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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.9.0.0 (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 (with transport of solid bodies and bed-load transport flood-control works, flood-induced damage; domain spatial coverage of some hundreds of squared kilometres) and fast landslides, sloshing tanks, sea waves and hydroelectric plants.

With Copyright 2005-2018 (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, Emanuela Abbate, Qiao Cheng.

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

* Scheme for dense granular flows. Reference: Amicarelli et al. (2017, IJCFD, [9]):

Amicarelli A., B. Kocak, S. Sibilla, J. Grabe; 2017; A 3D Smoothed Particle Hydrodynamics model for erosional dam-break floods; International Journal of Computational Fluid Dynamics, 31(10):413-434; DOI 10.1080/10618562.2017.1422731

* 3D SPH numerical scheme for the transport of solid bodies in free surface flows. Reference: Amicarelli et al. (2015, CAF, [7]):

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, [6]):

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, [122]):

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, [46]):

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 (e.g., 3D erosion criterion also with mixture-fixed bed interactions), 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 optimized executions |
| debug | SPHERA executable files compiled with gfortran/ifort for debug scalar executions |
| debug\_omp | SPHERA executable files compiled with gfortran/ifort for debug parallel 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 v.9.0.0 repository.

# Warranties and responsabilities

SPHERA v.9.0.0 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.9.0.0

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.9.0.0 need the following citation: “SPHERA v.9.0.0 (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).

SPHERA should also be cited 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.9.0.0 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.9.0.0 is available on GitHub ([184]). 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 citations);
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);
7. be interested in attending free internships on SPHERA at RSE as academic students (Bachelor Degree, Master Degree and PhD students).

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 (RSE can delete program units since a certain version).

SPHERA authors and “official users” need to activate a free account on github.com (with recognizable name, surname and affiliation) and “fork” SPHERA, by clicking on the icon “fork” in the official SPHERA public repository ([184; 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). The option “watch” might be insufficient to receive the whole news about the code repository: a hidden email address can be added in your private account under the web page https://github.com/<your\_github\_user\_ID>/SPHERA/settings/notifications to be notified on all the repository modifications.

If any activity dedicated to SPHERA is declared to RSE, that activity might be reserved by RSE for a specific user during a specific period to avoid redundancy and conflicts between users.

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: first FOSS release (SPHERA v.8.0). Executable codes.

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|  |

Figure 5.2. SPHERA on GitHub: first FOSS release (SPHERA v.8.0). Documentation.

|  |
| --- |
|  |

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 (commit 13Jun2018).

|  |
| --- |
|  |

Figure 5.5. SPHERA on GitHub: master branch. Input files (commit 13Jun2018).

|  |
| --- |
|  |

Figure 5.6. SPHERA on GitHub: master branch. Source code (commit 13Jun2018).



Figure 5.7. SPHERA indexed at SPHERIC web site (August 2018, extract from the list of the 13 SPH codes indexed at http://spheric-sph.org/sph-projects-and-codes ).

# The scheme for transport of solid bodies and the Semi-Analytic approach as a boundary treatment scheme for fixed boundaries

After 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.

The following sub-sections provide details on: improving 3D rotations (Sec.6.4); the sliding friction force (Sec.6.2); the body-boundary normal reaction force under sliding (at null normal velocity, Sec.6.3); the normal restitution coefficient (Sec.6.6).

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 ([10]), *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 2*h*, 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, [83]; Macia et al., 2012, [121]; Mayrhofer et al., 2013, [131]; Ferrand et al., 2013, [57]; Amicarelli et al., 2013, [6]).

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, [203]; Amicarelli et al., 2015, [7]; Di Monaco et al., 2011, [46]); sloshing tanks (Souto-Iglesias et al., 2006, [188]; Delorme et al., 2009, [42]; Amicarelli et al., 2013, [6]); wave motion (e.g., Patel et al., 2009, [156]; Antuono et al., 2011, [14]; Liu et al., 2013, [118]; Omidvar et al., 2012a, [149]); hydraulic turbines (Marongiu et al., 2010, [125]); fast landslides (e.g., Kumar et al., 2013, [102]); erosion and bed-load transport (Manenti et al., 2012, [122]); liquid jets (e.g., Koukouvinis et al., 2013, [100]); pollutant dispersion; astrophysics (e.g., Price & Monaghan, 2007, [164]); magneto-fluid dynamics (e.g., Price, 2012, [162]); multi-phase and multi-fluid flows (e.g., Kajtar & Monaghan, 2012, [95]).

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

This section relies on [46] and [7], whose reading is 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, [210]). Its basic features are deeply described in Di Monaco et al. (2011, [46]) 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”; [210]):

|  |  |
| --- | --- |
|  | (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 [46]) hypothesizes the following linearization and assumptions to compute f in *Vh’*:

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

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

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

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 .

|  |  |
| --- | --- |
|  |  |

Under free-slip conditions, the tangential component of the velocity vector in the truncated portion of the kernel support is:

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

whereas it assumes the following expression under no-slip conditions:

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

where *t* is the vector tangential to the wall surface, as defined by its local orientation.

The normal component of the velocity vector in the truncated portion of the kernel support, no matter about the slip conditions, reads:

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

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

Thus, the associated velocity vectors can be assigned to the truncated portion of the kernel support both under no-slip conditions:

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

and free-slip conditions:

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

together with the following velocity differences, both under free-slip conditions:

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

and no-slip conditions:

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

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:

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

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):

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

where *as*represents a new acceleration term due to the fluid-body interactions, *M* is the artificial viscosity (Monaghan, 2005, [138]), *m* the particle mass and *r* the relative distance between the neighbouring and the computational particle.

Zeroing (molecular) viscosity reduces CPU time. A configuration with no-slip conditions and null viscosity makes sense if it is demonstrated that the value of viscosity is ininfluential.

No-slip conditions might possibly provide the same results as free-slip conditions if both the following conditions are satisfied: the test case approximately provides no-slip conditions even if free-slip conditions are used; dx is small enough.

If no-slip conditions can be used with body transport, then they are more convenient than free-slip conditions in terms of CPU time.

The second-to-last term of (6.16) is defined by Di Monaco et al. (2011, [46]). It is a viscous term, whose formulation is mixes Cleary’s and Morris’ formulations (Basa et al., 2009, [18]):

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

where ** and *r,2* are negligible constants avoiding divergent behaviours. In case ** and *r* do not tend to zero, then (6.17) assumes the following form:

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

One considers Morris’ term (Basa et al., 2009, [18]):

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

and that the following expression:

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

is a factor analogous to Cleary’s formulation (Basa et al., 2009, [18]):

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

It follows that (6.18) is equal to Morris’ term only in case of uniform density and viscosity:

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

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

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

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 [7], whose reading is suggested for further details.

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

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

The first formula of (6.24) represents the balance equation of the momentum of a solid rigid body, which translates with no rotation around its barycentre. The second formula of (6.24) represents the balance equation of the momentum of a solid rigid body which rotates with no translation of its barycentre; it is the balance equation of the body angular momentum.

The following kinematics formulae are used for time integrating the body velocity and angular velocity to obtain the barycentre position and the orientation of the body:

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

where ** is the vector of the angles lying between the body axes and the global reference system.

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

The first formula of (6.24) represents the balance equations for the momentum.*FTOT* is the global/resultant force acting on the solid body. The last formula of (6.24) expresses the balance equation of the body angular momentum, where ** denotes the angular velocity of the generic body.. *MTOT* represents the associated torque acting on the body and the matrix of the moments of inertia of the computational body (Einstein’s notation works for the subscript “*l*”):

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

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

One considers the final formulation of the second formula of (6.24). When the first/second term in the squared parentheses is negligible, then the resulting rotation is called torque-free/torque-induced precession. The minor effect of the torque-free term on a torque-induced precession is called nutation.

Torque-free precession occurs when the integral of the external forces, internal forces and external torques are null, but the integral of the internal torques is non-null. The internal torques are induced by the internal forces. These normal and shear stresses within the body material are necessary to permit the centripetal accelerations of the material points of the body.

Torque-free precessions are prevented if at least one of the following requirements is satisfied: body symmetry around the current rotation axis; body symmetry around the plane normal to the current rotation axis and passing for the body barycentre; null angular velocity.

The inverse of the matrix of the moment of inertia acts like a rotation matrix for the torque in the second formula of (6.24) and thus can induce a change in the rotation axis in the presence of an external torque. Torque-induced precession is prevented if at least one of the following conditions is satisfied: body symmetry around the current rotation axis; body symmetry around the plane normal to the current rotation axis and passing for the body barycentre; null torque.

In order to solve the system (6.24), we need to model the global force and torque, as described in the following. The resultant force is composed of several terms:

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

*G* represents the gravity force, whereas *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). In case of inertial and quasi-inertial fluid flows, we do not need to refer to neither turbulence scheme nor tangential stresses (simplifying hypothesis). Nonetheless, shear forces can be represented under more generic conditions (Sec.6.2).

Gravity is always active. The expressions “gravity deactivated” (input file template) only refers to the activation of drag and reaction forces, which temporarily balances gravity components, during an impingement or in case of sliding. The approximations refer to drag and reaction forces, not to gravity.

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

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

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 (6.24) 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:

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

Time integration of (6.24) 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 vector sum of the velocity of the corresponding body barycentre and the relative velocity:

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

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* is the body rotation matrix):

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

At the moment, the following simplifications are assumed: the drag force *TF* is not represented; each body is given in input a uniform density.

* 1. Improving 3D rotations

The equations:

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

are not exact and represent a limit when working with the a rotation matrix based on Euler angles: the first equation of (6.32) is exact only for 1D rotations, the second one is never exact (non-commutative property of the rotation matrices based on Euler angles).

The following formula represents a generalized Euler-Newton equation for 3D rotations and provides exact results in 3D:

|  |  |
| --- | --- |
|  | (6.33) |

Consider rotation matrices based on Euler’s theorem ( “each 3D rotation can be represented as a 1D rotation about a generic axis” of a unique rotation angle R). This approach is also called “matrix to axis-angle” and is used by Rodrigues formula to define the rotation matrix:

|  |  |
| --- | --- |
|  | (6.34) |

where the rotation axis is represented by the unit vector *nR*.

The cross-product matrix is a skew symmetric matrix:

|  |  |
| --- | --- |
|  | (6.35) |

The expansion of *Rij* reads:

|  |  |
| --- | --- |
|  | (6.36) |

In 2D, the Rodrigues’ rotation matrix is equal to Euler’s rotation matrix.

The rotation angle depends on the angular velocity and the time step duration:

|  |  |
| --- | --- |
|  | (6.37) |

When working with rotation matrices, Gimbal lock can be only prevented by Rodrigues formula.

So far, SPHERA only applies the approach described in this section to provide output data in order to initialize a following restarted simulation. In this frame, SPHERA determines the rotation matrix which provides a rotation from the initial time of the former simulation to a generic time for which output data are available for a following restarted simulation. This represents an approximated procedure which only guarantees a correct re-initialization of the relative position of the first body particle. As the body centre of mass is correctly imposed, the error in the body orientation (of a reinitialized simulation) is limited.

However, the approach of this section could be used in a more generic way to reproduce the exact body orientation in the body dynamics balance equations at every time step (Sec.6.3).

Hereafter is reported the procedure to determine the rotation matrix to move from a first vector (the relative position of the first body particle at the initial time) to a second vector (the relative position of the first body particle at a generic output time).

The rotation axis unit vector is estimated as follows:

|  |  |
| --- | --- |
|  | (6.38) |

The cross product is not sufficient to distinguish between *R* and (**-*R*):

|  |  |
| --- | --- |
| , but don’t use | (6.39) |

However, consider that *R* from the cross product automatically and correctly provides an angle between 0 and ** (sin(*R*) is non-negative).

The sine and cosine functions of the rotation angle read:

|  |  |
| --- | --- |
| , | (6.40) |

Provided its sine and cosine functions, the value of the rotation angle can be estimated by means of the “atan2” function:

|  |  |
| --- | --- |
|  | (6.41) |

Once obtained the rotation axis and angle, Rodrigues formula is used to build the rotation matrix and rotate the whole body by means of a single rotation, from the initial time to the time chosen.

* 1. Reaction forces

Following the superposition principle of effects, the reaction forces of a generic body dynamics configuration are computed as vector sums of the reaction forces associated with two different configurations: the associated hyperstatic configuration and the associated dynamic configuration in the absence of other forces. Under hyperstatic conditions, the system of governing equations concern 6 balance equations (associated with the 6 degrees of freedom of the 3D body) and n compatibility equations (representing the deformation consistency among different parts of the same body).

The contributions to the reaction forces in the dynamic configuration should superpose the effects of the following dynamics mechanisms: 1D impingements in any direction in 3D; 1D sliding in any direction in 3D; pitch; roll; yaw.

SPHERA treats hyperstatic conditions as a dynamic configuration with spurious negligible oscillations: the relative velocities between the solid elements allow to dynamically develop the reactions necessary to maintain the hyperstatic configuration. The normal reaction in SPHERA is formally null, if the normal velocity is zero. However, according to Monaghan (2005, (Monaghan, 2005)), the normal forces of the boundary force particles dynamically restore the normal reaction forces. This approach is similar to a simple spring-model approach, but the reactions are triggered by the relative velocities, not the relative positions. In any case, these relative velocities and the associated displacements should be negligible with respect to the spatial resolution of the simulation.

SPHERA directly treats 1D impingements in 3D and 1D sliding mechanisms in 3D. SPHERA models the boundary reaction forces associated with the pitch and roll mechanisms thanks to the particle-based assessment of both the impact velocity and the sliding friction limiter. Instead, SPHERA does not represent the boundary reaction forces to the yaw mechanism as the simulated sliding friction force is based on a body approach. Treating the sliding friction force as the vector sum of particle-based friction forces would allow in future to treat the reaction forces associated with the yaw dynamics mechanism.

Contrarily to the normal reaction force, which is exerted gradually during the particle interaction, the sliding friction force is instantaneously applied at its maximum value as the particle interaction begins. This is correct in the frame of rigid bodies and point contacts. On the other hand, the formulation for the normal reaction guarantees the correct representation of the bouncing velocity, no matter about the maximum force. This means that the maximum normal reaction could be reproduced either instantaneously or gradually for rigid bodies. However, the current modelling of sliding friction might represent a systematic overestimation especially in case of curved surfaces (e.g., a wheel rolling on a flat plate) due to the artificial increase of the contact surface and the contact time (a point contact is replaced by a distributed contact). Possible solutions are: the reduction of the influence region just for sliding friction; an alternative gradual activation of sliding friction as if the solids were deformable. Nonetheless, curved surfaces are not currently permitted when initializing a rigid body.

