicular to the wall frontier, is equal to the same component of the frontier velocity (non-penetration condition). The model adopts a 1D LPRS (Linearized Partial Riemann Solver) to impose boundary conditions at the wall elements and semi-particles. The 1D LPRS is an up-wind scheme, also used in SPH-ALE modelling (Marongiu et al., 2010, [100]), which allows wall pressure being approximately compatible with the 3D pressure and velocity fields in the inner domain (constrained to the frontier kinematics).

The definition of the initial conditions (“L”, “Left”) of the 1D LPRS are described by means of a first order spatial reconstruction scheme.

For each interaction (“0a”) between a surface element (“a”) and a fluid particle (“0”), the LPRS initial conditions are defined at the position of the wall element. Here the model estimates density and the velocity components, by means of a first-order spatial reconstruction scheme around he computational particle (f alternatively refers to density and every velocity component):

|  |  |
| --- | --- |
|  | (8.7) |

The velocity vector is projected along the normal of the surface wall element to obtain un.

The solution (\*) of the LPRS (at the wall element position) provides a reconstructed density value, whereas the associated pressure comes from the EOS (mono-phase formulation):

|  |  |
| --- | --- |
|  | (8.8) |

So far, the model has estimated several values of pressure, at each wall element. The following SPH approximation of these values (summation over all the neighbouring fluid particles) provides a unique pressure value for the surface element:

|  |  |
| --- | --- |
|  | (8.9) |

* 1. Semi-particle volume

The volume of a semi-particle is defined in Amicarelli et al. (2013, [5]):

|  |  |
| --- | --- |
|  | (8.10) |

where kd represents the semi-particle shape coefficient and kw the semi-particle depth coefficient.

The exact assessment of the shape coefficient is not an easy task. However, some exact solutions for noticeable cases are evaluated, both in 2D and 3D, based on the hypothesis of uniform angles (in the same configuration) with the number of adjacent faces equal to D (number of the spatial dimensions). From those exact values, Amicarelli & Agate (2015, [3]) derive this interpolating formula:

|  |  |
| --- | --- |
|  | (8.11) |

where naf represents the number of adjacent elements actually detected and the subscript “i” here represents the generic adjacent element. The angles i lie between a generic surface element and each of the adjacent elements. According to the adopted formalism, the model needs to add 180° at the original assessment, in case the angle between the element normal vectors varies between -90° and +90°. The reference formula for i reads:

|  |  |
| --- | --- |
|  | (8.12) |

* 1. DB-SPH inlet and outlet sections

The inlet and outlet sections are represented by special surface elements, which are characterized by the following parameters: position, normal vector, null area (or length), pressure. Inlet and outlet surface elements allow detecting the computational particles, which are selected to impose inlet and outlet boundary conditions. The model search these particles within an influence sphere of characteristic length , where Lc represents the size of the inlet/outlet section. This search is very fast, but approximated: the accuracy of this simplified procedure depends on the test case. Once the interested computational particles are found, Dirichlet boundary conditions are assigned in terms of pressure and/or velocity components.

The inlet section is also interested by the following procedure, which reduces the SPH truncation errors. The free surface in the inlet region is made wavy to optimize the distribution of the fluid particles. The characteristic wave length is dx/2. The displacements are always perpendicular to the inlet normal. Two pattern regularly alternate. A white noise, with amplitude of dx/10, is finally added to the particle positions.

# The numerical model: time integration schemes (Leapfrog, Euler, Heun)

Time integration is ruled by a second-order Leapfrog scheme (refer to [176] for stability analysis and time integration schemes in SPH modelling), as described in Amicarelli et al. (2015, [6]) and Di Monaco et al. (2011, [39]):

|  |  |
| --- | --- |
|  | (9.1) |

Two alternative explicit Runge-Kutta time integration schemes are also implemented: Euler scheme (RK1; first order) and Heun scheme (RK2, second-order).

According to RK1, the generic parameter f is integrated as follows:

|  |  |
| --- | --- |
|  | (9.2) |

The scheme above can be rearranged in the following form:

|  |  |
| --- | --- |
|  | (9.3) |

where the subscripts here represent the time step ID.

RK2 assumes the following form:

|  |  |
| --- | --- |
|  | (9.4) |

This 2-stage formulation implies 2 stages (sub-loops) for each time step. During the first stage, the temporary value fRK1,i+1 is computed. During the second stage, the time step value fRK2,i+1 is assessed. However, several procedures do not need a double loop (e.g., the neighbouring search algorithm, the estimation of the time step duration, the inlet/outlet section management, the result printing, the erosion criterion).

# Developer guide

* 1. SPHERA v.8.0: synthetic description of the program units

The following sub-sections briefly describe all the program units of SPHERA v.8.0, according to their reference folder.

* + 1. Program units for the boundary conditions (“BC”)

The folder “BC” contains all the program units for the boundary conditions of the inlet and outlet sections (Table 10.1).

* + 1. Program units for the continuity equation

The folder “BE\_mass” contains all the program units to compute the Right Hand Side (RHS) of the continuity equation and the procedures of “partial smoothing” for pressure (Table 10.2).

* + 1. Program units for the momentum equation

The folder “BE\_momentum” contains the program units to compute the RHS of the momentum equation and the procedures of “partial smoothing” for velocity (Table 10.3).

* + 1. Program units for the transport of solid bodies in free surface flows

The folder “Body\_Transport” contains the program units exclusively dedicated to the transport of solid bodies in free surface flows (Amicarelli et al., 2015, [6]; Table 10.4).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| CancelOutgoneParticles\_2D | To count and delete the outgoing particles on boundaries of type "leve", "flow", "velo", "crit", "open". |
| CancelOutgoneParticles\_3D | To count and delete the outgoing particles on boundaries of type "leve", "flow", "velo", "crit", "open". Deletion occurs in 2 different ways:  a) If the particle belongs to a particle zone (maxzone) with the highest index (the only zone where both particle number reduction and increase are allowed), then the outgoing particle (npi) is replaced by the last particle (nag) in the particle array pg, and the total number of particle becomes nag=nag-1; simultaneously, the index of the last particle of the zone is changed (Partz(maxzone)%limit(2));  b) Otherwise, simply pg(npi)%cella = 0 (particle out of the domain boundaries). |
| FindFrame | It finds extremes of the rectangular frame which contains the boundary mib. |
| FindLine | Finds extremes of the rectangular frame which contains the boundary mib. |
| GenerateSourceParticles\_2D | To generate new source particles to simulate inlet fluid flow (only in 2D and with one inlet section). |
| GenerateSourceParticles\_3D | To generate new source particles at the inlet section (only in 3D and with one quadrilateral inlet section). |
| IsParticleInternal2D | To check whether a particle is internal to the 2D domain. |
| IsParticleInternal3D | To check whether a particle is internal to the 3D domain or not. It checks if point Px() is internal to the perimeter mib. It returns 'true' (positive check) or 'false'. The perimeter can be both convex or concave. |
| NormFix | Minor program unit. |
| NumberSectionPoints | Minor program unit. |
| PreSourceParticles\_2D | To generate new source particles at the inlet section (only in 2D and with one inlet section). |
| PreSourceParticles\_3D | To generate new source particles at the inlet section (only in 3D and with one quadrilateral inlet section). |
| VelLaw | To impose an input kinematics to particles. |

Table 10.1. Program units for the boundary conditions of the inlet/outlet sections (“BC”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| CalcPre | Particle pressure estimation. |
| inter\_EqCont\_2D | To accumulate contributions for the 2D continuity equation. Computation of velocity gradients and the second invariant of the strain-rate tensor. |
| inter\_EqCont\_2D | To accumulate contributions for the 3D continuity equation. Computation of velocity gradients and the second invariant of the strain-rate tensor. |
| inter\_SmoothPres | To calculate a corrective term for pressure. |
| PressureSmoothing\_2D | Partial smoothing for pressure (Di Monaco et al., 2011), also with DB-SPH boundary treatment scheme. |
| PressureSmoothing\_3D | Partial smoothing for pressure (Di Monaco et al., 2011), also with DB-SPH boundary treatment scheme. |

Table 10.2. Program units for the continuity equation (“BE\_mass”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| Diffumorris | Minor subroutine. |
| inter\_EqMoto | Computation of the momentum equation RHS (with DB-SPH boundary treatment scheme, Shepard's coefficient and gravity are added at a later stage) and the energy equation RHS (this last equation is not validated). |
| inter\_SmoothVelo\_2D | To calculate a corrective term for velocity. |
| inter\_SmoothVelo\_3D | To calculate a corrective term for velocity. |
| viscomon | Monaghan (2005) artificial viscosity term. It is also active for separating particles. Volume viscosity term is neglected in the momentum equation. |
| viscomorris | Morris term in the momentum equation. |

Table 10.3. Program units for the momentum equation (“BE\_momentum”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| Body\_dynamics\_output | .txt output files for body transport in fluid flows. |
| body\_particles\_to\_continuity | Contributions of the body particles to the continuity equation. |
| body\_pressure\_mirror | Computation of the body particle pressure (Amicarelli et al., 2015, CAF) |
| body\_pressure\_postpro | Post-processing for body particle pressure. |
| body\_to\_smoothing\_pres | Contributions of body particles to pressure partial smoothing (Amicarelli et al., 2015, CAF) |
| body\_to\_smoothing\_vel | Contributions of body particles to velocity partial smoothing (Amicarelli et al., 2015, CAF) |
| Gamma\_boun | Interpolative function defined by Monaghan (2005) for boundary force particles (Amicarelli et al.,2015,CAF). |
| Input\_Body\_Dynamics | Input management for body transport in fluid flows. |
| RHS\_body\_dynamics | To estimate the RHS of the body dynamics equations (Amicarelli et al.,2015,CAF). |

Table 10.4. Program units for the transport of solid bodies in free surface flows (“Body\_Transport”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| mixture\_viscosity | To compute the mixture viscosity of the bed-load transport layer. |
| Viscapp | Constitutive equation with tuninig parameters (validated in Manenti et al.,2012,JHE) |

Table 10.5. Program units for the constitutive equation (“Constitutive\_Equation”; SPHERA v.8.0).

* + 1. Program units for the constitutive equation

The folder “Constitutive\_Equation” contains the program units for the constitutive equation (Table 10.5).

* + 1. Program units for the boundary treatment scheme DB-SPH

The folder “DB\_SPH” contains those program units, which are exclusively dedicated to the boundary treatment scheme DB-SPH (Amicarelli et al., 2013, [5]; Table 10.6).

* + 1. Program units for the erosion criterion

The folder “Erosion\_Criterion” contains those program units, which are exclusively dedicated to the 2D erosion criterion of Manenti et al. (2012, [98]) and its further developments (Table 10.7).

* + 1. Program units on geometry (i.e., analytic geometry, algebra, …)

The folder “Geometry” contains the program units dedicated to analytic geometry, algebra and coordinate changes (Table 10.8).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| adjacent\_faces\_isolated\_points | Provided 2 adjacent triangular/quadrilateral faces, it finds at least 2 vertices not in common, at least one per face. They are ID\_face1\_iso and ID\_face2\_iso. In case the faces are not adjacent, then false\_hyp=.true. |
| BC\_wall\_elements | Wall element density and pressure (Amicarelli et al., 2013, IJNME). |
| DBSPH\_find\_close\_faces | Finding the adjacent surface elements of a given surface element, both using 3D -triangular elements- and 2D -quadrilateral raw elements- configurations (DB-SPH). |
| DBSPH\_IC\_surface\_elements | Initialization of wall surface elements (Amicarelli et al., 2013, IJNME). |
| DBSPH\_inlet\_outlet | Impose boundary conditions at the inlet and outlet sections (DB-SPH boundary treatment scheme). |
| DBSPH\_kinematics | Imposing input kinematics for the DB-SPH elements (linear interpolation of input data). |
| Gradients\_to\_MUSCL | 0th-order consistency estimation of velocity and density gradients for the MUSCL reconstruction (to feed the Partial Linearized Riemann Solver; Amicarelli et al., 2013, IJNME). |
| Gradients\_to\_MUSCL\_boundary | Estimation of the boundary terms for the MUSCL reconstruction scheme (DB-SPH), in case they are required in input. |
| Import\_ply\_surface\_meshes | To import the surface meshes (generated by SnappyHexMesh -OpenFOAM-), as converted by Paraview into .ply files. This subroutine is mandatory and activated only for the DB-SPH boundary treatment scheme. |
| semi\_particle\_volumes | To compute the semi-particle shape coefficients and volumes. |
| viscomorris\_wall\_elements | Wall element contributions to Morris' viscosity term. |
| wall\_elements\_pp | Smoothing wall element values for post-processing. Post-processing the wall surface element values (provided a selected region). Post-processing the hydrodynamic normal force on DBSPH surface elements (provided a selected region). Post-processing the wall surface element values (provided selected element IDs). |
| wavy\_inlet | To provide a very slightly wavy flow at the inlet section. Each particle layer is staggered by 0.5dx with respect to the previous and the following ones, which are instead aligned each other. This numerical feature reduces the SPH truncation errors at the DB-SPH inlet sections. A white noise is also added. (Amicarelli et al., 2013, IJNME). |

Table 10.6. Program units for the boundary treatment scheme DB-SPH

(“DB\_SPH”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| compute\_k\_BetaGamma | To compute k\_BetaGamma=teta\_c/teta\_c,00. k\_BetaGamma is the ratio between Shields critical non-dimensional stress for a generic 3D slope (teta\_c) and its analogous value defined by Shields diagram (teta\_c,00) on flat bed. |
| fixed\_bed\_slope\_limited | Forced deposition (or no erosion) for particles at least 2h below the fixed bed (as it is defined in the associated column) during the same time step: i.e. the maximum slope of the fixed bed is 2h/2h. This avoids eventual too fast propagation of erosion along the vertical (erosion is an interface phenomenon). |
| MohrC | Mohr-Coulomb 2D erosion criterion (Manenti et al., 2012, JHE). Shields erosion criterion works better (Manenti et al., 2012, JHE). |
| Shields | 3D erosion criterion based on the formulation of both Shields-van Rijn 2D criterion and Seminara et al.(2002) 3D criterion. 2D Shields erosion criterion based on pure fluid - fixed bed interactions (Manenti et al., 2012, JHE). Extension for bed load transport layer - fixed bed interactions (Amicarelli et al., CAF, submitted). Extension to the third dimension (Amicarelli et al., CAF, submitted). k=3d\_90 (Manenti et al., 2012, JHE; Amicarelli et al., CAF, submitted). Shields threshold for low Re\* (Amicarelli et al., CAF, submitted). |

Table 10.7. Program units for the erosion criterion (“Erosion\_Criterion”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| area\_quadrilateral | Computation of the area of a generic quadrilateral from the coordinates of its vertices. |
| area\_triangle | Computation of the area of a generic triangle, provided the coordinates of its vertices. |
| dis\_point\_plane | Computation of the distance between a point and a plane. |
| distance\_point\_line\_2D | Computation of the distance between a point and a plane. |
| distance\_point\_line\_3D | Computation of the distance between a point and a line in 3D. |
| IsPointInternal | Checking wheather a point with local normal coordinates csi() is internal to a given face, whose code is fk (=1 triangle, =2 parallelogram). |
| line\_plane\_intersection | Computation of the intersection point, if unique, between a line and a plane. |
| LocalNormalCoordinates | Given the local coordinates PX(1 to 2) of a point P laying on the plane of the boundary face nf, the procedure assigns to csi(1 to 3) the normal coordinates of the point Q corresponding to P in the inverse linear tranformation. |
| Matrix\_Inversion\_2x2 | Computation of the inverse (inv) of a provided 2x2 matrix (mat). |
| Matrix\_Inversion\_3x3 | Computation of the inverse (inv) of a provided 3x3 matrix (mat). |
| MatrixProduct | Returning in CC the product between matrices AA and BB. nr: number of rows of AA and CC. nc: number of columns of BB and CC. nrc: number of columns of AA = number of rows of BB. |
| MatrixTransposition | Returns in AAT(n,m) the transposed matrix of AA(m, n). |
| point\_inout\_polygone | Test to evaluate if a point lies inside or strictly outside a polygone (a triangle or a quadrilateral). |
| quadratic\_equation | To solve a quadratic equation. |
| reference\_system\_change | Transformation of coordinates, expressed in a new reference system. |
| three\_plane\_intersection | Computation of the intersection of 3 planes. |
| Vector\_Product | To return in ww the cross product of vectors uu and vv. |
| vector\_rotation | Rotation of a given vector, provided the vector of the rotation angles (3D). |

Table 10.8. Program units on Geometry (“Geometry”; SPHERA v.8.0).

* + 1. Program units for the initial conditions (IC)

The folder “IC” contains the program units on the management on the initial conditions (Table 10.9).

* + 1. Draft program units for the turbulent dispersion of granular material

For sake of completeness with respect to the previous versions of the code, the folder “Interface\_dispersion” contains the draft program unit “inter\_CoefDif”. This computes a corrective term for particle velocity around the interface “mixture - pure fluid”.

* + 1. Program units for the main algorithms

The folder “Main\_algorithm” contains the main program (“main”) and the program units for the main code algorithms (both in 2D and 3D), the memory management and the Leapfrog time integration scheme (Table 10.10).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| GeneratePart | Particle positions (initial conditions). |
| initialization\_fixed\_granular\_particle | To initialize the most of the fixed SPH mixture particles (bed-load transport). |
| SetParticleParameters | Setting initial particle parameters. |
| SetParticles | Particle coordinates (initial conditions). |
| SubCalcPreIdro | Hydrostatic pressure profiles (in case they are imposed as initial conditions). |

Table 10.9. Program units for the initial conditions (“IC”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| Gest\_Dealloc | Deallocations. |
| Gest\_Trans | Introductory procedure for the main algorithm. |
| Loop\_Irre\_2D | 2D main algorithm. |
| Loop\_Irre\_3D | 3D main algorithm. |
| sphera | Main program unit. |

Table 10.10. Program units for the main algorithms (“Main\_algorithm”; SPHERA v.8.0).

* + 1. Modules

The folder “Modules” contains the Fortran modules of SPHERA v.8.0. (Table 10.11).

* + 1. Program units for the neighbouring search, the smoothing operators and the interface detection.

The folder “Neighbouring\_Search” contains the program units for the neighbouring search, the kernel function and derivatives and the detection of the interfaces for the bed-load transport (Table 10.12).

* + 1. Program units for post-processing

The folder “Post\_processing” contains the program units to post-process the code results (Table 10.13). The main output files report the following parameters:

* flow rate hydrographs at the flow rate monitoring sections;
* 2D fields of the maximum values of the specific flow rate and the free surface height;
* time evolution of the interfaces of the bed-load transport model;
* time evolution of the main fluid dynamics variables (pressure and velocity) along the monitoring lines and points;
* hydrographs of the free surface height along the monitoring points;
* application log of SPHERA;
* 2D fields of the main fluid dynamics and SPH variables (“.vtu” and “.pvd” file formats) for Paraview (graphic FOSS) visualization;
* frontier geometry for the boundary treatment SA-SPH (“.vtk” format for Paraview);
* output files of the boundary treatment scheme DB-SPH (ref.: folder “DB\_SPH”);
* output files on the transport of solid bodies in free surface flows (ref.: folder “Body\_dynamics”).
  + 1. Program units for pre-processing

The folder “Pre\_processing” cntains the program units (Table 10.14) to pro-process the input files of SPHERA, which are:

* main input file (“.inp” format is defined in SPHERA v.8.0; user-defined name);
* file list for the DB-SPH surface meshes (“surface\_mesh\_list.inp”);
* ensemble of the files of the DB-SPH surface meshes (“.ply” format), which can be generated by means of SnappyHexMesh (FOSS mesh generator, OpenCFD Ltd) or Paraview.

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| Dynamic\_allocation\_module | Module to define dynamically allocated variables. |
| Hybrid\_allocation\_module | Module to define derived types of both dynamically and statically allocated variables. (Di Monaco et al., 2011, EACFM; Manenti et al., 2012; JHE; Amicarelli et al., 2013, IJNME; Amicarelli et al., 2015, CAF). |
| I\_O\_diagnostic\_module | To provide global interfaces to the subroutine diagnostic. |
| I\_O\_ENG\_module | Minor module |
| I\_O\_file\_module | Module for I/O. |
| I\_O\_ITA\_module | Minor module |
| I\_O\_language\_module | Minor module |
| SA\_SPH\_module | Module for the semi-analytic approach (boundary treatment scheme) of Di Monaco et al. (2011, EACFM). |
| Static\_allocation\_module | Module to define global (and statically allocated) variable. |
| Time\_module | Module for time recording. |

Table 10.11. Fortran modules (“Modules”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| CalcVarLength | Neighbouring search (pre-conditioned dynamic vector), relative positions, kernel functions/derivatives, Shepard's coefficient, position of the fluid-sediment interfaces along each background grid column. |
| CellIndices | To return the indices (i,j,k) of the cell (nc) in a 3D domain with ni\*nj\*nk cells. |
| CellNumber | To return the ID of the cell of indices (i,j,k). |
| CreaGrid | To create the background positioning grid. |
| InterFix | Minor program unit |
| OrdGrid1 | Ordering the numerical elements on the background positioning grid. |
| ParticleCellNumber | To return the ID of the grid cell where particle np is located. If particle is outside of the grid, it returns -1. |
| SearchforParticleZone\_3D | It returns in "partizone" the highest index of wet cells. In case no cell is wet, "partzone = sourzone" ("sourzone"is the inlet section cell). |
| w | kernel function |