* 1. Sliding friction force

The formulation of the current section refers to a single body interacting with multiple frontiers. It might be revised for a single body interacting with multiple bodies. The current code version assumes a unique friction angle applies to all the body-frontier interactions.

The overall normal of the neighbouring frontiers is the unit vector aligned with the vector sum of the neighbouring normals. In case of need, this sum might be weighted in a proper manner.

* + 1. Aerial stage (non-negative value for the input friction angle and body-frontier interactions)

The simulated and exact formulation (*\**) for the sliding friction force are equal:

|  |  |
| --- | --- |
|  | (6.42) |

where ** is the sliding friction angle, the subscript “*dry*” refers to dry conditions, *sw* is the unit vector parallel to the local frontiers and with direction opposite to the velocity vector of the body barycentre (projected on the local DEM).

The coefficient of sliding friction (*sf*) reads:

|  |  |
| --- | --- |
|  | (6.43) |

The absolute value for the exact formulation reads:

|  |  |
| --- | --- |
|  | (6.44) |

where the cosine of the slope angle is obtained by means of a dot product:

|  |  |
| --- | --- |
|  | (6.45) |

The direction of the sliding friction force is the opposite to the velocity direction of the centre of mass of the computational body.

The following limiter applies to the sliding friction force:

|  |  |
| --- | --- |
|  | (6.46) |

where  is the maximum particle velocity (all over the computational body) tangential to the interacting local frontier elements.

* + 1. Aerial stage (negative value for the input friction angle or body-body interactions)

The sliding friction force (*Ts*: drag force on a body under body-boundary interactions) is approximately represented by means of a tangential force, which balances the tangential component of gravity:

|  |  |
| --- | --- |
|  | (6.47) |

Its absolute value is:

|  |  |
| --- | --- |
|  | (6.48) |

where *DTM* is the slope angle and *k* the unit vector aligned with the vertical axis:

|  |  |
| --- | --- |
|  | (6.49) |

The removal of the gravity force component which is parallel to the bottom is equivalent to introducing an approximated sliding friction force, where the slope angle approximates the sliding friction angle.

|  |  |
| --- | --- |
|  | (6.50) |

This approximation might be acceptable, especially in case the sliding friction angle is unavailable.

Under this configuration, normal reaction does not provide any torque (nevertheless the limiter for the sliding friction force depends on the velocity of the solid particles interacting with the frontiers).

* + 1. Submerged stage

The sliding friction provided by a solid boundary to a wet body assumes the following form:

|  |  |
| --- | --- |
|  | (6.51) |

where *sw* is the unit vector parallel to the local frontiers and with direction opposite to the velocity vector of the body barycentre (projected on the local frontier surface). If this velocity is null, then the friction force is zero.

The maximum absolute value for the sliding friction reads:

|  |  |
| --- | --- |
|  | (6.52) |

where ** is here the sliding friction angle (the current code version assumes a unique value for all the body-frontier interactions).

As the direction of the sliding friction force is always opposite to the velocity direction of the centre of mass of the computational body (after projection along *sw*), the following approximated limiter applies:

|  |  |
| --- | --- |
|  | (6.53) |

where is the maximum particle velocity (all over the portion of the computational body within the boundary-body interaction region) tangential to the interacting local frontier elements.

The sliding friction force contributes to the global torque. The application point of the friction force for any solid body is computed as the average position of the body particles involved in the "body particle - frontier" interactions. Each interaction has the same weight in this averaging process (every particle might be considered more than once).

The following hypotheses are assumed: all the surface body particles in contact with wet boundaries have a defined pressure; all the body-boundary interfaces are hydraulically connected with the fluid; normal reaction forces (with bodies and boundaries, included the current boundaries providing friction) are not considered to assess the sliding force.

All the SPH fluid particles within any solid body at the beginning of the simulation (initial conditions for the fluid particle positions in case of Fluid - Structure interactions), due to design, are removed before the simulation time starts.







* 1. Body-boundary normal reaction force under sliding (at null normal velocity)
     1. Aerial stage

The exact formulation is correctly represented:

|  |  |
| --- | --- |
|  | (6.54) |

This term is added to the body-boundary normal force in the main file of this documentation -Eq.(6.32)-. The overall normal of the neighbouring frontiers is the unit vector aligned with the vector sum of the neighbouring normals.

* + 1. Submerged stage

The normal reaction is formally null.

|  |  |
| --- | --- |
|  | (6.55) |

According to Monaghan (2005), the normal forces of the boundary force particles (6.32) dynamically restore the normal reaction force (body-boundary interactions), despite some body spurious oscillations (normal to the frontier) in the interaction zone (noise amplitude comparable with the spatial resolution).

|  |  |
| --- | --- |
|  | (6.56) |

* 1. Fluid-body interaction terms

This section relies on [7], whose reading is suggested for further details.

The fluid-body interaction terms rely on the boundary technique introduced by Adami et al. (2012, [1]), implemented and adapted for free-slip conditions (Amicarelli et al., 2015, [8]). 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 (6.15), used to treat solid frontiers (free-slip conditions):

|  |  |
| --- | --- |
|  | (6.57) |

Modelling the shear stress gradient term in the Navier-Stokes equation requires an alternative formulation to (6.57). The discretization of this term, which is coherent with the definition of the inter-particle velocity under no-slip conditions, assumes the following form:

|  |  |
| --- | --- |
|  | (6.58) |

Analogously, the fluid-body interaction term in the momentum equation (6.16) assumes the form:

|  |  |
| --- | --- |
|  | (6.59) |

where the subscript “*s0*” denotes a generic solid-fluid inter-particle interaction. The first term in the RHS of (6.59) is reported by Adami et al. (2012, [1]) whereas the last term will be discussed later on this section.

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):

|  |  |
| --- | --- |
|  | (6.60) |

The “wall” acceleration at the position of a generic body particle can then be derived by linearizing (6.60). This depends on the particular computational fluid particle “*0*” we are considering, so that we can refer to the interaction subscript “*s,0*”:

|  |  |
| --- | --- |
|  | (6.61) |

where *dln* is a vectorial length element along the centreline of the two particles, projected along the wall element normal.

One applies a SPH interpolation over all the pressure values estimated according to Adami et al. (2012, [1]) to derive a unique pressure value for a body particle:

|  |  |
| --- | --- |
|  | (6.62) |

In case of no-slip conditions, in-built motion interests all the acceleration components and the shear stress gradient term is involved; (6.60) is replaced by the following expression:

|  |  |
| --- | --- |
|  | (6.63) |

Analogously to (6.61), one obtains:

|  |  |
| --- | --- |
|  | (6.64) |

In case of no-slip conditions, (6.62) is replaced by the following expression:

|  |  |
| --- | --- |
|  | (6.65) |

which is at the moment approximated by this formula:

|  |  |
| --- | --- |
|  | (6.66) |

The pressure value of (6.62) or (6.66) is finally used in (6.59).

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 (6.65) -“*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 (6.65).

The assumption (6.60) 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 (6.65). Nevertheless, we prefer defining a maximum threshold for |*as*|, here equal to 10*g*.

The search for the fluid-body interaction normals is only carried out in case of free-slip conditions.

An improvement on the searching algorithm for the fluid-body interaction normals provides more accurate results and a computational time reduction with respect to Amicarelli et al. (2015, [8]), as described in the following. In that paper, the searching volume V*s* was defined as the parallelepiped described by the coordinates of the interacting particles:

|  |  |
| --- | --- |
|  | (6.67) |

This caused some issues (i.e. searching area close to zero or no accurate result for the searching algorithm) under the following configurations: interacting particles having almost the same value for one coordinate; surface solid particle being one of the interacting particles. To solve these issues, the new searching algorithm extends the searching region, which is here defined as the intersection between the two identical spheres centred at the interacting particle positions and radius equal to the inter-particle distance (Figure 6.1). The new definition of the searching volume reads:

|  |  |
| --- | --- |
|  | (6.68) |

where *d*(…) (m) is here the distance between two points.

|  |
| --- |
|  |

Figure 6.1. Searching volume in fluid-body interactions to define the interaction normal to the fluid-body interface.

The search for the fluid-body interaction normals now explicitly reports possible fluid-solid mass penetrations (just in case of free-slip conditions). In case of penetration (allowed for rough spatial resolutions), the supplementary search for a formal normal now only involves surface body particles.

Two pressure limiters can be activated to treat the fluid-solid interface.

The “negative value pressure limiter” provides a minimum threshold:

|  |  |
| --- | --- |
|  | (6.69) |

The “positive value pressure limiter” acts as a LPRS and provides a maximum pressure threshold:

|  |  |
| --- | --- |
|  | (6.70) |

The maximum and minimum operators in the Right Hand Side of (6.70) apply to the whole domain.

Modelling the shear stress gradient term in the Navier-Stokes equation requires the introduction of an additional fluid-body coupling term in the Right Hand Side (RHS) of the fluid momentum equation. It is the last term of (6.59). The discretization of this coupling term, which takes into account the shear stress exchanged at the fluid-body interface, is derived in coherence with the SPH particle approximation in the inner domain.

The solid particle volume is computed as follows:

|  |  |
| --- | --- |
|  | (6.71) |

The inter-particle velocity *us0* represents the field of the fluid velocity virtually reconstructed within the portion of the kernel support, which is truncated by the solid body.

The component of the inter-particle velocity, which is normal to the interface, guarantees no mass penetration (symmetric conditions) at the interface:

|  |  |
| --- | --- |
|  | (6.72) |

Under no-slip conditions, the component of the inter-particle velocity, which is tangential (subscript “*T*”) to the interface, guarantees a uniform velocity gradient around the interface (if its position is assumed to be the average of the positions of the interacting particles):

|  |  |
| --- | --- |
|  | (6.73) |

where the unit vector *t* is tangential to the interface.

Under no-slip conditions, the difference between the inter-particle velocity and the fluid particle velocity in Eq. (51) is expressed as follows:

|  |  |
| --- | --- |
|  | (6.74) |

* 1. Solid-solid interaction terms

This section relies on [7], whose reading is suggested for further details.

The solid-solid interaction term in (6.27) -*Ps*- represents body-body and body-boundary 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, [138]) 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*:

|  |  |
| --- | --- |
|  | (6.75) |

The analytic function *fbfp* is symmetric with respect to the impact point. The dependence of (6.75) 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:

|  |  |
| --- | --- |
|  | (6.76) |

where *NBK\** is the number of boundary frontiers.

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*”:

|  |  |
| --- | --- |
|  | (6.77) |

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 (6.77) 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, [138]) and depends on *q*= *rjk*/*h*:

|  |  |
| --- | --- |
|  | (6.78) |

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 (0.1*c*) in the formulation of Monaghan (2005, [138]) 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:

|  |  |
| --- | --- |
|  | (6.79) |

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, (6.79) 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, (6.77) 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*, (6.77) would drastically under-estimate the impingement forces if the whole mass of the bodies did not lie within the impact zone (of depth 2*h*). 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:

|  |  |
| --- | --- |
| , | (6.80) |

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’*:

|  |  |
| --- | --- |
|  | (6.81) |

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

|  |  |
| --- | --- |
|  | (6.82) |

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 (6.81) 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):

|  |  |
| --- | --- |
|  | (6.83) |

The body-boundary forces are normalized by the number of neighbouring frontiers for a given body. This number is approximated by the maximum number of neighbouring frontiers of a single body particle belonging to the body.

* 1. Normal restitution coefficient

The simulated normal restitution coefficient (*Rn*) is equal to unity if all the following conditions are satisfied: homogeneous velocity of the solid particles belonging to the impinging body, impingement with a single frontier element, isolated impingement, body axes aligned with the frontier axes. Otherwise (real cases), the scheme for body-boundary force is dissipative and represents *Rn*<1. The equivalent value of the restitution coefficient might be estimated a posteriori.

# The scheme for dense granular flows

This section describes the mathematical and numerical models for dense granular flows (Amicarelli et al., 2017, [9], Sec.7.1) and its possible speed-up by means of a 2-interface 3D erosion scheme (Amicarelli & Agate, 2014, [5], Sec.7.2), which extends the (1-interface) 2D erosion scheme of Manenti et al. (2012, [122], Sec.7.2).

This mixture model for dense granular flows (e.g., bed-load transport, fast landslides) is consistent with the “packing limit” of the Kinetic Theory of Granular Flow (KTGF) and no tuning parameter is used to represent the mixture viscosity.

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

* 1. Mixture model for dense granular flows

This whole section constantly refers to Amicarelli et al. (2017, [9]), but some further details and more recent code updates.

This SPH model represents the mixture of pure fluid and non-cohesive solid granular material, under the “packing limit” of the Kinetic Theory of Granular Flow (KTGF, [16]) for dense granular flows. This limit refers to the maximum values of the solid phase volume fraction and is peculiar of bed-load transport (e.g., erosional dam breaks) and fast landslides.

The continuity equation for the fluid phase (“f”) can be expressed as follows ([16]):

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

where ** (kg×m-3) is density, ** the phase volume fraction, *u* (m×s-1) the velocity vector, *t* represents time and *x* (m) the position vector. Einstein’s notation applies to the subscript “*j*”, hereafter.

The continuity equation for the incompressible solid phase (“*s*”) can be expressed as follows ([16]):

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

The volume balance equation assumes the following form:

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

After defining the mixture density and velocity (the subscript “*m*” is always omitted):

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

the summation of (7.1) and (7.2) provides:

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

The model assumes that SPH particles are conservative (i.e. mixture particles do not exchange net mass fluxes with the surrounding environment), which is a reasonable hypothesis for high solid volume fractions in saturated soils, according to the “packing limit” of the Kinetic Theory of Granular Flow (KTGF, [16]):

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

Starting from (7.6), the model adopts a Weakly Compressible approach to obtain:

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

Following the multi-phase approach of [127], the SPH approximation of (7.7) can be expressed as follows:

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

where *n* is the unit vector normal to the frontier. The subscripts “*0*”, “*b*” and “*w*” refer to the computational particle, a neighbouring particle and a wall frontier, respectively. The integral boundary term is computed according to [46] and represents the effects of wall frontiers.

Considering the KTGF, the momentum equation for the fluid phase can be expressed as follows ([16]):

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

where *ij* (Pa) is the deviatoric (or shear) stress tensor, *g* (m×s-2) gravity acceleration and *p* (Pa) pressure. The last term depends on the relative velocity between the phases (filtration process) through the drag coefficient *Kgs* (kg×m-3×s-1).