Table 10.12. Program units for the neighbouring search, the smoothing operators and the interface detection (“Neighbouring\_Search”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| calc\_pelo | Post-processing to write the free surface height. |
| CalcVarp | To calculate physical quantities at a monitoring point. |
| CreateSectionPoints | Minor program unit |
| GetVarPart | Getting particle values. |
| Memo\_Ctl | Post-processing for monitoring lines and points. |
| Memo\_Results | To write detailed results for restart. Not recommended. |
| Print\_Results | Post-processing for the log file. |
| result\_converter | Post-processing for .vtu (fluid dynamics parameters) and .vtk (geometry) files for Paraview. |
| s\_ctime | Minor program unit |
| start\_and\_stop | Time recording. |
| sub\_Q\_sections | Writing flow rate at monitoring sections provided in input for the flow rate (only in 3D). |
| Update\_Zmax\_at\_grid\_vert\_columns | Updating the 2D array of the maximum values of the fluid particle height, for each grid columns (only in 3D). Printing the 2D field of the water depth (current time step), according to the output frequency chosen in the input file (only in 3D). Printing the 2D fields of the specific flow rate components (current time step), at the same frequency of the water depth (only in 3D). |
| write\_Granular\_flows\_interfaces | Post-processing the interfaces for bed-load transport phenomena. |
| write\_h\_max | To compute and write the 2D array of the maximum values of the water depth, at the nodes of the Cartesian topography, provided as input data (only in 3D). Same task for the 2D field of the maximum (over time) specific flow rates. |

Table 10.13. Program units for post-processing (“Post\_processing”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| defcolpartzero | On the particle colours for visualization purposes. |
| Diagnostic | Diagnostic (error) messages. |
| Gest\_Input | Input check and management. |
| Init\_Arrays | Minor program unit |
| ModifyFaces | To generate triangles from quadrilaterals (partitioning along the shortest diagonal) |
| ReadBedLoadTransport | Reading input data for bed-load transport. |
| ReadBodyDynamics | Reading input data for body trasnport in fluid flows (Amicarelli et al., 2015, CAF). |
| ReadCheck | Minor program unit |
| ReadDBSPH | Reading input data for the DB-SPH boundary treatment scheme (Amicarelli et al., 2013, IJNME). |
| ReadInput | Reading input data. |
| ReadInputBoundaries | Reading input data for the boundary treatment scheme SA-SPH (semi-analytic approach; Di Monaco et al., 2011, EACFM). |
| ReadInputControlLines | Reading monitoring lines. |
| ReadInputControlPoints | Reading monitoring points. |
| ReadInputControlSections | Reading control sections (not valid for the flow rate) |
| ReadInputDomain | Minor program unit |
| ReadInputDrawOptions | Minor program unit |
| ReadInputExternalFile | Minor program unit |
| ReadInputFaces | Minor program unit |
| ReadInputGeneralPhysical | Minor program unit |
| ReadInputLines | Minor program unit |
| ReadInputMedium | Minor program unit |
| ReadInputOutputRegulation | Minor program unit |
| ReadInputParticlesData | Minor program unit |
| ReadInputRestart | Minor program unit |
| ReadInputRunParameters | Minor program unit |
| ReadInputTitle | Minor program unit |
| ReadInputVertices | Minor program unit |
| ReadRiga | Minor program unit |
| ReadSectionFlowRate | Input management for the flow rate monitoring sections. |

Table 10.14. Program units for pre-processing (“Pre\_processing”; SPHERA v.8.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| AddBoundaryContribution\_to\_CE2D | To compute boundary terms for the 2D continuity equation (rodivV). Equation refers to particle npi. It performs implicit computation of gradPsuro. (Di Monaco et al., 2011, EACFM). |
| AddBoundaryContribution\_to\_CE3D | To compute boundary terms for the 3D continuity equation (rodivV). Equation refers to particle npi. It performs implicit computation of gradPsuro. (Di Monaco et al., 2011, EACFM). |
| AddBoundaryContributions\_to\_ME2D | To compute boundary terms for the 2D momentum equation (gradPsuro, ViscoF). Equations refer to particle npi. (Di Monaco et al., 2011, EACFM). |
| AddBoundaryContributions\_to\_ME3D | To compute boundary terms for 3D momentum equation (gradPsuro, ViscoF). Equations refer to particle npi. It performs implicit computation of gradPsuro. (Di Monaco et al., 2011, EACFM). |
| AddElasticBoundaryReaction\_2D | To add supplementariìy normal boundary reaction to support eventual insufficient pressure gradient boundary term. In case of few neighbouring particles and presence of normal component of mass force (gravity). The normal reaction is computed with the formula R=(c0^2/d) ln(zi/d) [for zi<d], stemming from the compressible reaction of the fluid, where:  c0^2 = E/ro0 is the square of the sound speed within the fluid;  zi is the distance of the particle Pi from the boundary face;  d is a reference distance from which the reaction is added.  Check that the elastic boundary reaction never works.  To compute the boundary integral IntWdS  (Di Monaco et al., 2011, EACFM). |
| AddElasticBoundaryReaction\_3D | To add supplementary normal boundary reaction to support eventual insufficient pressure gradient boundary term. In case of few neighbouring particles and presence of normal component of mass force (gravity). The normal reaction is computed with the formula R=(c0^2/d) ln(zi/d) [for zi<d], stemming from the compressible reaction of the fluid, where:  c0^2 = E/ro0 is the square of the sound speed within the fluid;  zi is the distance of the particle Pi from the boundary face;  d is a reference distance from which the reaction is added.  Check that the elastic boundary reaction never works. (Di Monaco et al., 2011, EACFM). |
| BoundaryMassForceMatrix2D | Generation of the generalised boundary mass force matrix RN, on the base of the cosine matrix T and the parameter Fi. (Di Monaco et al., 2011, EACFM) |
| BoundaryMassForceMatrix3D | Generation of the generalised boundary mass force matrix RN, on the base of the cosine matrix T and the parameter Fi. (Di Monaco et al., 2011, EACFM) |
| BoundaryPressureGradientMatrix3D | To generate the pressure gradient matrix RRP, based on the cosine matrix T and the parameter vector Psi. (Di Monaco et al., 2011, EACFM) |
| BoundaryReflectionMatrix2D | Generation of the generalised reflection matrix R, based on the cosine matrix T and the parameters PsiS and PsiN. (Di Monaco et al., 2011, EACFM) |
| BoundaryVolumeIntegrals2D | To compute the boundary volume integrals IntWdV. (Di Monaco et al., 2011, EACFM) |
| CompleteBoundaries3D | (Di Monaco et al., 2011, EACFM) |
| ComputeBoundaryDataTab | To calculate the array to store close boundaries and integrals. (Di Monaco et al., 2011, EACFM) |
| ComputeBoundaryIntegralTab | To compute local coordinates (x,y,z) of a grid of points, regularly distributed on the semisphere z<0 (radius = 2h), whose centre is the origin O of local axis. The semisphere will be superposed to the influence sphere (kernel support) of a generic particle near a plane boundary face, and oriented in such a way that the axis (x,y,z) coincide with the face local axes (r,s,n). In the first three columns of the array BoundaryIntegralTab() the coordinates (x,y,z) of each point are stored; in the forth column the relative d\_alpha (portion of solid angle relative to the point, necessary for integrations) is stored. BITcols = 4. (Di Monaco et al., 2011, EACFM) |
| ComputeBoundaryVolumeIntegrals\_P0 | (Di Monaco et al., 2011, EACFM) |
| ComputeKernelTable | To pre-compute and store in kerneltab(0:ktrows,0:ktcols) the following values:  kerneltab(0:ktrows, 0) = rob = rb/h  kerneltab(0:ktrows, 1) = Int W\* ro2 dro (from rob to 2)  kerneltab(0:ktrows, 2) = Int dW\*/dro ro dro (from rob to 2)  kerneltab(0:ktrows, 3) = Int dW\*/dro ro^2 dro (from rob to 2)  kerneltab(0:ktrows, 4) = Int dW\*/dro ro^3 dro (from rob to 2)  (Di Monaco et al., 2011, EACFM) |
| ComputeSurfaceIntegral\_WdS2D | Computing the surface integral of kernel W along the segments intercepted by the kernel support (radius=2h) of the particle i, whose local coordinates are xpi=LocXY(1,icbs) and ypi=LocXY(2,icbs), on the adjacent boundary side icbs. (Di Monaco et al., 2011, EACFM) |
| ComputeVolumeIntegral\_WdV2D | Computing the integral of WdV extented to the volume delimited by the kernel support (radius=2h) of the particle i, whose local coordinates are xpi=LocXY(1,icbs) and ypi=LocXY(2,icbs), and the adjacent boundary side icbs. (Di Monaco et al., 2011, EACFM) |
| DefineBoundaryFaceGeometry3D | To define boundary faces from 3D geometry. (Di Monaco et al., 2011, EACFM) |
| DefineBoundarySideGeometry2D | Definition of the boundary sides. (Di Monaco et al., 2011, EACFM) |
| DefineBoundarySideRelativeAngles2D | Detection of the previous adjacent side and associated relative angle (for each boundary side). (Di Monaco et al., 2011, EACFM) |
| DefineLocalSystemVersors | To define the directional cosines of the local reference system. (Di Monaco et al., 2011, EACFM) |
| EvaluateBER\_TimeStep | (Di Monaco et al., 2011, EACFM) |
| FindBoundaryConvexEdges3D | To look for possible edges with an associated convex geometry. Their geometrical data are saved in BoundaryConvexEdge as TyBoundaryConvexEdge. (Di Monaco et al., 2011, EACFM) |
| FindBoundaryIntersection2D | To find the intersection segment between the kernel support of particle i, whose local coordinates are xpi=LocXY(1,icbs) and ypi=LocXY(2,icbs), and the straight boundary side iside=Cloboside(icbs), which lies on the local x-axis and extends from x=0 to bsidelen = BoundarySide(iside)%Length. It returns:  xpmin: minimum abscissa of intersected segment  xpmax: maximum abscissa of intersected segment  interlen: length of the intersected segment  (Di Monaco et al., 2011, EACFM) |
| FindCloseBoundaryFaces3D | To finds the "close" boundary faces, i.e. those faces located at a distance from the particle npi smaller than or equal to 2h. It returns:  Ncbf: number of close boundary faces  Clobface(1 to Ncbf): list of close boundary faces  LocX(1:SPACEDIM,Ncbf): local coordinates of particle npi with respect each boundary side  The algorithm looks for the boundary faces intersected by the cell boxes of the reference frame located all around particle npi, and cancels the repeated ones. (Di Monaco et al., 2011, EACFM) |
| FindCloseBoundarySides2D | To finds the "close" boundary sides, i.e. those sited at a distance from particle npi<=2h. It returns:  Ncbs: number of close boundary sides (= 0, 1, 2)  Cloboside(1:Ncbs): list of close boundary sides  LocXY(1:PLANEDIM,1:Ncbs): local coordinates of particle npi with respect each boundary side (vertex V1)  (Di Monaco et al., 2011, EACFM) |
| GridCellBoundaryFacesIntersections3D | To find the boundary faces intercepted by each frame cell of the grid nc[1,NumCells]. In the generic row nc of the vector CFBFPointers(1 to NumCells,1 to 2), it sets:  in the first column: the number of the intercepted faces  in the second column: the pointer to CFBFVector, where the list of intercepted faces begins  Searching is based on a principle of exclusion and is carried out in two phases:  First phase: for every cell, it excludes (as possibly intercepted) the faces, whose vertices all lie in one of the semispaces (defined by the planes containing the cell faces), which do not include the cell itself.  Second phase: for every remaining face, it verifies if all the 8 cell vertices belong to one of the semispaces defined by the plane containing the face. In the positive case, the face is excluded.  (Di Monaco et al., 2011, EACFM) |
| InterpolateBoundaryIntegrals2D | Interpolation in table "BoundIntegralTab(:,:)", defined in module "SA\_SPH\_module", the values in columns "Colmn(nc), nc=1, Ncols" corresponding to the input value "x" to be interpolated, in turn, in column 0.  It returns:  Func(nc), nc=1, Ncols : values interpolated in columns Col(nc), nc=1, Ncols  (Di Monaco et al., 2011, EACFM) |
| InterpolateTable | It interpolates values in the array "Table()" with "nrows" rows and "ncols" columns. Independent variables are in column 0 of Table():  nicols: number of columns of dependent variables to be interpolated  icol(): list of columns of dependent variables to be interpolated  ivalue(): list of the "nicols" interpolated values  (Di Monaco et al., 2011, EACFM) |
| IWro2dro | Computes a SA-SPH definite integral (Di Monaco et al., 2011, EACFM) |
| J2Wro2 | Computes a SA-SPH definite integral (Di Monaco et al., 2011, EACFM) |
| JdWsRn | Computes a SA-SPH definite integral (Di Monaco et al., 2011, EACFM) |
| SelectCloseBoundarySides2D | Selecting among the close boundary sides, those that really give contribution to the equations of particle 'npi'. It returns:  IntNcbs: number of close boundary sides, which give contribution (= 0, 1, 2)  Intboside(1:IntNcbs): list of close boundary sides, which give contribution  IntLocXY(1:PLANEDIM,1:Ncbs): local coordinates of particle np with respect each boundary side, which gives contribution  (Di Monaco et al., 2011, EACFM) |
| WIntegr | Computing a SA-SPH definite integral (Di Monaco et al., 2011, EACFM) |