The momentum equation for the solid phase can be expressed as follows ([16]):

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

Provided the volume equation and the definitions of the mixture velocity and density, the sum of (7.9) and (7.10) provides:

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

Considering the assumption on conservative SPH particles, the shear stress gradient term of the fluid phase can be expressed as follows ([16]):

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

where ** (Pa×s) represents viscosity. Under the hypothesis of plain strain, the shear stress gradient term is represented by [174] (visco-plastic model for dry granular material based on internal friction), by means of a parameter, which KTFG names frictional viscosity, as described in the following.

The pressure of the solid phase is treated as follows:

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

where (Pa) are the effective stresses along the principal directions and (Pa) is the mean effective stress ([174] refers to a smoothed approximation of the 3D Mohr-Coulomb criterion; the extension to Mohr-Coulomb-Terzaghi criterion for saturated soils is straightforward). The shear stress gradient term in the momentum equation can be expressed as follows ([174]):

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

where ** (rad) is the internal friction angle, *eij* (s-1) is the strain-rate tensor and *I2*(*eij*) (s-2) represents its second invariant (formulation for incompressible fluids). One may notice that the term (7.14) is potentially unstable at high internal friction angles and that, in the “packing limit” of the KTGF, the shear stress terms of the collisional-kinetic regime are zeroed. Eq.8.14 can be rearranged as follows:

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

The strain-rate tensor reads:

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

whereas its second invariant (in case of free divergence flows) assumes the following expression:

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

Renormalization (Randles & Libertsky, 1996, [167]) applies to the velocity derivatives in (7.17), only for 2D simulations:

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

The KTGF introduces the following definition for the frictional viscosity *fr* (Pa×s):

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

to obtain:

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

Eq.(7.20) is consistent with internal friction, as it does not depend on the magnitude of the strain-rate tensor.

In analogy to the Navier-Stokes equation (for incompressible flows), under the strong but accepted hypothesis of smooth spatial variations of fr, (7.20) provides:

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

which is valid in the “packing limit” of the KTGF (i.e. for *s* close enough to the value of 0.59, which is the maximum attainable volume fraction for a sheared inelastic hard sphere fluid, [103]). The model then defines the mixture total pressure *p* (Pa) as:

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

One may consider that the mean effective stress can only be formulated under simplifying assumptions (e.g., *x*, *y* and *z* need to be the principal axes). Thus,  is computed as the difference between the total pressure and the fluid pressure:

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

Both fluid and solid pressures are limited to positive values as soils, which are either fully saturated or dry, do not bear tension. Considering the continuity equation, the momentum equation for the mixture can be rearranged as:

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

where *εs,p* = ca.0.59 and H(x) is the Heaviside step function:

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

Assuming SPH conservative particles implies that the velocity of each phase is basically equal to the one of the mixture:

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

Considering (7.22) and the assumption of SPH conservative particles, (7.24) reduces to:

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

where the mixture viscosity ** is finally defined as:

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

and **(m2×s-1) is the mixture kinematic viscosity.

Following the multi-phase approach of [127], with the boundary treatment method proposed by [46], the SPH approximation of (7.27) becomes:

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

where *r* (m) is the distance between two interacting particles*,* whereas *M* (m2×s-1) stands for the artificial viscosity ([138]). The boundary value *uSA* (m×s-1) of the velocity in the external portion *Vh’* (m3) of the kernel support is assigned according to [46]. So far, the last term, representing the bottom drag, has been validated in 2D.

The artificial viscosity is always activated, both for approaching and separating particles (the latter configuration was not considered in Di Monaco et al., 2011, [46]):

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

Despite its formulation as a mono-phase mixture, the model needs to adopt a simplified approach to represent fluid pressure in the granular material. This parameter can be related to two different soil conditions: uniform fully saturated soil and uniform dry soil (the first condition being applied to all the test cases in this study):

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

where the subscript “*blt-top*” refers to the top of the bed-load transport layer (or the layer of saturated material). Eq.(7.31) assumes a 1D filtration flow parallel to the slope of the granular material. This simplifying hypothesis is still consistent with SPH conservative particles; radis the topographic angle at the top of the bed-load transport layer and lies between the local interface normal *nblt-top* and the vertical:

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

The angle limiter in (7.32) allows one to assign null *pf* values in case of slope anomalies (very rare and unstable).

The mixture pressure is computed by means of a barotropic equation of state (linearized around a reference state indicated by subscript “ref”):

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

It has been shown that the artificial speed of sound *c* (m/s) in the Weakly-Compressible approach should be at least 10 times greater than the maximum velocity to reduce the pressure error associated to artificial compressibility effects below 1% ([127]). A unique speed of sound can be chosen (i.e. the highest among the SPH particle values, no matter about their phase volume fractions).

In order to reduce the computational time and avoid the unbounded growth of (7.19), a threshold for the mixture viscosity can be defined (*max*). Mixture particles with a higher viscosity are considered in the elasto-plastic regime of soil deformation and are kept fixed, whereas their pressure is derived from the mixture particles flowing above them. The threshold value is assumed to be high enough not to influence the simulation. At a fixed time step, *max* does not influence even the computational time (the Courant-Friedrichs-Lewy *CFL* numbercriterion dominates over the viscous term criterion), if the following condition is satisfied:

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

It follows that the time step duration is more probably ruled by either the CFL stability criterion, if the spatial resolution is coarse enough, or the viscous term stability criterion, if the spatial resolution is fine enough. In this case, it might be convenient to adopt a multi-step approach, where the time integration of the equations of motion for the fluid particles would be obtained with a longer time step than the one needed for the mixture particles.

No-slip conditions are suggested to be imposed on solid walls for 2D simulations at very fine spatial resolutions. The associated solid boundaries are in general in contact with the bottom of the fixed bed, so the choice of a no-slip rather than a slip condition did not play any role. On the other hand, for 3D simulations imposing free-slip conditions is suggested. In fact, the depth of the granular material layer is generally high enough and the interactions with solid walls quite exclusively concern either fluid particles at high Reynolds number or mixture particles with null velocities, so that the choice of a slip condition everywhere appeared to be an appropriate compromise. Nevertheless, no-slip conditions should be in general applied to those mobile mixture particles which are interested by a locally laminar regime. This issue, which plays a minor role in the test cases of Amicarelli et al. (2017, [9]), represents a matter of on-going developments.

The present model does not need any tuning for the mixture viscosity. The only case-dependent numerical parameters refer to the spatial resolution (*dx*, *h*) and possibly to *CFL* number.

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:

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

The sound speed (*cref*) should be at least 10 times (Monaghan, 2005, [138] assumed *Cp,max*=2; 5 times *Cp,max* for higher pressure peaks) higher than the maximum velocity in the fluid (WC approach). This position (constant *AWC* equal to 10) provides a maximum relative error on density of 1%, whereas the assumption *AWC*=4.5 increases the density relative error to 5% (Monaghan, 2005, [138]).

The velocity scale *Uscale* reads:

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

where *Ymax* is the maximum water depth and  is the maximum absolute value of velocity (the maxima operate both over the whole simulated time and the whole 3D domain space).

In order to impose the initial pressure field for granular flows, a dynamic setup of hydrostatic conditions is suggested within the elasto-plastic layer because “mono-phase” hydrostatic conditions are instantaneously imposed.

One notices that *εs,p* is used in the balance equations of this model, but the value of *εs* at the initial conditions should respect the mass conservation of the mixture, which is not necessarily under the packing limit at the beginning of the simulations. Sometimes, the void ratio *ev* is available instead of the phase volume fractions. The mixture porosity is related to the void ratio by means of the following expression:

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

Under these circumstances, the initial density of the solid phase is assessed as function of the mixture specific weight, the porosity, the fluid density and the gravity acceleration:

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

* 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, [122]), 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, [208]) reads:

|  |  |
| --- | --- |
|  | (7.39) |

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

|  |  |
| --- | --- |
|  | (7.40) |

where ks is a roughness length scale with ks=3d50 as an approximation for ks=3d90. It is a local erosion criterion, thus roughness is computed locally, instead of adopting a formulation for bed forms ([121]).

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, [122]) and those associated to the similarity theory or the SNBL:

|  |  |
| --- | --- |
|  | (7.41) |

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:

|  |  |
| --- | --- |
|  | (7.42) |

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:

|  |  |
| --- | --- |
|  | (7.43) |

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:

|  |  |
| --- | --- |
|  | (7.44) |

*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, (7.44) 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:

|  |  |
| --- | --- |
|  | (7.45) |

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):

|  |  |
| --- | --- |
|  | (7.46) |

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:

|  |  |
| --- | --- |
|  | (7.47) |

The transversal slope angle ** is defined as:

|  |  |
| --- | --- |
|  | (7.48) |

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, [177]):

|  |  |
| --- | --- |
|  | (7.49) |

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, [143]) for a fluid flow around a sphere:

|  |  |
| --- | --- |
|  | (7.50) |

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

|  |  |
| --- | --- |
|  | (7.51) |

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:

|  |  |
| --- | --- |
|  | (7.52) |

where *zint* is the interface height. A formula for the lift coefficient is derived, by interpolating the experimental data of Seminara et al. (2002, [177]):

|  |  |
| --- | --- |
|  | (7.53) |

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:

|  |  |
| --- | --- |
|  | (7.54) |

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.

* 1. A simplified approach for soil liquefaction

This section refers to Amicarelli et al. (2016, [7]).

A simplified approach is implemented for soil liquefaction, by means of linearized pore pressure functions, depending on the critical number *N* of equivalent uniform cycles:

|  |  |
| --- | --- |
|  | (7.55) |

where the subscript “*nq*” represents “no-quake” conditions, *NL* the critical value of *N* (when liquefaction occurs) and *N*/*NL* is named cyclic number ratio.

In case the liquefaction time (*tliq*) is known and *fliq* is approximately linear, (7.55) becomes:

|  |  |
| --- | --- |
|  | (7.56) |

where *tq0* and *tqf* are the quake starting and ending times.

# The DB-SPH boundary treatment scheme

This section describes the “Discrete Boundary” (DB) - SPH method for boundary treatment (Amicarelli et al., 2013, [114]). 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: DB-SPH particle approximation and modifications of the balance equations (Sec.8.1); 1D Linearized Partial Riemann Solver (Sec. 8.2); semi-particle volume (Sec.8.3); DB-SPH inlet and outlet sections (Sec.8.4); shear stress boundary terms (Sec.8.5).

* 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, [57]) 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, [57]).

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, [57]):

|  |  |
| --- | --- |
|  | (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, [57]), 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, [125]), 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, [6]):

|  |  |
| --- | --- |
|  | (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.

* 1. Shear stress boundary terms

This section refers to Amicarelli et al. (2016, [7]), whose reading is suggested for further details.

The shear stress boundary terms of Ferrand et al. (2013, [57]) are adapted to treat mobile frontiers and integrated in the boundary treatment scheme of Amicarelli et al. (2013, [6]). Such a scheme is potentially suitable to represent the bottom drag between saturated granular material and a base rock, even during an earthquake.

The boundary terms above appear in the Right Hand Side of the momentum equation and are due to both surface wall elements and semi-particles. In the first case, one obtains:

|  |  |
| --- | --- |
|  | (8.13) |

where ** is the integral Shepard coefficient and n the normal to any wall surface (neighbouring) element “*a*” of area *a*.

Considering the derivation chain rule, one obtains:

|  |  |
| --- | --- |
|  | (8.14) |

Once provided the similarity law of the viscous sub-layer, aligned the friction velocity vector with fluid velocity close to wall and assumed mobile frontiers, one can write:

|  |  |
| --- | --- |
|  | (8.15) |

where *d0* is the distance between the computational particle and the surface wall element.

Assuming a continuous field for the shear stress, the last term of (8.15) can be expressed as a SPH approximation and normalized by the discrete Shepard coefficient (**):

|  |  |
| --- | --- |
|  | (8.16) |

Thus, the shear stress boundary terms due to the surface wall elements are:

|  |  |
| --- | --- |
|  | (8.17) |

The analogous term due to the semi-particles “*s*” reads:

|  |  |
| --- | --- |
|  | (8.18) |

# Time integration schemes (Leapfrog, Euler, Heun)

Time integration for both fluid and solid body particles is ruled by a second-order Leapfrog scheme (refer to [212] for stability analysis and time integration schemes in SPH modelling), as described in Amicarelli et al. (2015, [7]) and Di Monaco et al. (2011, [46]):

|  |  |
| --- | --- |
|  | (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).

Time integration is constrained by the following stability criteria:

|  |  |
| --- | --- |
|  | (9.5) |

where *dt* (s) is the time step duration and *CFL* the Courant-Friedrichs-Lewy number. Following [1], the viscous term stability parameter is set to *C*=0.05.

An a-priori estimation of the elapsed time (*te*) can assume the following form:

|  |  |
| --- | --- |
|  | (9.6) |

where *D* is thedomain dimensionality and *A* varies from 1 to 2.

Under the simplifying hypothesis that the particle system of equations are independent, one obtains (at a fixed time step duration):

|  |  |
| --- | --- |
|  | (9.7) |

In case all the time steps are ruled by the *CFL* criterion, then *A*=1 and the following relationships are valid (at a fixed number of particles):

|  |  |
| --- | --- |
| thus | (9.8) |

In case all the time steps are ruled by the stability criterion on the viscous term, then *A*=2 and the following relationships are valid (at a fixed number of particles):

|  |  |
| --- | --- |
| thus | (9.9) |

In order to understand which stability criterion dominates, one considers the following ratio:

|  |  |
| --- | --- |
|  | (9.10) |

Provided a time step, if the ratio (9.10) is greater than 1, then the *CFL* criterion dominates. Otherwise, the viscosity stability criterion dominates.

When the *CFL* criterion dominates, the maximum viscosity has never any effect on *dt* if this condition is respected:

|  |  |
| --- | --- |
|  | (9.11) |

The elapsed time also depends on the global specific surface of the fluid domain. The highest the latter, the lowest the first. The global specific surface of the fluid domain is related to the mean number of neighbouring particles.

# The substation-flooding damage scheme

A substation-flooding damage model is presented and integrated in SPHERA (Amicarelli et al., 2018, [3]). The model distinguishes the damage due to power outages from the damage to the components of the electrical substations.