Table 10.15. Program units for the boundary treatment scheme SA-SPH (“SA\_SPH”, SPHERA v.8.0)

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| time\_integration\_body\_dynamics | Euler time integration for body transport in fluid flows. |
| Euler | Explicit RK1 time integration scheme (Euler scheme). |
| Heun | Heun scheme: explicit RK2 time integration scheme. |
| inidt2 | Initial time step. |
| rundt2 | Time step computation according to stability constraints (inertia terms, visosity term, interface diffusion -not recommended-). Plus. a special treatment for Monaghan artificial viscosity term and management of low-velocity SPH mixture particles for bed-laod transport phenomena. |
| Stoptime | Stopping time. |
| time\_integration | Explicit Runge-Kutta time integration schemes |

Table 10.16. Program units for time integration (“Time\_integration”; SPHERA v.8.0).

* + 1. Program units for the boundary treatment scheme SA-SPH

The folder “SA\_SPH” contains the program units, which are exclusively dedicated to the boundary treatment scheme SA-SPH (Di Monaco et al., 2011, [39]; Table 10.15).

* + 1. ***Program units for managing Fortran character variables***

Three minor program units are implemented to manage Fortran character variables: “GetToken”, “lcase” and “ltrim” (folder “Strings”).

* + 1. Program units for time integration

The folder “Time\_integration” contains those program units, which concern RK1 and RK2 time integration schemes (Table 10.16).

* 1. Style formatting

SPHERA developers follow the basic rules on Fortran 95 coding, adhere as much as possible to SPHERA file format and the following style formatting rules:

1. Please use the subroutine labels at the beginning of each program unit (title and description) and of sub-section (“modules”, “declarations”, “explicit interfaces”, “allocations”, “initializations”, “statements”, “deallocations”).
2. Please use Fortran 95 standard and portable procedures to be compiled with both gfortran and ifort.
3. A generic program unit has to be named as the associated file (without file extension) to have simpler dependencies in the makefile. As a consequence, one file per program unit is allowed and vice versa.
4. Please write since the first column of each line.
5. Please use 3 blank spaces for indentation.
6. Please use 1 blank space only before and after any mathematical operator in the Right Hand Side of each assignment and when a blank space is clearly convenient in terms of readability. Otherwise, blank spaces are used only for indentation (and within comments). For example, “endif” and “enddo” better replace “end if” and “end do”. Further, no blank space is present between a procedure and its arguments (e.g. write(\*,\*)).
7. For readability and printability, do not write beyond column 80. Here the symbol “&” is put for a new line.
8. Please follow this variable order for declarations: parameters, “inout” variables, local variables, external functions. For each of the previous variable set, please following the following sub-order: scalars, 1D arrays, …, nD arrays. Provided the same dimensionality, variable declarations follow this “sub-sub-order”: “logical”, “integer”, “double precision”, “character”, derived types.
9. A comment begins with “! <capitol letter>“ (there is a blank space after “!”).
10. Any logical expression is written within brackets (e.g., “(a==b).and.(c==d)”).
11. Automatic indentation is allowed only with blank spaces instead of tabs (but the makefile).
12. No multiple statements on a line (do not use “;” as a statement separator).
13. Do not go to a new line with “&” under the section “declarations”.
14. Keywords are written in lower case letters (e.g.: do,if,…).
15. Comments are written in UK English.

Please, use Microsoft Equation Editor to update the equations of this file or to add new equations.

# User guide

SPHERA installation is straightforward (Sec.11.1), even because the executable files are already compiled (with ifort and gfortran, also in debug mode).

SPHERA GitHub repository contains a sequence of input files, whose associated test cases are either reported on International Journal papers or represent their analogous simplifications. Please refer to SPHERA main references (Sec.1), the numerical model (Secs.6,7,8,9) and the verbose template for SPHERA main input file (Sec.11.2). This template defines and comments all the input parameters. Finally, SPHERA v.8.0 validations are reported in Sec.11.3.

* 1. Installation

SPHERA source and executable files are distributed on a dedicated Git repository on GitHub ([151]). In case of need, do not hesitate to use SPHERA contact email address (Sec.1).

SPHERA executable files are released for Linux OS (compilers: both ifort and gfortran, with OpenMP libraries).

The only mandatory argument (in the command line) of the chosen executable file is the name of the main input file (without the format extension ”.inp”).

* 1. Commented template of the main input file of SPHERA v.8.0

Figure 11.1 reports the commented template of the main input file of SPHERA v.8.0.

The comments define all the input parameters and describe the meaning of their possible values. Further, suggested or default values are reported.

|  |  |
| --- | --- |
| **Test case** | **Reference for detailed descriptions** |
| 2D\_erosional\_dam\_break\_SPHERA\_demo | (simple test case, rough resolution) |
| 2jets\_plate\_DBSPH\_high\_res | Amicarelli et al. 2013 (IJNME) |
| 2jets\_plate\_DBSPH\_low\_res | Amicarelli et al. 2013 (IJNME) |
| 2jets\_plate\_SASPH\_low\_res | Amicarelli et al. 2013 (IJNME) |
| Archimede | (simple test case, rough resolution) |
| asymmetric\_wedge\_20deg\_light | Amicarelli et al. 2015 (CAF) |
| asymmetric\_wedge\_20deg\_medium | Amicarelli et al. 2015 (CAF) |
| body-body\_impact\_asymmetric | Amicarelli et al. 2015 (CAF) |
| body-body\_impact\_low\_vel | Amicarelli et al. 2015 (CAF) |
| body-body\_impact\_symmetric | Amicarelli et al. 2015 (CAF) |
| body-boundary\_impact | Amicarelli et al. 2015 (CAF) |
| body-boundary\_impact\_low\_vel | Amicarelli et al. 2015 (CAF) |
| dam\_break\_2\_bodies | Amicarelli et al. 2015 (CAF) |
| dam\_break\_2D\_demo | (simple test case, rough resolution) |
| dam\_break\_multi-body | Amicarelli et al. 2015 (CAF) |
| jet\_body-plate | Amicarelli et al. 2015 (CAF) |
| jet\_plate\_DBSPH | Amicarelli et al. 2013 (IJNME) |
| jet\_plate\_DBSPH\_low\_res | Amicarelli et al. 2013 (IJNME) |
| jet\_plate\_SASPH\_low\_res | Amicarelli et al. 2013 (IJNME) |
| symmetric\_wedge\_20deg\_light | Amicarelli et al. 2015 (CAF) |
| symmetric\_wedge\_20deg\_medium | Amicarelli et al. 2015 (CAF) |
| water\_box\_free\_surface | (simple test case, rough resolution) |
| water\_tank-body | (simple test case, rough resolution) |

Table 11.1. Input files in SPHERA GitHub repository.

version.subversion !

! SPHERA main input file: template and comments

!----------------------------------------------------------------------------------------------------------------------------------

! SPHERA (Smoothed Particle Hydrodynamics research software; mesh-less Computational Fluid Dynamics code).

! Copyright 2005-2015 (RSE SpA)

! SPHERA authors and email contact are provided in SPHERA documentation.

! This file is part of SPHERA.

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! GNU General Public License for more details.

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! along with SPHERA. If not, see <http://www.gnu.org/licenses/>.

!----------------------------------------------------------------------------------------------------------------------------------

##### TITLE #####

title ! title (of the test case, string)

##### END TITLE #####

##### DOMAIN #####

! Input parameters for spatial resolution and boundary treatment scheme

D BC\_string ! D(spatial dimensionality)=2(2D),3(3D); BC\_string(Boundary

! treatment scheme)=semi(SA-SPH),dbsph(DB-SPH)

dx h/dx r ! The third parameter ("r") is optional and provides a white noise

! to the IC particle positions

##### END DOMAIN #####

##### VERTICES #####

! Input parameters for the boundary vertices of the fluid domain

! The DB-SPH boundary treatment scheme requires the

! vertices of the parallelepiped domain as a "contour" and the "fictitious

! air reservoirs"

! The SA-SPH boundary treatment scheme requires the vertices of the wall

! frontiers

! In absence of a declared origin, the first vertex is fictitious, equal to the

! and does not belong to any boundary (only useful for Paraview)

1 Vertex\_x Vertex\_y Vertex\_z ! (first vertex data)

! ... ! (other vertices)

Last\_vertex\_ID Vertex\_x Vertex\_y Vertex\_z ! (last vertex data)

##### END VERTICES #####

! If (D==2D): start

##### LINES #####

! 2D input parameters for the boundary lines of the fluid domain

! 2D boundary lines for wall frontiers, inlet/outlet sections, fluid reservoirs.

! In case of DB-SPH boundary treatment scheme, the code requires the lines of

! the parallelepiped domain as a "perimeter" and the "air reservoirs".

! In case of SA-SPH boundary treatment scheme, the code requires the

! lines of the boundaries

1 line\_1\_vertex\_1 ... line\_1\_vertex last line\_1\_Boundary\_ID

! first line data

... ! other records

line\_last\_ID line\_last\_vertex\_1 ... line\_last\_vertex\_last line\_last\_Boundary\_ID

##### END LINES #####

! If (D==2D): end

! If (D==3D): start

##### FACES #####

! 3D input parameters for the boundary faces of the fluid domain

! 3D boundary faces for wall frontiers, inlet/outlet sections, fluid reservoirs.