Considering the power outages (blackout events), a vulnerability and “proxy” damage (in time units, not in monetary units) model is presented. This assumes, as a simplifying hypothesis of no redundancy of the electric grid, that the failure of an electrical substation triggers a blackout event in a grid branch (no matter about its length and connections). The assessment of the overall vulnerability of the electric grid and the global damage (in monetary units) due to flood-related blackout events is out of the targets of this code version and needs the following elements: the coupling of the present model with a power grid model; the maps of the exposed population, the values of the public (also environmental) and private goods, the activities affected by the blackout and their flood-related vulnerability curves. On the other hand, considering the components of the electrical substations, a complete (direct and tangible) damage model is presented.

The substation-flooding damage model estimates the following physical quantities, at every electrical substation: the Probability of a power Outage Start (*POS*) as function of the maximum substation water depth; the Expected power Outage Status (*EOS*), at the level of the single electrical substations (in the absence of power grid redundancy); Expected Outage Time/duration (*EOT*, s); the flood-related vulnerability and damage (euros) limited to the components of the electrical substations.

* 1. Mathematical models

The mathematical models of the substation-flooding damage scheme separately considers both blackout events (Sec.10.1.1) and the components of the electrical substations (Sec.10.1.2).

* + 1. Proxy damage and vulnerability to flood-induced blackout events, in the absence of redundancy (at the level of the single electrical substations)

A proxy damage quantifies in time units (not in monetary units) the damage due to blackout events triggered by substation flooding. One assumes that the malfunction of a substation determines a blackout event in a branch of the power grid (simplifying hypothesis of no redundancy).

The breakdown in the electrical energy supply is analysed only considering the power outage events and neglecting the damage due to brownouts (voltage drops).

The Probability of an Outage Start (*POS*) (i.e. the probability of triggering a blackout event) at a fixed time is smaller than (or equal to) the probability of occurrence of a blackout event at the same time (*EOS*, “Expected Outage Status”) because the latter also depends on the blackout events which might start previously.

The procedure of HAZUS-MH (2011, [86]) considers a threshold water depth of *Yth*=1.2m for blackout events associated with the flooding of electrical substation. However, the above procedure does not mention neither data nor the method to elaborate them. Holmes (2015, [88]) explains that the above threshold value is overestimated. In particular, the majority of the UK electrical substations has shown a threshold of *Yth*=0.30m (Crawford & Seidel, 2013,[39]). Considering this value and a maximum threshold of *Yth,max*=0.50m, Holmes (2015, [88]) provides a linear relationship between the probability of an Outage Start and water depth, here assumed as spatial average over the territory belonging to the electrical substation (*Ysub*, m):

|  |  |
| --- | --- |
|  | (10.1) |

The above relationship has been validated on other open-field data (Holmes, 2015, [88]).

The “Expected Outage Status” is defined as a binary variable which represents either the expected presence (*EOS*=1) or the expected absence (*EOS*=0) of a blackout event at a fixed time, at the level of the single electrical substation:

|  |  |
| --- | --- |
|  | (10.2) |

*EOS* is unity if at least once, during the period before the on-going time (*t*=*t\**) lasting the restoration time of the electrical infrastructures (t*rei,e*), *POS* is greater than 0.5.

The values of t*rei,e* are commonly greater for smaller substations with less redundancy. This characteristic time has been quantified by several authors: Chow et al. (1996, [35]) report the interval *trei*=0’-500’; Maliszewski & Perrings (2012, [122]) suggest an average value of *trei,e*=99’ and a maximum value of *trei,max*=330’. Both the above references consider a typical value of *trei* smaller than two hours. However, their analyses only consider blackout events under normal (non-extreme) environmental conditions. Reed (2008, [168]) proposes to use a particular realization of the “gamma” probability density function, for *trei* on blackouts induced by intense meteorological and flood events.

Considering a null minimum value and a maximum value (under the worst hypothesis) of 22 hours (95th percentile of the “gamma” distribution of Reed -2008, [168]-), the present model assumes an expected restoration time of 11 hours (*trei,e*=39’600s), in the absence of further data and in favour of safety.

The system (10.1)-(10.2) represents a formulation of the vulnerability of the single electrical substation to the flood-induced blackout events, in the absence of redundancy.

The “Expected Outage Time” (*EOT*, s) is here defined as the expected cumulated duration of the sub-periods of blackout:

|  |  |
| --- | --- |
|  | (10.3) |

where *∆t* is the model time step duration. The subscripts “*0*”, “*f*” and “*i*” represent initial conditions, final conditions and a generic time step, respectively. A blackout event can involve several interruptions and the following relationship is assumed: *EOT*≥*trei,e*. Eq.(10.3) represents a formulation of the “proxy” damage (quantified in time units) due to flood-induced blackout events, in the absence of redundancy(at the level of the single substations).

* + 1. Flood-induced damage to the components of the electrical substations

This mathematical model assesses the (direct and tangible) damage induced by floods to the components of the electrical substations (*Dsub*). This damage model is complete as it quantifies both vulnerability and damage (the latter in monetary units):

|  |  |
| --- | --- |
|  | (10.4) |

The value of the electrical substations (*Va,sub*) can be expressed in US dollars (HAZUS-MH, 2011, [86]):

|  |  |
| --- | --- |
|  | (10.5) |

but SPHERA works in euros (currency exchange rate of February 2018):

|  |  |
| --- | --- |
|  | (10.6) |

*Vu,sub* is the vulnerability of an electrical substation with respect to the (direct and tangible) flood-induced damage involving the substation components. This model provides a regression curve (6th degree polynomial function) for *Vu,sub*, after elaboration of the point values reported by HAZUS-MH (2011, [86]):

|  |  |
| --- | --- |
|  | (10.7) |

where the maximum value of the substation water depth *Ysub,max* refers to the period simulated until the on-going time (*t*=*t\**). The regression procedure provides the following constants: *a*=-1.22877·10-6m-6, *b*=1.92478·10-5m-5, *c*=8.4216·10-6m-4, *d*=-0.00119121m-3, *e*=0.00390726m-2, *f*=0.0170243m-1.

* 1. The numerical models

The numerical models of the substation-flooding damage scheme discretize the mathematical models of Sec.10.1. At the beginning of the simulation the following procedures are executed:

* identification of the DEM vertices internal to the polygons (representing the electrical substations in plan view);
* assessment of the areas of the above polygons (represented by triangles, quadrilaterals, pentagons and hexagons);
* initializations of the variables of the electrical substations.

At the end of each output writing time step of the damage model, the following procedures are executed for every electrical substation:

* assessment of the variable *Ysub* as spatial average of the water depth values at the DEM vertices within the polygon of the electrical substation;
* update of the variable *Ysub,max*;
* assessment of the variables *POS* and *EOS*;
* update of the variables *EOT*, *Dsub* and*Vu,sub*;
* writing of the output file for the vulnerability and damage variables.

The water depths at the DEM points are saved and stored until the following time step.

As an example, the map of the Italian electrical stations, substations and transmission lines is available at MATTM (2018, [133]). It is useful to activate the layer of OpenStreetMap and the “aerial view” of Bing to detect the electrical stations (squares), substations (polygons) and transmission lines (lines), as well as the electricity pylons (nodes/points). Contrarily, the feature “Atlarete Linee” seems more imprecise (some symbols of the electrical stations would represent electricity pylons; the electrical substations do not seem to represent the nodes of the transmission power grid).

# The modelling chain

An overview of the numerical modelling chain of SPHERA is reported in Figure 11.1.

Published at the end of 2014, the dataset SRTM3 (USGS, [192]) provides a repository of DEM (“Digital Elevation Models”) with an almost global cover and spatial resolution of 1” (in terms of geographical coordinates) or ca.31m (maximum/coarser spatial resolution in terms of cartographic coordinates). With respect to the former free DEM datasets (finest spatial resolution of 3”), SRTM3 has permitted a relevant improvement in using Open-Access DEM. The SRTM3 products are available in the format “.tif”. Considering its global coverage, SRTM3 provides a root-mean-square error on heights of ca.6m, even though the error kurtosis is very high ([170]). However, these estimations refer to almost the whole terrestrial surface, included the high-latitude regions where errors are definitely higher.

The software tool GDAL (OSGEO, [65]), the main QGIS library, can be used as an independent code. In the frame of the present modelling chain, GDAL allows to convert the DEM file format “.tif” in the alternative format “.dem”.

DEM2xyz (RSE SpA, [39]) reads the DEM file (“.dem” format), converts the geographic coordinates in Cartesian coordinates over a regular grid and writes the resulting DEM on an output file (“.xyz” format), possibly coarsening the spatial resolution.

Paraview (Kitware, [153]) reads the “.xyz” output file of DEM2xyz and elaborates a 2D Delaunay grid starting from the DEM vertices. Paraview also allows to cut the numerical domain (the cuts have to be far enough from the water bodies not to disable the procedures to extrude the water bodies from the DEM), circumscribes the water bodies, draws the possible filing/digging regions, detects the dam toe and the most upstream point over the coastline of the water bodies.

The above information, derived by Paraview, is transferred over the main input file of DEM2xyz, which is executed again to modify the already computed DEM, by reconstructing the bathimetry below the water bodies and the possible assignation of the digging/filling regions (uniform height within the same region), after a verification/modification on the normal vectors to the surface elements of the DEM. At this point, Paraview is used again to draw those geometrical figures which are necessary to initialize some variables in the main input file of SPHERA, in order to detect water bodies, earth-filled dams and monitoring elements.

The numerical tool ply2SPHERA\_perimeter (RSE SpA, [160]) converts the DEM “.ply” file in two distinct output files. They have the same format as the sections “VERTICES” and “FACES” of the main input file of SPHERA. It is the vertices and faces of the portion of the DEM within the numerical domain of SPHERA.

In case the boundary treatment method of Sec.8 is used, SnappyHexMesh (OpenFOAM, OpenCFD Ltd, [153]) is used as a surface grid generator for the initial positioning grid of the DB-SPH elements.

Once the sections “VERTICES” and “FACES” are obtained from ply2SPHERA\_perimeter and the input file for the positioning surface grid is produced by SnappyHexMesh, one completes the remaining sections of the main input file of SPHERA.

This 3D CFD-SPH code is executed to simulate the propagation of floods in non-stationary regime with transport o granular material and solid bodies (the other application fields the code has been applied to are: fast landslides, sea waves; sloshing fuel tanks; hydroelectric plants).

The output files of SPHERA which contain the profiles (1D) of the fluid dynamics variables are visualized by means of Gnuplot (Williams & Kelley, [69]), which returns the output file in the “.eps” format. These files are read by GSView (Ghostgum Software Pty Ltd, [79]) and converted in the “.png” format. The profiles simulated are compared with the analogous experimental (or numerical) profiles available from experimental images or the scientific literature (indexed journals; Open-Data archives). In these cases it is normally admitted the digitization of experimental

|  |
| --- |
|  |

Figure 11.1. FOSS / Freeware / Open-Data tools of the modelling chain for SPHERA.

and numerical profiles from published sources by means of Engage Digitizer (Mitchell et al., [48]), with proper citation of the source, in order to validate the code.

The output files of SPHERA which contains the synthetic fluid dynamics fields need a following elaboration by means of Grid Interpolator (RSE SpA, [79]).

Paraview shows the (2D and 3D) fluid dynamics fields produced by SPHERA and returns the associated image files. These are concatenated in “.gif” animations by means of Image Magick (ImageMagick Studio LLC, [90]). The compression of these animations, necessary in case the concatenation involves many files, is carried out by means of Virtual Dub ([213]), which returns an “.avi” video output file.

The RSE tools of the present numerical chain (i.e. SPHERA, DEM2xyz, ply2SPHERA\_perimeter, Grid Interpolator) are developed by means of a series of numerical tools: gedit (GNOME Foundation, [66], text editor), gfortran (GNU, Free Software Foundation, [69]; Fortran compiler), gmake (GNU, Free Software Foundation, [72]; for the Makefile execution), gdb (GNU, Free Software Foundation, [66]; debugger), gprof (GNU, Free Software Foundation, [76]; profiler for scalar executions), Valgrind (Valgrind Developers, [204]; memory management tool), Scalasca (Forschungszentrum Jülich & TU Darmstadt, [173]; code profiler for OMP executions). The RSE tools are developed and distributed with no charge by means of Git (Torvalds et al., [69]; main “Distributed Version Control System” -DVCS-) and GitHub (GitHub Inc, [70]; main platform for Git-managed software).

The numerical modelling chain is based on free tools: FOSS, freeware or OpenData.

FOSS tools are defined as “Free/Libre and Open-Source Software” by the Free Software Foundation ([62]). The FOSS tools of the modelling chain are: gedit, gfortran, gmake, gdb, gprof, Valgrind, Scalasca, Git, GDAL, Paraview, DEM2xyz, SnappyHexMesh, ply2SPHERA\_perimeter, SPHERA, Grid Interpolator, Image Magick, Gnuplot, Engage Digitizer, Virtual Dub.

“Freeware” tools are simply free software. Two freeware tools are used in the reference modelling chain: GitHub (for public repositories) and GSView.

“Open-Data” tools are databases available upon public and free access like SRTM3, which belongs to the modelling chain.

The FOSS tools gfortran, gprof and Scalasca can be possibly replaced with more effective codes such as: ifort (Intel Corporation, [91]; Fortran compiler); idb (Intel Corporation, [91]; Fortran debugger); cpuinfo (Intel Corporation, [91]; code profiler for OMP executions); ITAC, Trace Analyzer and VTUNE (Intel Corporation, [91]; code profiler for OMP/MPI executions); Advisor (Intel Corporation, [91]; profiler for executions with code vectorization); TotalView (Rogue Wave Software, [199]; code debugger for parallel executions). Analogously, it is possible to support or replace the other elements of the modelling chain with more effective software, if available (e.g., a DEM with finer spatial resolution).

The replacement of a free tool with a proprietary tool (available with charge) is normally a reversible procedure which does not alter the functioning of the modelling chain.

# Developer guide

The developer guide is represented by the following sub-sections: a synthetic description of the program units (Sec.12.1); the style formatting (Sec.12.2); the modifications with respect to SPHERA v.8.0 (Sec.12.3).

* 1. SPHERA v.9.0.0: synthetic description of the program units

The following sub-sections briefly describe all the program units of SPHERA v.9.0.0, 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 12.1).

* + 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 12.2).

* + 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 12.3).

* + 1. Program units for the transport of solid bodies

The folder “Body\_Transport” contains the program units exclusively dedicated to the transport of solid bodies (Amicarelli et al., 2015, [7]; Table 12.4).