! In case of DB-SPH boundary treatment scheme, the code requires the faces of

! the parallelepiped domain as a "perimeter" and the "air reservoirs".

! In case of SA-SPH boundary treatment scheme, the code requires the

! the boundary faces

! Vertex list clockwise (normal vector exiting the frontier/domain;

! view from the semi-space of the normal vector): not the best convention

! The last vertex ID is 0 in case of triangular faces

! SA-SPH boundary normal vectors and reservoir face normal vectors point inward

! (clockwise list of points if looking from outside the fluid domain). For

! "perimeter" boundaries: the vertices have to be adjacent, but there is no rule

! about the vertex order (better anticlockwise).

1 face\_1\_vertex\_1 ... face\_1\_vertex last face\_1\_Boundary\_ID

! first face data

... ! other records

face\_last\_ID face\_last\_vertex\_1 ... face\_last\_vertex\_last face\_last\_Boundary\_ID

##### END FACES #####

! If (D==3D): end

##### BOUNDARIES #####

! Input parameters for the fluid domain boundaries delimited by

! lines(2D)/faces(3D)

! In case of DB-SPH boundary treatment scheme, the parallelepiped domain

! (mandatory) is formally represented by a fictitious SA-SPH frontier, which

! is only used to generate the background positioning grid.

! 1st boundary

Boundary\_name !

Boundary\_ID !

Boundary\_type ! Boundary\_type = fixed(wall frontier),perimeter

! (fluid reservoir),source(inlet section),open,

! tapis (not recommended)

! If (Boundary\_type=="fixed"): start

Shear\_stress\_coefficient ! Shear\_stress\_coefficient=1.0(no-slip),

! 0.(free-slip)

RGBColor !

! If (Boundary\_type=="fixed"): end

! If (Boundary\_type=="perimeter"): start

fluid\_ID !

colour\_pattern colour\_ID ! colour\_pattern=uniform,bends; colour\_ID=009EA8

! if (motion\_type=std): start

motion\_type IC\_velocity\_x IC\_velocity\_y IC\_velocity\_z slip\_condition

! motion\_type=std; slip\_condition=0.0

! if (motion\_type=std): end

! if (motion\_type=law): start

motion\_type n\_records ! motion\_type=law; n\_records(number of records for

! the imposed kinematics)

time\_1 u\_1 v\_1 w\_1 1

...

time\_n\_records u\_n\_records v\_n\_records w\_n\_records n\_records

! (list of records for the imposed

! 3D translational kinematics: time, vector

! velocity, record\_ID)

! if (motion\_type=law): end

IC\_pressure\_type IC\_pressure\_value

! IC\_pressure\_type=pa(uniform pressure),qp

! (hydrostatic conditions),pl(hydrostatic pressure

! based on the maximum level of an assigned fluid;

! IC\_pressure\_value=(uniform pressure value for pa),

! (free surface height for qp), (equivalent free

! surface level of the on-going fluid for pl)

IC\_reservoir\_type Car\_top\_zone

! IC\_reservoir\_type=1(vertices and faces),2(from

! Cartesian topography); Car\_top\_zone = boundary ID

! of underlying topography(influence only if

! IC\_reservoir\_type==2)

! If (IC\_reservoir\_type==2): start

dx\_CartTopog H\_res ! dx\_CartTopog(spatial resolution of the Cartesian

! topography); H\_res(height of the reservoir free

! surface)

ID\_first\_vertex ID\_last\_vertex

! ID\_first\_vertex,ID\_last\_vertex(ID of the first and

! and the last vertices of the reference topography)

n\_circum nag\_aux ! n\_circum(number of vertices circumscribing

! the horizontal projection of the reservoir)=3,4;

! nag\_aux(rough overestimation of the number of

! fluid particles in the reservoir)

circum\_1\_x circum\_1\_y ! First point of the 2D figure circumscribing the

! horizontal projection of the reservoir

... ! other point/s of the 2D figure above

circum\_last\_x circum\_last\_y ! last point of the 2D figure above

dam\_zone\_ID n\_circum\_dam

! dam\_zone\_ID; dam\_zone\_n\_vertices(number of

! vertices of the 2D figure circumscribing the

! horizontal projection of the

! dam zone)=3,4

circum\_dam\_1\_x circum\_dam\_1\_y

! First point of the 2D figure circumscribing the

! horizontal projection of the dam zone

... ! other point/s of the 2D figure above

circum\_dam\_last\_x circum\_dam\_last\_y

! last point of the 2D figure above

! If (IC\_reservoir\_type==2): end

! If (Boundary\_type=="perimeter"): end

! If (Boundary\_type=="open"): start

RGBColor

! If (Boundary\_type=="open"): end

! If (Boundary\_type=="source"): start

flowrate 0. ! flowrate(inlet velocity \* inlet area); 0.

pa IC\_pressure !

RGBColor

! If (Boundary\_type=="source"): end

! ... ! other boundaries

! n-th boundary

! ... ! Data of the last boundary

##### END BOUNDARIES #####

##### DBSPH #####

! Input parameters for the DB-SPH boundary treatment scheme

dx\_f/dx\_w MUSCL\_boundary\_flag k\_w ! dx\_f/dx\_w(ratio between the fluid particle

! size and the wall element size);

! MUSCL\_boundary\_flag(logical flag to

! activate boundary terms for MUSCL); k\_w

! (semi-particle depth coefficient)

n\_monitor\_points n\_monitor\_regions ! n\_monitor\_points; n\_monitor\_regions=0,1(to

! estimate the Force along x-direction)

! if (n\_monitor\_points>0): start

ID\_wall\_element\_monitor\_1 ... ID\_wall\_element\_monitor\_n

! if (n\_monitor\_points>0): end

! if (n\_monitor\_regions>0): start

xmin,xmax,ymin,xmax,zmin,zmax ! (monitoring region vertices)

! if (n\_monitor\_regions>0): end

imposed\_kinematics\_records flag\_in-built\_monitors

! imposed\_kinematics\_records(number of

! records, which describe a possible imposed

! kinematics;

! flag\_in-built\_monitors(logical): flag for

! in-built motion of control lines and

! DB-SPH frontiers

! if (imposed\_kinematics\_records==1): start

time\_1 velocity\_x\_1 velocity\_x\_2 velocity\_x\_3

! ... ! other possible records

time\_last velocity\_x\_last velocity\_x\_last velocity\_x\_last

! (records for the imposed translational

! kinematics to frontiers)

! if (imposed\_kinematics\_records==1): end

n\_inlet n\_outlet ! n\_inlet(number of inlet sections)

! n\_outlet(number of outlet sections)

! if (n\_inlet>1): start

x\_inlet\_1 y\_inlet\_1 z\_inlet\_1 n\_x\_inlet\_1 n\_y\_inlet\_1 n\_z\_inlet\_1 velocity\_x\_inlet\_1 velocity\_y\_inlet\_1 velocity\_z\_inlet\_1 L\_inlet\_1

... ! (other possible records)

x\_inlet\_last y\_inlet\_last z\_inlet\_last n\_x\_inlet\_last n\_y\_inlet\_last n\_z\_inlet\_last velocity\_x\_inlet\_last velocity\_y\_inlet\_last velocity\_z\_inlet\_last L\_inlet\_last

! inlet section data: position, normal,

! velocity, length.

! if (n\_inlet>1): end

! if (n\_outlet>1): start

x\_outlet\_1 y\_outlet\_1 z\_outlet\_1 n\_x\_outlet\_1 n\_y\_outlet\_1 n\_z\_outlet\_1 velocity\_x\_outlet\_1 velocity\_y\_outlet\_1 velocity\_z\_outlet\_1 L\_outlet\_1

... ! (other possible records)

x\_outlet\_last y\_outlet\_last z\_outlet\_last n\_x\_outlet\_last n\_y\_outlet\_last n\_z\_outlet\_last L\_outlet\_last p\_outlet\_last

! outlet section data: position, normal,

! length, pressure

! if (n\_outlet>1): end

##### END DBSPH #####

##### BED LOAD TRANSPORT #####

! Input parameters for bed-load transport (blt) scheme

erosion\_criterion\_ID ID\_main\_fluid ID granular

! erosion\_criterion\_ID=0(no bed-load

! transport),1(Shields-Seminara),2(Shields

! without blt-fixed bed interactions),3

! (Mohr-Coulomb, not recommended);

! ID\_main\_fluid(medium of

! the main fluid); ID granular

! (medium of the blt layer)

! if (erosion\_criterion\_ID>0): start

velocity\_fixed\_bed erosion\_flag ! velocity\_fixed\_bed(velocity threshold

! -e.g. equal to velocity scale/100- to

! detect the fixed bed); erosion\_flag=0

! (activated far from fronts); 1(inactive),

! 2(active everywhere)

viscosity\_blt\_formula deposition\_at\_frontiers Gamma\_slope\_flag

! viscosity\_blt\_formula(in the bed-load

! transport layer)=1(Chauchat-Médale 2010

! CMAME),2(Chezy-like),3(diluted viscosity),

! 4(lambda(Bn));deposition\_at\_frontiers=1

! (imposed),0(not imposed); Gamma\_slope\_flag

! =1(Gamma slope angle computed),0(null)

n\_monitor\_lines dt\_out erosion\_convergence\_criterion n\_max\_iterations

! n\_monitor\_lines(number of monitoring lines

! aligned with x- or y-axis); dt\_out(writing

! time step); erosion\_convergence\_criterion

! (convergence criterion for the erosion

! criterion); n\_max\_iterations(maximum

! number of iterations for the erosion

! criterion)

Chezy\_friction\_coefficient ! Chezy\_friction\_coefficient(default=0.005)

x\_min\_dt x\_max\_dt

y\_min\_dt y\_max\_dt

z\_min\_dt z\_max\_dt ! Vertices of the parallelepiped, within

! which the mixture particles can influence

! the time step estimation

line\_ID ! monitoring line ID for blt

x\_line y\_line ! monitoring line is defined by variable or

! fixed (-999.) x- and y-coordinates

! if (erosion\_criterion\_ID>0): end

##### end BED LOAD TRANSPORT #####

##### medium #####

! Input parameters for the fluids

fluid\_type ! fluid\_type=liquid,granular

fluid\_ID !

! If (fluid\_type==liquid): start

density bulk\_modulus

! If (fluid\_type==liquid): end

! If (fluid\_type==granular): start

solid\_phase\_density solid\_phase\_bulk\_modulus

!

! If (fluid\_type==granular): end

Monaghan\_alpha Monaghan\_beta ! Monaghan alpha (artificial viscosity),

! Monaghan beta (=0, artificial viscosity)

diffusion\_coefficient settling velocity coefficient

! null recommended values (i.e. inactive

! parameters)

0. 0. 0.

! If (fluid\_type==liquid): start

dynamic\_viscosity !

roughness\_coefficient ! null recommended values (i.e. inactive

! parameter)

! If (fluid\_type==liquid): end

! if ((fluid\_type==granular).and.(erosion\_criterion\_ID==1)): start

delta ! delta(internal friction angle in degrees,

! even if the code works in radians)

effective\_porosity d\_50 d\_90 !