* + 1. Program units for the constitutive equation

The folder “Constitutive\_Equation” contains the program units for the constitutive equation (Table 12.5; Amicarelli et al., 2017, IJCFD).

|  |  |
| --- | --- |
| **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). |
| 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 12.1. Program units for the boundary conditions of the inlet/outlet sections (“BC”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| CalcPre | Particle pressure estimation. |
| Continuity\_Equation | To accumulate contributions for the 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 12.2. Program units for the continuity equation (“BE\_mass”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **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). |
| velocity\_smoothing | To calculate a corrective term for velocity. |
| velocity\_smoothing\_SA\_SPH\_2D | To calculate a corrective term for velocity. |
| velocity\_smoothing\_SA\_SPH\_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 12.3. Program units for the momentum equation (“BE\_momentum”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **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 12.4. Program units for the transport of solid bodies in free surface flows (“Body\_Transport”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| mixture\_viscosity | To compute the frictional viscosity and the mixture viscosity for dense granular flows (KTGF packing limit). (Amicarelli et al., 2017, IJCFD) |
| Viscapp | Constitutive equation with tuning parameters (validated in Manenti et al.,2012,JHE) |

Table 12.5. Program units for the constitutive equation (“Constitutive\_Equation”; SPHERA v.9.0.0).

* + 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, [6]; Table 12.6).

* + 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, [122]) and its further developments (Table 12.7).

* + 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 12.8).

|  |  |
| --- | --- |
| **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\_BC\_shear\_viscosity\_term | Computation of the contributions to the numerator of the boundary shear viscosity term in DB-SPH-NS. |
| 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). |
| DBSPH\_velocity\_gradients\_VSL\_SNBL | Computation of the velocity gradients in the Viscous Sub-Layer of the Surface Neutral Boundary Layer. The gradients are used in the DB-SPH BC shear viscosity term (DB-SPH-NS). For wall elements, the numerator and the denominator (wall element Shepard coefficient without contributions from semi-particles) are updated independently. Their ratio is computed in "DBSPH\_BC\_shear\_viscosity\_term": here are summed their contributions. To compute the kinematic viscosity of the semi-particles (before Shepard correction). Contributions to the discrete Shepard coefficient of wall elements depending on fluid particles (not on semi-particles). |
| drafts | Wall element contributions for Monaghan artificial viscosity term. |
| 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. |
| 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 12.6. Program units for the boundary treatment scheme DB-SPH

(“DB\_SPH”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **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. |
| drafts | Mohr-Coulomb 2D erosion criterion (Manenti et al., 2012, JHE). Shields erosion criterion works better (Manenti et al., 2012, JHE). |
| 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). |
| 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 12.7. Program units for the erosion criterion (“Erosion\_Criterion”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| area\_hexagon | Computation of the area of a generic hexagon from the coordinates of its vertices. |
| area\_pentagon | Computation of the area of a generic pentagon from the coordinates of its vertices. |
| 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\_convex\_non\_degenerate\_polygon | Test to evaluate if a point lies inside or strictly outside a polygon. A point is internal to the polygon if its distances from the lines passing for the polygon sides (no matter about the number of sides, but they must be taken in either a clockwise or an anti-clockwise order), have all the same sign of a generic polygon vertex not belonging to the selected side -a null distance is always a positive test for internal points-). The maximum number of polygon sides is now equal to 6 (triangles, quadrilaterals, pentagons and hexagons can be treated). Polygons must be convex and non-degenerate (a n-side polygon should have n vertices, not more). |
| point\_inout\_hexagon | Test to evaluate if a point lies inside or strictly outside a generic hexagon. The hexagon is partitioned into 4 triangles (P1P2P6,P2P5P6,P2P3P5,P3P4P5). A point is internal to the hexagon if it is internal to one of its triangles. |
| point\_inout\_pentagon | Test to evaluate if a point lies inside or strictly outside a generic pentagon. The pentagon is partitioned into 3 triangles (P1P2P5,P2P3P5,P3P4P5). A point is internal to the pentagon if it is internal to one of its triangles. |
| point\_inout\_quadrilateral | Test to evaluate if a point lies inside or strictly outside a generic quadrilateral. The quadrilateral is partitioned into 2 triangles (P1P2P3,P1P3P4). A point is internal to the quadrilateral if it is internal to one of the triangles. |
| 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\_axis\_angle | Provided 2 vectors, this subroutine computes the rotation axis and the rotation angle which allow rotating from the unit vector aligned with the first vector to the unit vector aligned with the second vector. |
| vector\_rotation\_Euler\_angles | 3D rotation of a given vector, provided the vector of Euler's angles (3D). |
| vector\_rotation\_Rodrigues | 3D rotation of a given vector, provided the rotation axis and the rotation angle, based on Rodrigues formula. |

Table 12.8. Program units on Geometry (“Geometry”; SPHERA v.9.0.0).

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

The folder “IC” contains the program units on the management on the initial conditions (Table 12.9).

* + 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 12.10).

|  |  |
| --- | --- |
| **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). |
| 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. |
| SetParticleParameters | Setting initial particle parameters. |
| SetParticles | Particle coordinates (initial conditions). |
| SubCalcPreIdro | Hydrostatic pressure profiles (in case they are imposed as initial conditions). |

Table 12.9. Program units for the initial conditions (“IC”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **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 12.10. Program units for the main algorithms (“Main\_algorithm”; SPHERA v.9.0.0).

* + 1. Modules

The folder “Modules” contains the Fortran modules of SPHERA v.9.0.0. (Table 12.11).

* + 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 12.12).

* + 1. Program units for post-processing

The folder “Post\_processing” contains the program units to post-process the code results (Table 12.13). 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;
* 3D 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”).

Monitor interpolations should take into account the influence of SA-SPH frontiers in the program unit “interpolations\_for\_monitoring\_element”. However, it is cumbersome to perform a SA-SPH neighbouring search starting from a point (not a particle): it would be smarter (despite the approximation) to find the closest fluid particle, consider its SA-SPH neighbouring frontiers and interpolate (as for partial smoothing). Instead, a simpler solution is implemented:

* while assessing contributions to the interpolation for the monitoring element from fluid particles, find the closest fluid particle within the kernel support of the monitoring element;
* at the end of the program unit, if the possible closest fluid particle has neighbouring SA-SPH frontiers, then the interpolation are replaced by this particle value, else keep the interpolation. It seems smarter to refer to the closest fluid particle as the particle values are already representative of their kernel support.

SPHERA returns the time series of the maximum height (file “.plb”) and the minimum height (file “.zlft”) of the free surface. The latter represents the position of the lowest water-air interface, along a generic vertical monitoring line. This quantity seems proper to assess the water depth, obtained after difference with the height of the underlying solid surface. The algorithm searches in the positioning grid the lowest height of the free surface (from the bottom towards the top of a monitoring line) and stops at the first positioning cell which is empty and has at least one cell filled of water below (along the vertical). The filtering procedure is based on pinpointing air masses between portions of liquid along a vertical monitoring line. This procedure might be improved integrating an additional control on the possible detachment between the lowest portion of the local liquid sub-domain and the underlying solid surface.

* + 1. Program units for pre-processing

The folder “Pre\_processing” cntains the program units (Table 12.14) to pro-process the input files of SPHERA, which are:

* main input file (“.inp” format is defined in SPHERA v.9.0.0; 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\_file\_module | Module for I/O. |
| 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 12.11. Fortran modules (“Modules”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **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. |
| w | kernel function |

Table 12.12. Program units for the neighbouring search, the smoothing operators and the interface detection (“Neighbouring\_Search”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| calc\_pelo | Post-processing to write the free surface height. |
| CalcVarp | To calculate physical quantities at a monitoring point. |
| cat\_post\_proc | To concatenate the ".txt" output files and remove the original ones. |
| CreateSectionPoints | Minor program unit |
| electrical\_substations | output assessment and writing for electrical substations (only in 3D). Output (time series): Probability of an Outage Start (POS), Expected Outage Status (EOS), Expected Outage Time (EOT, time series update of its expected scalar value), Damage to the Substation Beyond Outage (Dsub, time series update of its expected scalar value), Substation Vulnerability (Vul). Output depends on Ysub (spatial average of the fluid/mixture depth at the DEM grid points, within the substation polygon). |
| GetVarPart | Getting particle values. |
| interface\_post\_processing | Post-processing the interfaces for bed-load transport phenomena. |
| 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 | To print 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 12.13. Program units for post-processing (“Post\_processing”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **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 12.14. Program units for pre-processing (“Pre\_processing”; SPHERA v.9.0.0).

|  |  |
| --- | --- |
| **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 12.15. Program units for the boundary treatment scheme SA-SPH (“SA\_SPH”, SPHERA v.9.0.0)

|  |  |
| --- | --- |
| **Program unit** | **Synthetic Description** |
| Euler | Explicit RK1 time integration scheme (Euler scheme). |
| Heun | Heun scheme: explicit RK2 time integration scheme. |
| time\_step\_duration | Computation of the time step duration (dt) according to stability constraints (CFL condition, viscosity term stability criterion, interface diffusion criterion -not recommended-). Plus, a special treatment for Monaghan artificial viscosity term and management of low-velocity SPH mixture particles for bed-load transport phenomena. |
| stoptime | Stopping time. |
| time\_integration | Explicit Runge-Kutta time integration schemes |
| time\_integration\_body\_dynamics | Euler time integration for body transport in fluid flows. |

Table 12.16. Program units for time integration (“Time\_integration”; SPHERA v.9.0.0).

* + 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, [46]; Table 12.15).

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

Three minor program units are implemented to manage Fortran character variables: “GetToken” and “lcase” (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 12.16).

* 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.

* 1. Modifications with respect to SPHERA v.8.0

Hereafter is reported the list of modifications of SPHERA v.9.0.0, with respect to SPHERA v.8.0, according to git format.

commit de264ca645593d9a4c3a6acc41b7c204e4d088b8

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Aug 3 12:19:36 2018 +0200

Minor modifications.

commit 75f50318377f954661da8de607e7e22693215902

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Aug 3 10:33:56 2018 +0200

Minor modifications.

Folders "bin", "debug", "debug\_omp": executable files of SPHERA v.9.0.0 are

available.

commit 8f786fe307de381ddfcf76d1fecbecbc73afe182

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Aug 1 12:13:29 2018 +0200

Minor modifications. Input. Modifications on the following test cases:

"db\_squat\_obstacle.inp"; "db\_body\_exp\_UniBas.inp".

commit b6bbfc2c18b584981cfa3f6448f520fdcef58c61

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Jul 25 10:04:45 2018 +0200

Modifications in progress for the release version SPHERA v.9.0.0.

Input. New and updated tutorials for SPHERA v.9.0.0.

Postprocessing. “\*wall\_IDs\*” files and “\*wall\_regions\*” files are

concatenated (subroutine "cat\_post\_proc").

Pre-processing. Bug fixed on 2D restart: arrays “GCBFVector” and

“GCBFPointers” only work in 3D.

commit abf4371b9e3032f53b7a143a5f3d7ebfaf82ac1b

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Apr 4 16:07:56 2018 +0200

SPHERA v.9.0.0.

Version update in the program unit labels. Version string update for the

input file check ("static\_allocation\_module.f90"). The Makefile is ready for

a free optimized gfortran execution. Update of the description on the major

numerical developments of the code.

commit 3e5b2fa8c5f4aef0fd6277d4565767a1ec845f4e

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Apr 3 11:33:50 2018 +0200

Minor modifications.

Input. Tutorial: "Alpe\_Gera\_dbf\_Lanzada\_substations" .

commit b3e92d3ab826955c61f187974950463c5697e14c

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Mar 14 08:51:55 2018 +0100

Minor modifications.

Documentation. Appendix update. Bulk modulus assignment.

commit 61ba5309eb85e2157ba8a2d1a768fbe800e96fac

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Mar 5 16:00:50 2018 +0100

Minor modifications.

Input. New tutorials: "SPH\_udb\_Kim2015JH\_scenario1\_dx\_0\_025m\_gate.inp",

"SPH\_udb\_Kim2015JH\_scenario1\_dx\_0\_025m\_no\_gate.inp",

"SPH\_udb\_Kim2015JH\_scenario1\_dx\_0\_050m\_gate.inp",

"SPH\_udb\_Kim2015JH\_scenario1\_dx\_0\_050m\_no\_gate.inp",

"SPH\_udb\_Kim2015JH\_scenario2\_dx\_0\_025m\_gate.inp",

"SPH\_udb\_Kim2015JH\_scenario2\_dx\_0\_025m\_no\_gate.inp",

"SPH\_udb\_Kim2015JH\_scenario2\_dx\_0\_050m\_gate.inp",

"SPH\_udb\_Kim2015JH\_scenario2\_dx\_0\_050m\_no\_gate.inp".

commit 97320bc16e12849638ed13405efbab7c7d1ec427

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Feb 26 17:29:14 2018 +0100

Minor modifications.

Post\_processing. Fix on the subroutine "electrical\_substations.f90" for

restarted simulations.

commit 646d653b0b4edb8fbb0dd42d7941fd1770e2dfa1

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Feb 22 14:59:48 2018 +0100

Minor modifications. Post\_processing. Fix on the formula for vulnerability in

the program unit "electrical\_substations.f90".

commit a71647aea6ca74cfb758364678db78e622d8c659

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Feb 21 17:35:05 2018 +0100

Minor modifications.

commit bc6339cfb892d6536d86e87e9b1ffa56475731b9

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Feb 19 12:00:10 2018 +0100

Minor modifications.

Post\_processing. Subroutine "cat\_post\_proc.f90": fix on substations.

commit 6b21ef95d1dbfb14156909a629d5772d07617460

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Feb 16 18:09:04 2018 +0100

Minor modifications.

Post\_processing. Subroutine "cat\_post\_proc.f90": fix on substations.

Post\_processing. Subroutine "electrical\_substations.f90": iterative

allocation and deallocation checks are not written anymore.

commit 31a8cb6398a413a8654a9396934cb093c8dc4d30

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Feb 16 13:19:35 2018 +0100

Minor modifications.

Pre\_processing. A generic vertex of any electrical susbtation only needs 2

coordinates.

commit 18b5258f2a5b4fa39d9a2b5c46ac6bfe109aeb06

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Feb 15 16:27:15 2018 +0100

Minor modifications.

Geometry. New program units (after compilation): “area\_hexagon”,

“area\_pentagon”.