! if ((fluid\_type==granular).and.(erosion\_criterion\_ID==1)): end

! if ((fluid\_type==granular).and.(erosion\_criterion\_ID>1)): start

! Alternative to the reference blt scheme

cohesion viscosity\_max tuned\_viscosity

! cohesion; viscosity\_max,tuned\_viscosity (

! tuning parameters for viscosity)

delta ! delta(internal friction angle in degrees,

! even if the code works in radians)

roughness\_coefficient d\_50 erosion\_model

! roughness\_coefficient; d\_50; erosion\_model

! =shields,mohr

max\_step\_still ! max\_step\_still(number of time steps during

! which mixture particles are kept still)

! if ((fluid\_type==granular).and.(erosion\_criterion\_ID>1)): end

##### end medium #####

##### BODY DYNAMICS #####

! Input parameters for the scheme on body transport in fluid flows

n\_bodies dx/dx\_body imping\_body\_grav

! n\_bodies(number of transported solid

! bodies); dx/dx\_body(ratio between fluid

! particle size and body particle size);

! imping\_body\_grav=0(gravity always

! active, recommended value),1(gravity

! inactive until the first impact

! body-fluid)

! if (n\_bodies>0): start

ID\_first\_body n\_elem ! ID\_first\_body=1; n\_elem(number of

! elements of the body)

body\_mass !

pos\_CM\_x pos\_CM\_y pos\_CM\_z ! pos\_CM(position of the centre of mass at

! t=0)

Ic\_flag ! Ic\_flag=0,1(mass moment of inertia is

! imposed)

! if(Ic\_flag==1): start

Ic(1,1) Ic(1,2) Ic(1,3) !

Ic(2,1) Ic(2,2) Ic(2,3) !

Ic(3,1) Ic(3,2) Ic(3,3) !

! if(Ic\_flag==1): end

alfa\_x alfa\_y alfa\_z ! alfa(rotation angles of the body axis with

! respect to the reference system axis at

! t=0)

pos\_rotC\_x pos\_rotC\_y pos\_rotC\_z ! pos\_rotC(centre of rotation just to

! configure the initial orientation in the

! global reference system)

vel\_CM\_x vel\_CM\_y vel\_CM\_z ! vel\_CM(velocity of the centre of mass at

! t=0)

omega\_x omega\_y omega\_z ! omega(angular velocity of the body at t=0)

imposed\_kinematics\_flag n\_records ! imposed\_kinematics\_flag=0,1(kinematics is

! imposed); n\_records(number of records,

! which desrcibe the imposed kinematics)

first\_ID\_element ! first\_ID\_element=1(of body 1)

L\_x L\_y L\_z ! L\_x,L\_y,L\_z(side lengths of the element)

pos\_CM\_elem\_x pos\_CM\_elem\_y pos\_CM\_elem\_z

! pos\_CM\_elem(position of the centre of mass

! of the element at t=0)

alfa\_elem\_x alfa\_elem\_y alfa\_elem\_z ! alfa\_elem(rotation angles of the body axis

! with respect to the reference system axis

! at t=0)

face\_xmin\_flag face\_xmax\_flag face\_ymin\_flag face\_ymax\_flag face\_zmin\_flag face\_zmax\_flag

! (integer flags to activate the normal

! vectors of surface body particles only

! if face\_...\_flag=1; x/y/z\_min/max

! indicates the 6 faces of the element

! -parallelepiped-)

xmin xmax ymin ymax zmin zmax ! (spatial limits -in the global reference

! system before the initial rotation- to

! deactivate particle masses if((x>=xmin).

! or.(x<=xmax).or.(y>=ymin).or.(y<=ymax).or.

! (z>=zmin).or(z<=zmax)) foor boolean

! operations on elements/body)

... ! (other element records)

... ! (last element record)

!

... ! (other body records)

!

... ! (last body record)

! if (n\_bodies>0): end

##### end BODY DYNAMICS #####

##### RUN PARAMETERS #####

! Input parameters for time integration, partial smoothing and memory management

final\_time final\_time\_step ! (the run stops when reaching either the

! final time or the final time step)

CFL Leapfrog\_flag scheme\_order factor dt\_alfa\_Mon

! CFL, Leapfrog\_flag=1(Leapfrog time

! integration scheme),0(explicit RK time

! integration schemes); scheme\_order(time

! integration scheme order, but for Leapfrog

! is "1"); factor(=0., weighting factor to

! estimate dt); dt\_alfa\_Mon(logical flag

! making Monaghan artificial viscosity

! coefficient to influence dt)

teta\_p, teta\_u var ! teta\_p,teta\_u(coefficients for partial

! smoothing of pressure and velocity); var=A

COEFNMAXPARTI COEFNMAXPARTJ body\_part\_reorder

! COEFNMAXPARTI:max0(max number of fluid

! particles)=COEFNMAXPARTI\*nag;

! COEFNMAXPARTJ:maxb(max number of

! neighbours)=COEFNMAXPARTJ\*(4h/dx)^D;

! body\_part\_reorder(DB-SPH)=0(fixed

! frontiers),1(mobile frontiers)

MAXCLOSEBOUNDFACES MAXNUMCONVEXEDGES

! MAXCLOSEBOUNDFACES(max number of

! neighbouring boundary face per fluid

! particle); MAXNUMCONVEXEDGES(max number

! of edges)

GCBFVecDim ! GCBFVecDim(rough overestimation of the

! number of Grid Cell - Boundary Face

! intersections (SA-SPH)

density\_thresholds\_flag ! density\_thresholds\_flag=0(default, no

! density limiters),1(density limiters for

! debug)

##### end RUN PARAMETERS #####

##### general physical properties #####

! Input parameters for gravity and reference pressure

! 3D case: start

gravity\_acceleration\_x gravity\_acceleration\_y gravity\_acceleration\_z

! 3D case: stop

! 2D case: start

gravity\_acceleration\_x gravity\_acceleration\_z

! 2D case: stop

reference\_pressure !

##### end general physical properties #####

!##### restart #####

! (this section is not active)

!##### end restart #####

##### output regulation #####

! Post-processing parameters for .txt files. The first two words (and the

! possible fourth) of each line are keywords.

results time dt\_out ! dt\_out(writing time step)

restart time dt\_restart ! dt\_restart(=99999., restart time step)

print partial log\_file\_frequency ! log\_file\_frequency (log file writing time

! step in terms of time step number)

control time dt\_out\_mon ! dt\_out\_mon(writing time step for

! monitoring elements)

level time dt\_out\_FS medium fluid\_ID

! dt\_out\_FS(writing time step for free

! surface post-processing); fluid\_ID

! if (IC\_source\_type==2): start

depth dt\_out dt\_out\_depth ! dt\_out\_depth(writing time step for 2D

! fields of water depth (h) and specific

! flow rate components (q\_x=u\_m\*h,q\_y=v\_m\*h))

! if (IC\_source\_type==2): end

##### end output regulation #####

##### draw options #####

! Post-processing parameters for Paraview file formats. The first two words

! of each line are keywords.

vtkconverter any dt\_out\_PV ! dt\_out\_PV(writing time step for Paraview

! .vtu files)

##### end draw options #####

##### control points #####

! Input parameters for monitoring points

x\_monitor\_point\_1 y\_monitor\_point\_1 z\_monitor\_point\_1

... ! (other monitoring points)

x\_monitor\_point\_n y\_monitor\_point\_n z\_monitor\_point\_n

##### end control points #####

##### control lines #####

! Input parameters for monitoring lines

line\_1\_label

! if(D==2D): start

edge\_1\_line\_1\_x edge\_1\_line\_1\_z

edge\_2\_line\_1\_x edge\_2\_line\_1\_z

! if(D==2D): end

! if(D==3D): start

edge\_1\_line\_1\_x edge\_1\_line\_1\_y edge\_1\_line\_1\_z

edge\_2\_line\_1\_x edge\_1\_line\_1\_y edge\_2\_line\_1\_z

! if(D==3D): end

line\_1\_number\_of\_discretization\_points

... ! (other possible monitoring line records)

##### end control lines #####

##### control sections #####

! (this section is not active)

##### end control sections #####

##### section flow rate #####

! Input parameters on monitoring sections for the flow rate

n\_sect dt\_out n\_fluid\_types ! n\_sect(number of the flow rate monitoring

! sections; dt\_out(writing time step for

! flow rates); n\_fluid\_types(number of fluid

! types (the first ID fluid types are

! selected)

first\_section\_ID ! first\_section\_ID=1

n\_vertices ! n\_vertices(number of vertices describing a

! monitoring section for the flow rate (3 or

! 4) of the first section

vertex\_1\_x vertex\_1\_y vertex\_1\_z

vertex\_2\_x vertex\_2\_y vertex\_2\_z

vertex\_3\_x vertex\_3\_y vertex\_3\_z

vertex\_4\_x vertex\_4\_y vertex\_4\_z

! vertices of the first section (in case of

! 3 vertices do not mind about the fourth

! point)

... ! other possible section records

##### end section flow rate #####

Figure 11.1. Commented template of the main input file of SPHERA v.8.0.

* 1. Validation of SPHERA v.8.0

SPHERA v.8.0 is validated on 44 test cases (Figure 11.2). Some of them are published on International Journals and were also carried out with previous versions of the code. Other minor test cases only represent very simple configurations. The remaining 13 test cases are still matter of study for on-going numerical developments and validations, although preliminary validations are published.

|  |  |  |  |
| --- | --- | --- | --- |
| **Test case**  **Brief description or reference (indexed International Journal)** | **Example image** | **Test case**  **Brief description or reference (indexed**  **International Journal)** | **Example image** |
| “2D\_erosional\_dam\_break\_SPHERA\_demo”  Simple and demonstrative 2D erosional dam break  (rough resolution)  SPHERA v.8.0 |  | “2jets\_plate\_DBSPH\_high\_res”  Amicarelli et al. (2013, IJNME)+  “2jets\_plate\_DBSPH\_low\_res”  Amicarelli et al. (2013, IJNME)+  “2jets\_plate\_SASPH\_low\_res”  Amicarelli et al. (2013, IJNME) |  |
| “Archimede”  Simple and demonstrative test case: solid cube leaned on still water (rough resolution)  SPHERA v.8.0 |  | “asymmetric\_wedge\_20deg\_light”  Amicarelli et al. (2015, CAF) |  |
| “asymmetric\_wedge\_20deg\_medium”  Amicarelli et al. (2015, CAF) |  | “Benchmark1\_SASPH”  Amicarelli et al. (2013, IJNME)+  “SPHERIC\_B1\_dam\_break\_DB-SPH”  Amicarelli et al. (2013, IJNME) |  |
| “Benchmark2\_SASPH”  Di Monaco et al. (2011, EACFM) +  “SPHERIC\_B2\_dam\_break\_DB-SPH”  Amicarelli et al. (2013, IJNME) |  | “body-body\_impact\_asymmetric”  Amicarelli et al. (2015, CAF)+  “body-body\_impact\_low\_vel”  Amicarelli et al. (2015, CAF)+  “body-body\_impact\_symmetric”  Amicarelli et al. (2015, CAF) |  |
| “body-boundary\_impact”  Amicarelli et al. (2015, CAF)+  “body-boundary\_impact\_low\_vel”  Amicarelli et al. (2015, CAF) |  | “dam\_break\_2\_bodies”  Amicarelli et al. (2015, CAF) |  |
| “dam\_break\_2D\_demo”  Simple and demonstrative test case on a 2D dam break  (rough resolution)  SPHERA v.8.0 |  | “dam\_break\_body\_UniBas”  Amicarelli et al. (2015, CAF) |  |
| “dam\_break\_multi-body”  Amicarelli et al. (2015, CAF) |  | “erosional\_dam\_break\_2D\_FraCap02Taipei”  Amicarelli & Agate (2014, SPHERIC) |  |
| “erosional\_dam\_break\_bed\_2D\_FraCap02”  Amicarelli & Agate (2014, SPHERIC) |  | “erosional\_dam\_break\_bed\_2D\_Spi05”  Amicarelli & Agate (2014, SPHERIC) |  |