Post\_processing. New functionality to monitor electrical substations. New

program unit (after compilation): “electrical\_substations”.

Post\_processing. Z\_fluid\_step now belongs to the module

"Dynamic\_allocation\_module" as "Z\_fluid\_max".

Pre\_processing. New program unit (after compilation): “ReadSubstations”.

Input. New/updated tutorials: "Alpe\_Gera\_dam\_break\_no\_volume\_correction.inp",

"Alpe\_Gera\_dam\_break\_no\_volume\_correction\_flood\_control\_dam.inp",

"Alpe\_Gera\_dam\_break\_volume\_correction.inp",

"Alpe\_Gera\_dam\_break\_volume\_correction\_flood\_control\_dam.inp",

"Alpe\_Gera\_double\_dam\_break\_no\_volume\_correction.inp",

"Alpe\_Gera\_double\_dam\_break\_volume\_correction.inp",

"ICOLD\_dam\_breach\_trunks.inp", "dam\_breach\_ICOLD\_DB-SPH\_BD.inp",

"edb\_2D\_FraCap02.inp", "edb\_2D\_FraCap02\_Taipei.inp", "edb\_2D\_Spi05.inp",

"edb\_ICOLD.inp", "edb\_KarlSand.inp", "edb\_Pon10.inp",

"rectangular\_side\_weir\_Fr\_0\_491.inp", "wave\_motion\_for\_WaveSAX.inp".

commit 98cee1d8218c2a09e70a8d396f7607a7dae48e67

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Nov 27 11:22:37 2017 +0100

Minor modifications.

commit 94a99094f1d798e143eaa6f25acb7ad0fa58bbff

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Sep 5 17:22:23 2017 +0200

Minor modifications.

SA\_SPH. An omp critical section is inserted in the program unit

“ComputeBoundaryDataTab”. The omp critical section “omp\_FBCE3D” of the

program unit “FindBoundaryConvexEdges3D” is extended.

Main\_algorithm. The omp critical sections “omp\_Ncbf\_Max” and

“omp\_Ncbf\_Max\_2” are inserted in the program unit “Loop\_Irre\_3D”.

commit ef8db5888fb2b76c7c62e6c55b1050a78b61cccc

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Sep 5 09:57:23 2017 +0200

Minor modifications.

BC. Program unit "CancelOutgoneParticles\_3D". The computation of a

line-plane intersection is corrected.

BC. Some omp critical sections are defined in the program units

"CancelOutgoneParticles\_3D" and "CancelOutgoneParticles\_2D".

Post\_processing. The free surface detected by the monitoring lines is

increased of dx/2 to consider that the free surface is located at the

edge (dx/2 over the particle barycentre) of the detected particles.

Time\_integration. The new program unit “time\_step\_duration” merges the old

program units “inidt2” and “rundt2”.

BE\_mass. The new program unit “Continuity\_Equation” merges the old program

units “inter\_EqCont\_3D” and “inter\_EqCont\_2D”.

BE\_momentum. The new program units “velocity\_smoothing”,

“velocity\_smoothing\_SA\_SPH\_2D” and “velocity\_smoothing\_SA\_SPH\_3D” merge

the old program units “inter\_SmoothVelo\_2D” and “inter\_SmoothVelo\_3D”.

Obsolete program units. The following obsolete program units are removed:

“I\_O\_ENG\_module”, “I\_O\_ITA\_module”, “I\_O\_language\_module”,

“SearchforParticleZone\_3D”, “ltrim”.

commit 3e57ac797faf6b48d16735db4f39f711b25c7eac

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Jun 13 15:39:10 2017 +0200

Minor modifications.

Documentation files. Sliding friction and normal reaction forces. On the

overall normal of the neighbouring frontiers.

commit 8b4a7d025d7b9fc4c3a11e25806fc9bc378e1589

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Jun 13 15:17:45 2017 +0200

Minor modifications.

Body transport. Dry stage (no neighbouring fluid particles) of body-frontier

interactions. Explicit formulation for the sliding friction force,

depending on the friction angle between the computational body and the

neighbouring frontier. The direction of the sliding friction force is the

opposite to the velocity direction of the centre of mass of the

computational body (projected on the local DEM plane). Present

approximations: a unique friction angle applies to all the body-frontier

interactions; the vector sum of the normal reaction force under sliding

and the sliding friction force provide no contribution to the body torque

(nevertheless the limiter for the sliding friction force depends on the

velocity of the solid particles interacting with the frontiers). In case

the input friction angle is negative, then sliding friction depends on

the local slope/interface angle (this always applies for body-body

interactions).

commit bf6ec5499859e874649a888007dfd2ac0255abcb

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri May 26 17:15:41 2017 +0200

Minor modifications.

Bug fixed. Post-processing. On the initialization of the arrays q\_max and

Z\_fluid\_max in a restarted simulation.

commit 5987d6bac30af5d8f29066e3c3f419bbf662f9b0

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue May 23 15:45:28 2017 +0200

Minor modifications.

SA-SPH. Input variable “laminar\_no-slip\_check” to enable/disable the local

check on the laminar regime to eventually activate no-slip conditions.

Formerly, “laminar\_no-slip\_check” was implicitely “.true.”.

commit cf90bc47da1f6ca87980d920b5621d13b5ee5b4c

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue May 23 11:35:55 2017 +0200

SA-SPH. No-slip conditions are activated in 3D (Di Monaco et al., 2011, EACFM):

assessment in progress.

commit 177afd0d84fa7e07b8ad5ebe839e24b477ad1bf0

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon May 15 17:53:16 2017 +0200

Minor modifications.

Body dynamics. Documentation file. An appendix is added. Meaning of

the following approximated configuration of SPHERA:

(imping\_body\_grav=1, imping\_body\_grav\_dry=0): clarifications on

gravity force, sliding friction force, body-boundary normal

reaction force under sliding, normal coefficient of restitution.

commit 211cd11398ae27e0ecb271932d8810602ee2daa4

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Mar 28 16:33:37 2017 +0200

Minor modifications.

Body transport. Additional option to deactivate gravity during any dry

impingement.

commit 03fc89e6c807cef61341a84df82aee26231c446e

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Mar 23 13:41:53 2017 +0100

Minor modifications.

Post-processing. Maximum body particle acceleration is available in the

application log.

Bug fixed. Body transport. Misprint on the definition of the variable

"imping\_body\_grav" on the template of the input file.

Bug fixed. Body transport. On the use of the variable

“time\_max\_no\_body\_gravity\_force”.

commit 338f8141e7ff06bdb656abd6de22dd6613fd31d1

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Mar 22 14:31:43 2017 +0100

Minor modifications.

Body transport. FSI (Fluid-Structure Interaction). Both free-slip (new

formulation) and no-slip conditions (Adami et al., 2012) are available.

So far, no-slip conditions have been used.

commit 8f3cbaf810caa49b85213bcdfed8f440e36b7d5b

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Mar 21 19:37:32 2017 +0100

Minor modifications.

Body transport. Limiter for maximum pressure values on the body surfaces.

This limiter only avoids extremely high and unphysical values.

commit d764eb10b7b19374e24f1cb8023a11ef02e1a0f1

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Mar 15 11:26:07 2017 +0100

Minor modifications.

Body transport. Input variable to activate a limiter which avoids pressure

negative values on the body surfaces.

commit 9f12acfbc42de0685fb7a22ea52cd7b7568ff9e5

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Mar 14 17:25:28 2017 +0100

Minor modifications.

Body transport. Input variable “time\_max\_no\_gravity\_gravity\_force”: gravity

force is deactivated until this time. No deactivation in case of negative

value.

Body transport. Input variable “time\_max\_no\_body\_frontier\_impingements”:

body-frontier impingements are deactivated until this time. No

deactivation in case of negative value.

commit 3b76a72dd26d5d12c55810587081c2d3459764d3

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Mar 14 15:32:14 2017 +0100

Minor modifications.

Bugs fixed. Pre-processing; Post-processing. On the restart procedure.

Bugs fixed. Post-processing. On the allocation of the arrays “q\_max”,

“h\_step”, “qx\_step”, “qy\_step”, “h\_max”.

commit f0272cf22412ffbca0f920f68e2cbe63ef9790af

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Mar 10 18:21:45 2017 +0100

Minor modifications.

Body transport. I/O management of the body orientation to initialize a new

simulation based on the data of a previous run (and with no need for a

restart procedure). The IC rotation matrix (to set body particle IC) is

based on Rodrigues’ formula (Euler’s theorem) and depends on the input

data. The IC orientation of a generic body (and a generic body element)

is provided in terms of rotation axis and rotation angle (instead of

Euler angles; ref.: input file template). The rotation axis and the

rotation angle are written in the output file “Body\_dynamics.txt” and

refer to the following times: initial time, current time. The vector

“alfa” is not read/written anymore in I/O management. Implemented as an

approximated procedure, the new modification only guarantees a correct

reinitialization of the relative position of the first body particle.

Nevertheless, as the body centre of mass is correctly reinitialized, the

error in the body orientation (of a reinitialized simulation) is limited.

commit e3ca4bdfa16e632f58865a580481f1939a0d5298

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Mar 7 13:36:51 2017 +0100

Minor modifications.

Bug fixed. Post-processing. Min./max. of the absolute value of the body

angular velocity on the application log.

Body transport. Rotation matrix computation is formally more accurate. No

influence on the test cases treated so far.

commit 7ffae125eb66f7da766d3193a1dee406934accd5

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Mar 3 15:27:12 2017 +0100

Minor modifications.

Bug fixed. IC. Allocation of the auxiliary variable z\_aux: dependency on the

"fictitious vertex" .

commit 33ea4ab906d8c07e8c5bc5936b235c438ae879a3

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Mar 3 11:38:02 2017 +0100

Minor modifications.

Body transport. The variable "alfa" (rotation angle of the body with respect

to the reference system) is reported in the output file

"Body\_dynamics.txt" .

commit db85a1c659d75e327081babbf0a58c8c3a9c14f1

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Mar 2 13:35:53 2017 +0100

Minor modifications.

IC. There is no constraint on the number of reservoirs which can be extruded

from topography (only one extruded reservoir was permitted).

Pre-processing. The numerical parameters nag\_aux (slight overestimation of

the total numer of fluid particles) does not depend anymore on the

reservoir. Other minor modifications on the template of the input file.

Bug fixed. IC. The upper particle ID of a given zone/reservoir is computed.

The parameter nag\_reservoir\_CartTopog is not used anymore.

commit 8e93fc0ab9884337e960f9c084d180cfb0448b6e

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Feb 22 15:55:57 2017 +0100

Minor modifications.

"z-coordinate" is available in the ".vtu" output files, no matter about the

configuration of the input files.

commit 221723dbaa0bad8ee33eaab6df505368e8bdfbeb

Merge: 83959e7 49c46ab

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Feb 3 10:44:31 2017 +0100

Merge branch 'master' into SPHERA\_v\_8\_0\_AA

commit 49c46abdbfc251ef6f7080e7acfa99e2c02af52b

Merge: afc1a53 02e427f

Author: Andrea Amicarelli (RSE SpA) <Andrea.Amicarelli@rse-web.it>

Date: Fri Feb 3 10:46:36 2017 +0100

Merge pull request #2 from SauroManentiUNIPV/SPHERA\_v\_8\_0\_SM

Limiting viscosity

commit 83959e73823a71a1794471d64ca82c3d73792476

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Feb 3 10:37:19 2017 +0100

Minor modifications.

Additional comments.

commit 02e427f68af69a7046cacb425377cec260996aba

Merge: 7161c7a afc1a53

Author: SauroManentiUNIPV <sauro.manenti@unipv.it>

Date: Wed Jan 25 10:23:45 2017 +0100

Manual merging of master into branch SPHERA\_v\_8\_0\_SM .

commit 7161c7a57e49a6c206f2042ce81506d12179992a

Author: SauroManentiUNIPV <sauro.manenti@unipv.it>

Date: Tue Jan 24 10:11:45 2017 +0100

Limiting viscosity.

commit afc1a5340b08fabdb664c1e33ab734931aada96e

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Jan 23 16:34:48 2017 +0100

Minor modifications.

Bug fixed. Body transport. On the reference system change in body-frontier

interactions in case of triangular frontier faces.

Bug fixed. On the allocation of the arrays of the maximum specific flow rate

and the maximum water depth duiring a restart run.

Bug fixed. DB-SPH. On the removal of the fictictious reservoirs at the

beginning of the simulation.

commit 45fcb6b07116b84f18f2e8aebcbf7fde0af335e9

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Jan 17 18:49:47 2017 +0100

Minor modifications.

Post-processing. More inclusive format specifiers in the application log.

commit 291635f710350286d15d92685d9ca0d7809098f6

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Jan 17 16:57:32 2017 +0100

Minor modifications.

Corrections on the management of the body transport arrays during the

restart procedures.

commit 2bd0c242874c61ff1e6828f534b3f80a16b7af11

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Jan 17 15:31:54 2017 +0100

Minor modifications.

Bugs fixed. Misprints.

commit 329ab71887d99bdb6a8fd76bf4b1a4a7701e8484

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Jan 17 15:06:26 2017 +0100

Minor modifications.

Bugs fixed. Checks on the allocation of some arrays for body transport.

commit 030b64e788b55403562d75dbb0e8d526b5121780

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Dec 22 11:06:58 2016 +0100

Minor modifications.

Bug fixed (post-processing). Allocation of the array of the specific flow

rate (q\_max) is function of the number of the topographic vertices

(instead of the positioning grid vertices).

commit 4e7f0a6adef6c1490adffdd0c9e20975af3f8900

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Nov 25 14:51:18 2016 +0100

Minor modifications.

New test case: ICOLD erosional dam break (on complex topography).

commit 4928313ac1ea3c46246944a8fbcb8bdb9b39fad1

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Nov 17 16:58:44 2016 +0100

Minor modifications.

Bug fixed. In the restart mode, the value of the variable “GCBFVecDim”

provided by the input file is not used. Instead, the restart file

provides the correct value.

Bug fixed. In the restart mode, the array “GCBFPointers” is correctly

allocated.

commit 6d6dec91f1b7f3a626d93a4f8d2ced5114d83d1e

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Nov 15 17:24:59 2016 +0100

Minor modifications.

Bug fixed. Variable “GCBFVector” is correctly allocated in the restart mode.

Variable “NumBSides” is correctly written and read in the restart mode.

commit 894697dd17c970d3dd2d832197eb3f0757d92f17

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Nov 9 12:00:49 2016 +0100

Minor modifications.

Bug fixed. New “if” constructs depending on the variable “diffusione”

(subroutines “rundt2” and “inidt2”). The bug might have caused minor

errors in estimating the time step duration (dt).

Bug fixed. Restored the mobile particle counting (to assess the variable

“indarrayFlu”; initialization section of the subroutine “LoopIrre3D”).

Bug fixed. Detection of the elastic strain rate regime (subroutine

“mixture\_viscosity”).

commit b96ae71e82ebe0daaa28025ba7eb0d701feb3aa4

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Oct 28 10:01:40 2016 +0200

Minor modifications.

Bed-load transport. Bug fixed in computing the mixture viscosity.

commit f328621c31a5ce4a98327f051a279122c8ea1fa2

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Oct 27 17:13:23 2016 +0200

Minor modifications.

Bug fixed. Bed-load transport. The wrong treatment of local uniform velocity

fields is deleted.

commit 84a39cbeea9b92e5101571ff53d689a4a1353b1b

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Oct 27 12:25:04 2016 +0200

Minor modifications.

Bug fixed. Mixture particles in the elastic-plastic strain regime (mixture

viscosity higher than the reference threshold): acceleration is zeroed in

3D by the subroutine “LoopIrre3D” (as in 2D; zeroing velocity is not

sufficient). Notice that the involved particles are held fixed.

commit df636281b5fdb7a8d4d78a972e824f73f605e4c3

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Oct 26 17:18:48 2016 +0200

Minor modifications.

Bug fixed. For those particles, which are held fixed, the dynamic viscosity

is formally set equal to the maximum/threshold frictional viscosity

(instead of fluid viscosity; subroutines “LoopIrre3D” and “LoopIrre2D”).

Due to the presence of several "if" constructs, which are based on

conditions depending on the particle viscosity, this modification may

influence the computation.

Bug fixed. The subroutine “Shields” is now properly called when using RK

time integration schemes (subroutine “LoopIrre3D”).

commit a49ded801956e8d1058be97bcbbeb0b4f488f802

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Oct 24 17:31:34 2016 +0200

Minor modifications.

Bed-load transport. Particles modify their mobility status (fixed/”sol” or

mobile/”flu”) only in the subroutine “Shields” (not anymore in the

subroutine “mixture\_viscosity”), according to the fixed bed detection (in

“CalcVarLength”), no matter about the cause of change (either the

velocity threshold or the maximum frictional viscosity). So far, the

momentum equation and the velocity smoothing procedures are skipped for

mixture particles in the elastic-plastic strain regime. This is not due

to the particle status (it is not “fixed” at this stage of the

algorithm), but to the particle viscosity, which is at least equal to the

frictional viscosity threshold (“if” condition on …%mu = …%mumx). This

modification already began with the previous commit.

Bugs fixed.

commit 385cddf18b53d2f650017bfab06f833f474f8ea6

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Oct 21 17:16:51 2016 +0200

Minor modifications. Auxiliary procedures are deleted. Notice that some SPHE

pre-processing tools are available at https://github.com/AndreaAmicarelli

(e.g., DEM2xyz -RSE SpA-, ply2SHERA\_perimeter -RSE SpA-).

commit c6266690a785ae390bcd40f8ef79f7f5d3e0c652

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Sep 23 18:19:56 2016 +0200

Minor modifications.

Bed-load transport. Restored the initial mobile particle counting in the

subroutines Loop\_Irre\_3D and Loop\_Irre\_2D, in the presence of the boundary

treatment SASPH.

Bed-load transport. The following redunant variables are erased:

Med()%modelloerosione, erosione, modelloerosione.

commit 7ad2b8c70b1f59afd966845884ddd2b01dd324ed

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Sep 16 18:39:43 2016 +0200

Minor modifications.

commit 28aab0183d8277001ecd19103945c70cd70b13a7

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Sep 13 08:07:28 2016 +0200

Minor modifications. The following test cases are published at SPHERIC 2016:

San\_Fernando\_Lower\_van\_Norman\_dam\_liquefaction.inp,

dike\_breach\_2D\_expSchHag12JHR\_ID13.inp,

erosional\_dam\_break\_Karlsruher\_sand.inp, spherical\_Couette\_flow.inp.

commit 293fa92960a8bbb4c56284883621a4d77a7d37ef

Merge: b0911f6 d7c4348

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Sep 13 07:56:04 2016 +0200

Merge branch 'master' into SPHERA\_v\_8\_0\_AA

commit d7c43486d6e90f52ab00c5a7ae95d671a058cdf8

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Sep 13 07:51:19 2016 +0200

input file for SPHERA v.8.0 (RSE SpA): Benchmark2\_SASPH. Copyright 2005-2016

(RSE SpA; authored by Antonio Di Monaco, Giordano Agate, Andrea Amicarelli).

References: Di Monaco et al. (2011, EACFM), Amicarelli et al. 2013 (IJNME).

commit b0911f667eca5adc2adf1d33792bbf54259c09ad

Merge: 2f4307a 7db30ab

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Sep 8 17:33:11 2016 +0200

Merge branch 'master' into SPHERA\_v\_8\_0\_AA

commit 7db30ab95c6a4b1508b4d37a1108edd1557495a7

Merge: 1a2e6e1 5e23337

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Sep 8 17:22:36 2016 +0200

Merge branch 'master' of https://github.com/AndreaAmicarelliRSE/SPHERA

commit 2f4307a43bc2e9b94c49dc0945b189c715b12491

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Sep 8 08:09:05 2016 +0200

Minor modifications.

commit 5e233370f4b5a885fbdc1dadde17dfb56600e48b

Merge: a7893bc f3041c0

Author: Andrea Amicarelli (RSE SpA) <Andrea.Amicarelli@rse-web.it>

Date: Mon Sep 5 11:02:15 2016 +0200

Merge pull request #1 from chqiao/patch-1

Minor modification. Format correction in the application log (for portability with gfortran compiler).

commit f3041c0219578af9dc7eb2f0e602395e9bef4450

Author: QIAO Cheng <qiaoch@yeah.net>

Date: Thu Aug 18 20:50:20 2016 +0800

Correct the write out format of headline

Correct the write out format problem of screen display which will make a error while compiling the code.

commit 1a2e6e1a61a836f31d84981e751ecb08e8b52c0e

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Jul 4 14:19:57 2016 +0200

Time integration. Two time integration coefficients are requestsed in input to

compute the time step duration: CFL and vsc\_coeff (coefficient for the

viscous stability criterion; default value: 0.05).

Restart procedure. In 3D, arrays GCBFVector & GCBFPointers are saved and read

in/from the restart file, whereas subroutine

GridCellBoundaryFacesIntersections3D is not called during a restarted run.

Auxiliary procedure. ply2SPHERA\_perimeter. An offset for z-coordinates can

be imposed from the input file.

commit a7893bcc577c3747b77b259e02d47df679b3a679

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Jun 13 13:17:55 2016 +0200

Minor modifications. Some new input files.

commit c6b5f503e88043c4c9a65e980732bf64b244c4c9

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Jun 13 13:04:48 2016 +0200

Bed-load transport. Lagrangian saturation scheme. Modification to obtain null

fluid pressure for thos (possible) dry mixture particles, which lie below

saturated mixture particles.

Minor modifications. New input files.

commit 032c13b87d9e1234ab46746d39703517d3ea54c1

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Jun 8 11:48:08 2016 +0200

Bed-load transport. New conservative Lagrangian scheme for saturation

conditions (hypothesis of stratified flows).

Mixture particles are either fully saturated or dry. The variable

saturated\_medium\_flag is added as an input logical variable to

indicate if a medium is fully saturated or dry. The mixture density is

computed accordingly.

The variable alfa\_WT (Water Table slope) is computed on the mixture

particle, which locally defines position of the water table). The

formulation for the fluid pressure depends on this angle, which

approximately represents the underground flow direction.

ID of the highest saturated mixture particle in the background grid

column. This local height is approximately representative of the top of

the fully saturated zone (under the hypothesis of stratified flows). This

parameter is stored in the array ind\_interfaces(i\_grid,j\_grid,6).

Bed-load transport. The redundant input variable ID\_granular is not requested

anymore.

Post-processing. The subroutine write\_Granular\_flows\_interfaces is split in

write\_Granular\_flows\_interfaces and interface\_post\_processing.

Bug fixed. Post-processing. Correction on format specifiers for the application

log file.

Bug fixed. Post-Processing. The subroutine cat\_post\_proc is now called by the

subroutine result\_converter. In other words, the .txt files are concatenated

each time new .vtu output files are written.

commit acc0448528c779745f4b6b1cf603680f2d16ed88

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu May 26 11:25:23 2016 +0200

Minor modifications.

commit e5363e585c2c4d10bf60ff0ad02fe90fb802ab44

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu May 26 08:35:40 2016 +0200

Post-processing. File concatenation of output .txt files is carried out

incrementally at each post-processing stage. Thus, the .txt output files are

concatenated even in case of a simulation stop or kill. New subroutine:

cat\_post\_proc.

Post-processing. PV and log files allow using a number of particles higher than

999’999.

commit 210d87f88e2d8c947ac046f06388bb12bdb0eae3

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue May 24 10:05:23 2016 +0200

Bug fixed. IC. The check on the particle array dimension (subroutine

SetParticles) is fixed.

commit 7beedef63de0f201c4620d65ee08d855fa206974

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue May 24 08:20:31 2016 +0200

Bug fixed. Geometry. Variable dis2 is correctly initialized in the subroutine

point\_inout\_convex\_non\_degenerate\_polygon. There were issues when the

variable dis was null.

commit 02123239afeb56f4c77c12a7b05f308542bf2d9b

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri May 20 18:44:50 2016 +0200

Bug fixed. Auxiliary procedure ply2SPHERA\_perimeter. Vertex IDs in face

definition are corrected with the proper offset.

Bug fixed. Bed-load transport. Granular\_flows\_options%saturation\_conditions is

treated element per element, with no array notation (typo in CalcVarLength).

commit 4f88ff84a3a1039ac5929acd3aa5961283210f23

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue May 17 18:11:37 2016 +0200

Bug fixed. Geometry. Invalidated vertex IDs of SA-SPH faces can have both null

and negative values (subroutine LocalNormalCoordinates).

commit 31dd699717332659fb3624c269613d34a620d819

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed May 11 16:11:00 2016 +0200

Bug fixed. Invalidated vertex IDs of SA-SPH faces can have both null and

negative values (subroutines ModifyFaces, IsParticleInternal3D).

commit e0781e73493bdf9883e8b0b6b72ee0d05a984cf3

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed May 11 11:36:10 2016 +0200

Bug fixed. Restart. Arrays Z\_fluid\_max, q\_max,

Granular\_flows\_options%minimum\_saturation\_flag and

Granular\_flows\_options%maximum\_saturation\_flag are allocated after reading

their dimensions from the restart file (ReadRestartFile).

New input files: Benchmark1\_dam\_break\_DBSPH, Benchmark2\_DBSPH,

dam\_break\_body\_UniBas, erosional\_dam\_break\_2D\_FraCap02\_Taipei,

erosional\_dam\_break\_bed\_2D\_FraCap02, erosional\_dam\_break\_bed\_2D\_Spi05,

erosional\_dam\_break\_Pon10\_asym, flushing\_2D\_small\_granular\_flows,

flushing\_2D\_small\_granular\_flows\_erosion\_criterion\_2D\_complete,

flushing\_3D\_small\_slope\_B3\_granular\_flows\_erosion\_criterion\_2D\_complete,

flushing\_3D\_small\_slope\_B3\_granular\_flows\_erosion\_criterion\_3D\_complete,

ICOLD\_earth-fill\_dam\_breach\_long, ICOLD\_earth-fill\_dam\_breach\_short,

ICOLD\_earth-fill\_dam\_break, sloshing\_tank\_TbyTn\_0\_78,

sloshing\_tank\_TbyTn\_1\_07, submerged\_landslide.

commit 1c0f2e717dc7839f5c483bb9272a426bcf483de0

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu May 5 20:46:05 2016 +0200

Bug fixed. IC. Variable dx\_CartTopog is double precision, not an integer (issue

with gfortran).

Bug fixed. IC. Variable h\_reservoir (subroutine GeneratePart) was wrongly

declared and initialized.

commit 2691ab8ae7bf45fa114769a9de065d298258fa72

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed May 4 17:29:38 2016 +0200

Minor modifications.

commit 73fdcebece3447174d1f7c93a02fcac8c55e0ad9

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed May 4 13:18:45 2016 +0200

Bug fixed. SA-SPH. Run-time reduction of the number of nodes (local variable

nnodes in the subroutine DefineLocalSystemVersors) in 3D.

commit 7649c717d6d8ab257c14a306d31af88dd1c99685

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue May 3 16:25:49 2016 +0200

Bed-load transport. Additional saturation schemes: uniform dry soil

(saturation\_scheme=0), uniform fully saturated soil (saturation\_scheme=1).

The saturation scheme, which depends on time\_minimum\_saturation and

time\_maximum\_saturation, is represented by saturation\_scheme=2.

Bed-load transport. The mixture top interface normal is computed depending on

the mixture neighbours (instead of the fluid neighbours, which may be

absent) and a default vertical vector is added (in the absence of mixture

neighbours).

commit 04548f7c25312da841f83ad77b403b03969e16a3

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon May 2 15:00:35 2016 +0200

Minor modifications.

commit 6afe37c35135b449999a8817ddfd1cf64e686bf9

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon May 2 14:44:36 2016 +0200

Minor modifications.

commit e0970cddff774ceb89d6eff8d140eaf04c0f9c11

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon May 2 14:41:29 2016 +0200

Upgraded documentation of SPHERA v.8.0

commit 5b638350b97e3445654a441a37a2189e950cbe56

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Apr 28 11:29:06 2016 +0200

Bed-load transport. New saturation conditions. The fluid pressure formula

depends on the zone: phreatic zone, dry soil or infiltration zone. The

infiltration front linearly grows between its height at the time with

minimum saturation and those at the time with maximum saturation. The local

soil bottom is detected as an interface. So far, the time at minimum

saturation has to be smaller than (or equal to) the time at maximum

saturation. When t<=t\_min\_sat, there is always phreatic zone below the free

surface and dry soil elsewhere. When t>=t\_max\_sat, the saturation zones are

freezed at t\_max\_sat.

commit 217903d6caaae919c840640460ed3b87fb664f16

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Apr 27 11:29:40 2016 +0200

Bug fixed. Bed-load transport. Granular\_flows\_options%saturation\_flag is

treated by the restart procedures.

commit bcc458b5bb7261926fa3fc3df80ed85e69c9edda

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Apr 20 20:01:26 2016 +0200

Minor Modifications.

commit d4486112dc3a303a5e7baf648db6fa529a0aa1c2

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Apr 19 17:04:27 2016 +0200

Bed-load transport. Saturation state is computed up to the saturation freezing

time (input parameter).