|  |  |  |  |
| --- | --- | --- | --- |
| **Test case**  **Brief description or reference (indexed International Journal)** | **Example image** | **Test case**  **Brief description or reference (indexed**  **International Journal)** | **Example image** |
| “erosional\_dam\_break\_Pon10”  Amicarelli & Agate (2014, SPHERIC) |  | “flushing\_2D\_small\_granular\_flows”  Amicarelli & Agate (2014, SPHERIC)+ “flushing\_2D\_small\_granular\_flows\_erosion\_criterion\_2D\_complete”  Amicarelli & Agate (2014, SPHERIC)+  “flushing\_2D\_small\_tuned\_model\_and\_erosion\_criterion\_2D\_limited”  (Manenti et al., 2012, JHE) |  |
| “flushing\_3D\_small\_slope\_B3\_granular\_flows\_erosion\_criterion\_2D\_complete”  SPHERA v.8.0 +  “flushing\_3D\_small\_slope\_B3\_granular\_flows\_erosion\_criterion\_3D\_complete”  SPHERA v.8.0 |  | “ICOLD\_earth-fill\_dam\_breach\_long”  Amicarelli & Agate (2014, SPHERIC) +  “ICOLD\_earth-fill\_dam\_breach\_short”  Amicarelli & Agate (2014, SPHERIC) +  “ICOLD\_earth-fill\_dam\_break”  Amicarelli & Agate (2014, SPHERIC) |  |
| “jet\_plate\_DBSPH“  Amicarelli et al. (2013, IJNME) +  “jet\_body-plate”  Amicarelli et al. (2015, CAF)+  “jet\_plate\_DBSPH\_low\_res”  Amicarelli et al. (2013, IJNME)+  “jet\_plate\_SASPH\_low\_res”  Amicarelli et al. 2013 (IJNME) |  | “sloshing\_tank\_TbyTn\_0\_78”  Amicarelli et al. (2013, IJNME) |  |
| “sloshing\_tank\_TbyTn\_1\_07”  Amicarelli et al. (2013, IJNME) |  | “submerged\_landslide”  Amicarelli & Agate (2014, SPHERIC) |  |
| “symmetric\_wedge\_20deg\_light”  Amicarelli et al. (2015, CAF) |  | “symmetric\_wedge\_20deg\_medium”  Amicarelli et al. (2015, CAF) |  |
| “tsunami\_ISEC”  Guandalini et al. (2014, DAOE) |  | “water\_box\_free\_surface”  Simple and demonstrative 2D test case on hydrostatic conditions (rough resolution)  SPHERA v.8.0 +  water\_tank-body  Simple and demonstrative 2D test case on hydrostatic conditions and "fluid - solid body" interactions (rough resolution)  SPHERA v.8.0 |  |

Figure 11.2. Validations and applications of SPHERA v.8.0 (44 test cases).

In azure those test cases, whose input files are published on SPHERA GitHub repository (Table 1.1).

# FAQ

So far, no additional information is relevant.

# Beneficiary Lists on the licenses of the previous versions of the code

SPHERA transfer on GitHub (as GNU-GPL FOSS) allows avoiding the production of ad-hoc licenses for limited periods. For sake of completeness, this section collects the exhaustive lists of SPHERA licenses (they are all expired), which has been realised by RSE SpA (formerly ERSE SpA, formerly CESI RICERCA SpA, formerly CESI SpA - Ricerca di Sistema) for the previous versions of the code (before SPHERA v.8.0).

Hereafter the list of beneficiaries of the licences (all expired) of SPHERA source codes:

* E4 Computer Engineering (license for company use; the license was exclusively released to translate the code in CUDA language, in collaboration with RSE SpA; 2009; SPHERA v.3.2);
* Prof. Mario Gallati (University of Pavia; personal license for single-user for academic use, in the frame of a collaboration with RSE SpA funded by Ricerca di Sistema; 2009; SPHERA v.3.2).

Hereafter the list of beneficiaries of the licences (all expired) of SPHERA executable files:

* Dr. Raffaele Albano and Dean Prof. Aurelia Sole (University of Basilicata; SPHERA v.3.3, 17May2012-16May2013; SPHERA v.4.0, 21May2012-20May2013; SPHERA v.5.0, 14Nov2012-13Nov2013; SPHERA v.5.0.2, 03Apr2013-31Oct2013; SPHERA v.5.0.2, 01Nov2013-31Dec2013; SPHERA v.5.0.2 –without erosion criterion -, 01Jul2015-31Dec15);
* Ms. Luciana Giuzio and Prof. Aurelia Sole (University of Basilicata; SPHERA v.3.3, 17May2012-16May2013);
* Prof. Philippe Larroudé (University of Grenoble -FRA-; SPHERA v.4.0.5 -without RK time integration schemes, without DB-SPH method-, 06Apr2012-05Apr2013);
* Ms. Latifa Ziane and Prof. Mohammed Chérif Khellaf (University USTHB of Algiers, Algeria; SPHERA v.7.0, 01Jul2015-31Dec2015).

# Previous versions of the code

SPHERA v.8.0 includes all the relevant source files of the previous versions of the code.

Although these versions were not tracked on GitHub SPHERA repository (because the code was not written under a Git repository), the obsolete program units are kept as draft subroutines in (and only in) SPHERA v.8.0, just to keep them tracked on SPHERA GitHub repository. Further, Table 14.1 reports information on SPHERA v.7.0 files and their relationships with SPHERA v.8.0 program units.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Program unit (SPHERA v.7.0)** | **First author**  **(SPHERA v.7.0)** | **SPHERA 8.0 folder** | **SPHERA v.8.0 file** | **subroutine(s)/**  **function(f)/**  **module(m)/**  **main(p)** | **Notes** |
| CancelOutgoneParticles\_2D | undef. | BC | CancelOutgoneParticles.f90 | s |  |
| CancelOutgoneParticles\_3D | undef. | BC | CancelOutgoneParticles.f90 | s |  |
| FindFrame | undef. | BC | Sphera\_Tools.f90 | s |  |
| FindLine | undef. | BC | Sphera\_Tools.f90 | s |  |
| GenerateSourceParticles\_2D | Di Monaco | BC | GenerateSourceParticles.f90 | s |  |
| GenerateSourceParticles\_3D | Di Monaco | BC | GenerateSourceParticles.f90 | s |  |
| IsParticleInternal2D | undef. | BC | Sphera\_Tools.f90 | f |  |
| IsParticleInternal3D | undef. | BC | Sphera\_Tools.f90 | f |  |
| NormFix | undef. | BC | Sphera\_Tools.f90 | s |  |
| NumberSectionPoints | undef. | BC | Sphera\_Tools.f90 | f |  |
| PreSourceParticles\_2D | Di Monaco | BC | GenerateSourceParticles.f90 | s |  |
| PreSourceParticles\_3D | Di Monaco | BC | GenerateSourceParticles.f90 | s |  |
| VelLaw | undef. | BC | Sphera\_Tools.f90 | s |  |
| CalcPre | undef. | BE\_Mass | Sphera\_Tools.f90 | s | with commented subroutine on Mach check |
| inter\_EqCont\_2D | undef. | BE\_Mass | Inter.f90 | s |  |
| inter\_EqCont\_3D | undef. | BE\_Mass | Inter.f90 | s |  |
| inter\_SmoothPres | Di Monaco | BE\_Mass | Inter.f90 | s |  |
| PressureSmoothing\_2D | Di Monaco | BE\_Mass | PressureSmoothing.f90 | s |  |
| PressureSmoothing\_3D | Di Monaco | BE\_Mass | PressureSmoothing.f90 | s |  |
| diffumorris | undef. | BE\_Momentum | Sphera\_Tools.f90 | s |  |
| inter\_EqMoto | undef. | BE\_Momentum | Inter.f90 | s |  |
| inter\_SmoothVelo\_2D | Di Monaco | BE\_Momentum | Inter.f90 | s |  |
| inter\_SmoothVelo\_3D | Di Monaco | BE\_Momentum | Inter.f90 | s |  |
| viscomon | undef. | BE\_Momentum | Sphera\_Tools.f90 | s |  |
| viscomorris | undef. | BE\_Momentum | Sphera\_Tools.f90 | s |  |
| Body\_dynamics\_output | Amicarelli | Body\_Transport | Body\_dynamics.f90 | s |  |
| body\_particles\_to\_continuity | Amicarelli | Body\_Transport | Body\_dynamics.f90 | s |  |
| body\_pressure\_mirror | Amicarelli | Body\_Transport | Body\_dynamics.f90 | s |  |
| body\_pressure\_postpro | Amicarelli | Body\_Transport | Body\_dynamics.f90 | s |  |
| body\_to\_smoothing\_pres | Amicarelli | Body\_Transport | Body\_dynamics.f90 | s |  |
| body\_to\_smoothing\_vel | Amicarelli | Body\_Transport | Body\_dynamics.f90 | s |  |
| Gamma\_boun | Amicarelli | Body\_Transport | Body\_dynamics.f90 | f |  |
| Input\_Body\_Dynamics | Amicarelli | Body\_Transport | Body\_dynamics.f90 | s |  |
| RHS\_body\_dynamics | Amicarelli | Body\_Transport | Body\_dynamics.f90 | s |  |
| mixture\_viscosity | Amicarelli | Constitutive\_Equation | Granular\_flows.f90 | s |  |
| viscapp | Di Monaco | Constitutive\_Equation | Sphera\_Tools.f90 | s |  |
| adjacent\_faces\_isolated\_points | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| BC\_wall\_elements | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| DBSPH\_find\_close\_faces | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| DBSPH\_IC\_surface\_elements | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| DBSPH\_inlet\_outlet | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| DBSPH\_kinematics | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| Gradients\_to\_MUSCL | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| Gradients\_to\_MUSCL\_boundary | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| Import\_ply\_surface\_meshes | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| semi\_particle\_volumes | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| viscomon\_wall\_elements | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s | in drafts.f90 |
| viscomorris\_wall\_elements | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s | in drafts.f90 |
| wall\_elements\_pp | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| wavy\_inlet | Amicarelli | DB\_SPH | BC\_wall\_elements.f90 | s |  |
| compute\_k\_BetaGamma | Amicarelli | Erosion\_Criterion | Granular\_flows.f90 | s |  |
| fixed\_bed\_slope\_limited | Amicarelli | Erosion\_Criterion | Granular\_flows.f90 | s |  |
| MohrC | Manenti | Erosion\_Criterion | Crit\_Erosion.f90 | s | in drafts.f90 |
| Shields | Manenti | Erosion\_Criterion | Crit\_Erosion.f90 | s |  |
| area\_quadrilateral | Amicarelli | Geometry | Granular\_flows.f90 | s |  |
| area\_triangle | Amicarelli | Geometry | Granular\_flows.f90 | s |  |
| dis\_point\_plane | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| distance\_point\_line\_2D | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| distance\_point\_line\_3D | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| IsPointInternal | undef. | Geometry | Sphera\_Tools.f90 | f |  |
| line\_plane\_intersection | Amicarelli | Geometry | Granular\_flows.f90 | s |  |
| LocalNormalCoordinates | Di Monaco | Geometry | Sphera\_Tools.f90 | s |  |
| Matrix\_Inversion\_2x2 | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| Matrix\_Inversion\_3x3 | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| MatrixProduct | undef. | Geometry | Sphera\_Tools.f90 | s |  |
| MatrixTransposition | undef. | Geometry | Sphera\_Tools.f90 | s |  |
| point\_inout\_polygone | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| quadratic\_equation | Amicarelli | Geometry | Granular\_flows.f90 | s |  |
| reference\_system\_change | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| three\_plane\_intersection | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| Vector\_Product | undef. | Geometry | Sphera\_Tools.f90 | s |  |
| vector\_rotation | Amicarelli | Geometry | Body\_dynamics.f90 | s |  |
| GeneratePart | undef. | IC | Sphera\_Tools.f90 | s |  |
| initialization\_fixed\_granular\_particle | Amicarelli | IC | Granular\_flows.f90 | s |  |
| SetParticleParameters | Amicarelli | IC | Sphera\_Tools.f90 | s |  |
| SetParticles | undef. | IC | Sphera\_Tools.f90 | s |  |
| SubCalcPreIdro | Agate | IC | Sphera\_Tools.f90 | s |  |
| AggDens | undef. | Interface\_Dispersion | Sphera\_Tools.f90 | s | in drafts.f90 |
| inter\_CoefDif | undef. | Interface\_Dispersion | Inter.f90 | s | in drafts.f90 |
| inter\_SmoothVF | Manenti | Interface\_Dispersion | Inter.f90 | s | in drafts.f90 |
| check\_files | undef. | Main algorithm | Sphera\_Main.f90 | s | in sphera.f90 |
| Gest\_Dealloc | undef. | Main algorithm | Sphera\_Tools.f90 | s |  |
| Gest\_Trans | undef. | Main algorithm | Sphera\_Tools.f90 | s |  |
| Loop\_Irre\_2D | Di Monaco | Main algorithm | Loop\_Irre.f90 | s |  |
| Loop\_Irre\_3D | undef. | Main algorithm | Loop\_Irre.f90 | s |  |
| sphera | undef. | Main algorithm | Sphera\_Main.f90 | p | in sphera.f90 |
| AdM\_User\_Type | Di Monaco | Modules | AdM\_User\_Type.f90 | m | New name: Hybrid\_allocation\_module |
| ALLOC\_Module | undef. | Modules | Alloc\_Module.f90 | m | New name: Dynamic\_allocation\_module |
| BoundIntegralTab\_Module | Di Monaco | Modules | BoundIntegralTab\_Module.f90 | m | New name: SA\_SPH\_module |
| diagnostic\_module | undef. | Modules | Diagnostic\_Module.f90 | m | New name: I\_O\_diagsnostic\_module |
| english\_writime2 | undef. | modules | Sphera\_Tools.f90 | m | New name: I\_O\_ENG\_module |
| files\_entities | undef. | Modules | Files\_Entities.f90 | m | New name: I\_O\_file\_module |
| GLOBAL\_Module | undef. | Modules | Global\_Module.f90 | m | New name: Static\_allocation\_module |
| italiano\_writime2 | undef. | modules | Sphera\_Tools.f90 | m | New name: I\_O\_ITA\_module |
| language\_writime2 | undef. | modules | Sphera\_Tools.f90 | m | New name: I\_O\_language\_module |
| time\_usertype | undef. | Modules | Time\_UserType.f90 | m | New name: Time\_module |
| CalcVarLength | undef. | Neighbouring\_Search | Sphera\_Tools.f90 | s |  |
| CellIndices | undef. | Neighbouring\_Search | Sphera\_Tools.f90 | f |  |
| CellNumber | undef. | Neighbouring\_Search | Sphera\_Tools.f90 | f |  |
| CreaGrid | undef. | Neighbouring\_Search | Sphera\_Tools.f90 | s |  |
| InterFix | undef. | Neighbouring\_Search | Inter.f90 | s |  |
| OrdGrid1 | undef. | Neighbouring\_Search | Sphera\_Tools.f90 | s |  |
| ParticleCellNumber | undef. | Neighbouring\_Search | Sphera\_Tools.f90 | f |  |
| SearchforParticleZone\_3D | Di Monaco | Neighbouring\_Search | Sphera\_Tools.f90 | s |  |
| w | Di Monaco | Neighbouring\_Search | Boundaries.f90 | f |  |
| calc\_pelo | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| CalcVarp | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| CreateSectionPoints | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| GetVarPart | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| Memo\_Ctl | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| Memo\_Results | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| Print\_Results | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| result\_converter | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| s\_ctime | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| s\_secon2 | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| start\_and\_stop | Agate | Post-processing | Sphera\_Tools.f90 | s |  |
| sub\_Q\_sections | Amicarelli | Post-processing | Granular\_flows.f90 | s |  |
| Update\_Zmax\_at\_grid\_vert\_columns | Amicarelli | Post-processing | Granular\_flows.f90 | s |  |
| write\_Granular\_flows\_interfaces | Amicarelli | Post-processing | Granular\_flows.f90 | s |  |
| write\_h\_max | Amicarelli | Post-processing | Granular\_flows.f90 | s |  |
| writime2 | undef. | Post-processing | Sphera\_Tools.f90 | s |  |
| defcolpartzero | undef. | Pre-processing | Sphera\_Tools.f90 | s |  |
| diagnostic | Agate | Pre-processing | Sphera\_Tools.f90 | s |  |
| Gest\_Input | undef. | Pre-processing | Sphera\_Tools.f90 | s |  |
| Init\_Arrays | undef. | Pre-processing | Sphera\_Tools.f90 | s |  |
| ModifyFaces | undef. | Pre-processing | Sphera\_Tools.f90 | s |  |
| ReadBedLoadTransport | Amicarelli | Pre-processing | ReadInputFile.f90 | s |  |
| ReadBodyDynamics | Amicarelli | Pre-processing | ReadInputFile.f90 | s |  |
| ReadCheck | undef. | Pre-processing | ReadInputFile.f90 | f |  |
| ReadDBSPH | Amicarelli | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInput | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputBoundaries | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputControlLines | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputControlPoints | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputControlSections | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputDomain | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputDrawOptions | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputExternalFile | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputFaces | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputGeneralPhysical | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputLines | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputMedium | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputOutputRegulation | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputParticlesData | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputRestart | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputRunParameters | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputTitle | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadInputVertices | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadRestartFile | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadRiga | undef. | Pre-processing | ReadInputFile.f90 | s |  |
| ReadSectionFlowRate | Amicarelli | Pre-processing | ReadInputFile.f90 | s |  |
| AddBoundaryContribution\_to\_CE2D | Di Monaco | SA\_SPH | AddBoundaryContribution.f90 | s |  |
| AddBoundaryContribution\_to\_CE3D | Di Monaco | SA\_SPH | AddBoundaryContribution.f90 | s |  |
| AddBoundaryContributions\_to\_ME2D | Di Monaco | SA\_SPH | AddBoundaryContribution.f90 | s |  |
| AddBoundaryContributions\_to\_ME3D | Di Monaco | SA\_SPH | AddBoundaryContribution.f90 | s |  |
| AddElasticBoundaryReaction\_2D | Di Monaco | SA\_SPH | AddBoundaryContribution.f90 | s |  |
| AddElasticBoundaryReaction\_3D | Di Monaco | SA\_SPH | AddBoundaryContribution.f90 | s |  |
| BoundaryMassForceMatrix2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| BoundaryMassForceMatrix3D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| BoundaryPressureGradientMatrix3D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| BoundaryReflectionMatrix2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| BoundaryVolumeIntegrals2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| CompleteBoundaries3D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| ComputeBoundaryDataTab | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| ComputeBoundaryIntegralTab | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| ComputeBoundaryVolumeIntegrals\_P0 | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| ComputeKernelTable | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| ComputeSurfaceIntegral\_WdS2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| ComputeVolumeIntegral\_WdV2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| DefineBoundaryFaceGeometry3D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| DefineBoundarySideGeometry2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| DefineBoundarySideRelativeAngles2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| DefineLocalSystemVersors | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| EvaluateBER\_TimeStep | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| FindBoundaryConvexEdges3D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| FindBoundaryIntersection2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| FindCloseBoundaryFaces3D | DI Monaco | SA\_SPH | Boundaries.f90 | s |  |
| FindCloseBoundarySides2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| GridCellBoundaryFacesIntersections3D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| InterpolateBoundaryIntegrals2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| InterpolateTable | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| IWro2dro | Di Monaco | SA\_SPH | Boundaries.f90 | f |  |
| J2Wro2 | Di Monaco | SA\_SPH | Boundaries.f90 | f |  |
| JdWsRn | Di Monaco | SA\_SPH | Boundaries.f90 | f |  |
| SelectCloseBoundarySides2D | Di Monaco | SA\_SPH | Boundaries.f90 | s |  |
| WIntegr | Di Monaco | SA\_SPH | Boundaries.f90 | f |  |
| GetToken | undef. | strings | Sphera\_Tools.f90 | f |  |
| lcase | undef. | strings | Sphera\_Tools.f90 | f |  |
| ltrim | undef. | strings | Sphera\_Tools.f90 | f |  |
| Euler | Amicarelli | Time\_Integration | time\_integration.f90 | s |  |
| Heun | Amicarelli | Time\_Integration | time\_integration.f90 | s |  |
| inidt2 | undef. | Time\_Integration | Sphera\_Tools.f90 | s |  |
| rundt2 | undef. | Time\_Integration | Sphera\_Tools.f90 | s |  |
| stoptime | undef. | Time\_Integration | Sphera\_Tools.f90 | s |  |
| time\_integration | Amicarelli | Time\_Integration | time\_integration.f90 | s |  |
| time\_integration\_body\_dynamics | Amicarelli | Time\_Integration | time\_integration.f90 | s |  |
| KeyDecoderCheck | Agate |  | KeyDecoderCheck.f90 | s | Erased permanently |
| sloshing\_tank\_control\_points | Amicarelli |  | DB-SPH\_hard\_coding.f90 | s | Erased permanently |

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# SPHERA registration

SPHERA v.8.0 Copyright is registered (“Registro pubblico speciale per i programmi per elaboratore, SIAE”, Italy).

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