Formal modifications. Variable it\_corrente is named on\_going\_time\_step. Variable

tempo is named simulation\_time.

commit 762d6356742461f6fd7f63a3bea8b3569bb9f8b8

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Apr 18 17:39:04 2016 +0200

Bug fixed. Bed-load transport. Corrected the threshold constraint for the angle

alfa\_TBT.

Bug fixed. Bed-load transport. Nearest neighbour searching is mandatory even in

the absence of any erosion criterion (for fluid phase pressure).

commit 7fef54266c4fe19ff36f231efd689f5487f64fc7

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Apr 15 19:32:41 2016 +0200

Bed-load transport. Improvement of the formula for fluid phase pressure

(simplifying assumption: 1D filtration with piezometric lines in the mixture

parallel to the local 3D slope of the mixture top).

Bed-load transport. Computation of the mixture top interface normal.

Bug fixed. Bed-load transport. The interfaces between mobile and fixed particles

are now computed only in the presence of an erosion criterion.

commit 505f3368f95bee0f4c48659960c54ffb25af4d61

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Apr 15 10:34:17 2016 +0200

Bed-load transport. The mean effective stress is now estimated as a difference

between the total stress and the pressure of the liquid phase. In general,

xyz axis are not the principal axis and the lateral pressure coefficient at

rest (K\_0) only represents granular material at rest). So far, the model

assumes hydrostatic conditions for the liquid pressure in the mixture. Mean

effective stress is zeroed if the computation provides a negative value.

Bed-load transport. The fluid particle ID on the fluid side of the bed-load

transport layer top interface is now computed even without any erosion

criterion. This ID is mandatory to estimate the fluid pressure within the

mixture.

commit a1c505d19ed8c738bf5b11e4cf24cada9f70ba2e

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Apr 14 12:29:53 2016 +0200

Bed-load transport. The formula for the mean effective stress is corrected

according to the plane strain hypothesis of Mohr-Coulomb-Terzaghi criterion.

commit 2faf3a21338281ad9d7bfef65a4ecf3a9aaffabe

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Apr 12 11:35:29 2016 +0200

Bug fixed. Bed-load transport. In the presence of mixture particles interested

by the frictional viscosity threshold, pg(...)%var=0 was missing when

smoothing velocities (both in 2D and 3D). For safety reasons, now the

variable vel replaces the variable var in time integration for trajectories

(Leapfrog scheme). However, at that point, the variable var should be equal

to the variable vel (in any case).

commit 4c9b23405a7d940dd9edeaba7dd46e9881f4de50

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Apr 8 11:46:26 2016 +0200

Bed-load transport. The mixture particles, which are affected by the frictional

viscosity threshold, are blocked.

commit 85f1ed9a63281a3321ac1a4d97c429b9cea9d258

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Apr 5 17:23:11 2016 +0200

Bed-load transport. Contribution of the fluid phase to the frictional viscosity

in the bed-load transport layer, just to avoid null values for the mixture

particles at the layer top. Elsewhere, this contribution is negligible.

Bug fixed. Erosion criterion. Corrected the "if construct" in case the critical

shear stress is close to zero.

commit 0ceee40754870bca2da34b939d023942092f22e3

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Apr 4 17:30:44 2016 +0200

Bed-load transport. Frictional viscosity is the mixture viscosity in

the bed-load trabnsport layer.

Bed-load transport. The mean effective stress replaces the vertical effective

stress, by means of the coefficient of lateral earth pressure at rest.

Bed-load transport. Formulations erased: Chauchat & Médale blt viscosity,

Einstein dilute viscosity, Chezy-like viscosity. Parameter erased:

Granular\_flows\_options%viscosity\_blt\_formula, Granular\_flows\_options%Bn,

Granular\_flows\_options %Chezy\_friction\_coeff. Parameters erased in the

input file: Granular\_flows\_options%viscosity\_blt\_formula,

Granular\_flows\_options %Chezy\_friction\_coeff.

Bed-load transport. In case of null strain rate tensor (uniform flow or still

material), then dtau/dx=0. This condition is fictitiously represented with a

null friction viscosity.

Bed-load transport. A viscosity threshold (mu\_max) is used as a limiter.

commit 170c499e99d49264f3dce944b281c684a8862fe2

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Mar 22 17:40:32 2016 +0100

Bug fixed. Restart: management of the variable Domain%start in ReadRestartFile.

Bug fixed. Restart: corrected file format o read the restart steps before the

requested one.

Bug fixed. Restart: only the sections “domain”, “boundaries“, “vertices” and

“faces” (main input file) are not read during a restart execution.

Bug fixed. Restart: correction on the first call of sub\_Q\_sections in case of

restart.

commit e5c50c6401eceafdb241db2ff1cc3a5a92ddb5e7

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Mon Mar 21 18:38:39 2016 +0100

Minor modifications.

commit cd7627020ff22d5180d11d8b8803af0038c91c4c

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Mar 17 13:33:30 2016 +0100

Minor modifications.

Bug fixed. Bed-load transport. Deactivation of the approach for liquefaction

if the liquefaction time equals zero (approach deactivation).

commit aad4a6e4c6753c5aca70598d8b6acbecaed44737

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Mar 16 17:54:31 2016 +0100

Minor modifications.

commit a10f63b8a3aa8e7f2e8e1b6b740a78a14db76ebc

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Mar 15 17:31:17 2016 +0100

Bed-load transport. Liquefaction only applies, in the presence of the free

surface along the vertical of the computational particle.

Bed-load transport. Effective stress is equal to the total pressure, in the

absence of the free surface along the vertical of the computational particle.

Bug fixed. BC, DB-SPH. Argument of wavy\_inlet is the inlet section ID, not the

boundary ID.

Bug fixed. Bed-load transport. Calling Shields in LoopIrre\_2D for DB-SPH (with

bed-load transport, even without erosion criterion). The corresponding 3D

correction is still missing.

Bug fixed. DB-SPH. Assigning surface\_mesh\_file\_ID to inlet and outlet DB-SPH

elements.

Bug fixed. DB-SPH. Zeroed variables Ncbs, IntNcbs and Ncbf when using DB-SPH.

Bug fixed. DB-SPH. SPH approximation of density with NMedium>1.

Bug fixed. DB-SPH. surface\_mesh\_file\_ID was not assigned in 2D

(Import\_ply\_surface\_meshes).

Bug fixed. Erosion criterion, DB-SPH. Mobile particles are counted after having

removed DB-SPH fictitious reservoir (once they were set equal to the the

number of particles in the domain).

Bug fixed (timing).

Tests (AA!!!) on multi-fluid DB-SPH.

commit 29a207b9fab8d8c5eb40cf584b39166f27dd2f26

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Feb 18 18:59:52 2016 +0100

SPH-blt-3Dbd.

Liquefaction (preliminary implementation). Linear pore pressure functions

(with respect to the cyclic number ratio).

commit f58226d86df2e433992cc6e8e27d681aff085b67

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Wed Feb 17 17:39:57 2016 +0100

SPH-blt-3Dbd: validations.

Minor modifications

DB-SPH. Graphical issue: avoided divisions by the discrete Shepard

coefficient for non-wet wall elements.

commit 53b464b89df692a5231ed578641928fd2c0c70f7

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Tue Feb 16 17:42:45 2016 +0100

SPH-blt-3Dbd: validations.

DB-SPH. New input logical variable: negative\_wall\_p\_allowed (pressure of wall

elements can be negative).

DB-SPH. New input logical variable FS\_allowed (free surface detection can be

avoided).

commit 29bbc8b7930280cf14d27d02a8a3639b6d108e6c

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Fri Feb 12 19:26:04 2016 +0100

SPH-blt-3Dbd: validations. Minor modifications.

commit ed52bd4c8c23bf34a3cdb5ddd2ac48a217dff921

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Feb 11 17:42:00 2016 +0100

SPH-blt-3Dbd: validations.

Momentum equation. Background pressure (Domain%prif) is now preliminarily implemented (it was only treated in pressure smoothing).

SPH-blt. The recently increase of dx/2 in the interface height (to compute effective pressure) is removed.

Bug fixed (pressure smoothing for 3D DB-SPH). This correction would improve the results of Amicarelli et al. (IJNME, 2013) on two 3D dam breaks.

commit fb5f6747b565785945171de5f5ba1ff7b60e9039

Author: AndreaAmicarelliRSE <Andrea.Amicarelli@rse-web.it>

Date: Thu Feb 4 18:32:11 2016 +0100

SPH-blt-3Dbd: validations.

Neighbouring search. Warning alert/ Error, in case the number of wall element neighbours is equal to / greater than the maximum number allowed.

DB-SPH. The upper limiter of the integral Shepard coefficient can be removed by means of an input variable.

Bug fixed (DB-SPH-NS-blt). Corrected the position of the line on: Shepard correction for the velocity gradient (times shear viscosity) of the semi-particles in the Viscous Sub-Layer of the Surface Neutral Boundary Layer.

Previously, it was erroneously executed for each fluid particle neighbour.

commit b1c20b4708ff71009fa3f8dca4f06f2a7765c860

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Fri Jan 29 17:53:00 2016 +0100

SPH-blt-3Dbd: validations.

SPH-blt-3Dbd. New variable DBSPH%slip\_ID.

SPH-blt-3Dbd. Ferrand et al. (2013, IJNMF) formulation: BC contributions (both terms) to viscosity shear stress term are null if the fluid particles are still. The formulation is adapted to moving boundaries.

SPH-blt. Added dx/2 to the top of the bed-load transport layer to improve the estimation of the effective stress.

Bugs fixed (DBSPH\_kinematics). A parallel do end was missing. Variables vel\_aux and omega\_aux are now shared variables in every omp cycle.

Bug fixed (Loop\_Irre\_3d and Loop\_Irre\_2d). Wrong if construct (accelerations were always null with DB-SPH). This bug was introduced after SPHERA v.8.0 and has not affected any study/release.

Bug fixed (Time\_integration). Corrected estimation of dt in the presence of only inlet sections and mixture reservoirs.

commit 1be37160f3fe0bd4096da30dd4ba2293b482f76b

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Wed Jan 27 19:03:15 2016 +0100

SPH-blt-3Dbd: validations.

Minor modifications (the bugs do not affect the results of previous studies):

Semi-particle (DB-SPH) viscosity is now normalized by means of the discrete Shepard correction.

Bug fixed on time integration. Neglecting mixture particles in CFL computation considered every non-fixed particle, fluid particles included.

Bug fixed on DB-SPH. vel\_aux and omega\_aux were used even in case of no imposed kinematics (and were not initialized). Now an “if construct” only selects wall elements related to a boundary with imposed kinematics (no need for

initializing vel\_aux and omega\_aux).

Bug fixed on DB-SPH. vel\_aux and omega\_aux were private (instead of shared) in a parallel do.

Bug fixed on time integration (initialization of done\_flag in 3D).

commit d6b2c2b4a506711b0f17c232ef774c485a126c33

Merge: 299175c 55981ad

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Mon Jan 25 10:29:33 2016 +0100

SPH-blt-3Dbd. Merging from master.

commit 299175c55faa00e40b995071e0f9af9c2a78773c

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Thu Jan 21 17:23:37 2016 +0100

SPH-blt-3Dbd: validation in progress. Test removed.

commit 9d138d56bce8b1d225f8aa226ade45e48f76f13e

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Thu Jan 21 17:19:33 2016 +0100

DB-SPH-NS-blt (or equivalently SPH-blt-3Dbd: SPH - bed-load trasnport - 3D bottom drag). Validation in progress. Minor errors fixed.

commit f4d8f7fdf8c9853eafc5b78b217c5d255dfc8d4b

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Wed Jan 20 18:44:52 2016 +0100

Merging issues completed. Fixed the merging conflict errors accidentally introduced in commit of 29Oct15, 10h26.

commit 403c02b80da9cc742c97910c91719ee28d7c96eb

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Wed Jan 20 14:52:19 2016 +0100

Merging issues. In progress.

commit 141f00c910da228cf71c3232ef28ab783db8d265

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Tue Jan 19 18:35:52 2016 +0100

Merging issues. In progress.

commit 55981ad8dacb54a5a2c204edbccca78f9bcb5715

Author: AndreaAmicarelliRSE <andrea.amicarelli@rse-web.it>

Date: Thu Nov 19 18:22:05 2015 +0100

SPHERA free software (FOSS). Signed SIAE registration application.

# User guide

SPHERA installation is straightforward (Sec.13.1), 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.13.2). This template defines and comments all the input parameters. Finally, SPHERA v.9.0.0 tutorials are discussed in Sec.13.3.

* 1. Installation

SPHERA source and executable files are distributed on a dedicated Git repository on GitHub ([184]). 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”).

The Makefile (under the folder “src”) allows compiling SPHERA under different configurations, as explained in Table 13.1. SPHERA is optimized by means of the following features: preprocessor directives (two macros are active); compilation options “-O2” (for both the compilers “gfortran” and “ifort”) and “-ipo” (for the compiler “ifort”).

|  |  |  |  |
| --- | --- | --- | --- |
| **Makefile variable** | **Suggested value** | **Executable**  **name:**  **SPHERA\_j\_abcdefghi** | **Description** |
| VERSION | v9\_UserInitials\_CommitData | j=VERSION | Master subversion compiled by the user |
| COMPILER | ifort | a=1 | Compiler |
|  | gfortran | a=2 |  |
| EXECUTION | optimized | b=1 | Execution mode |
|  | debug | b=2 |  |
| PARALLELIZATION | OMP | c=1 | parallel simulations |
|  | NO | c=2 | sequential simulations |
| PD\_SPACE | -DSPACE\_3D | d=3 | 3D (macro) |
|  | -DSPACE\_2D | d=2 | 2D (macro) |
| PD\_VERBOSITY | (blank space) | e=0 | Synthetic output |
|  | -DVERBOSITY | e=1 | Verbose output (macro, inactive) |
| PD\_KTGF | -DKTGF\_FULL | f=1 | KTGF scheme (dense granular flows) with possible 2-interface 3D erosion criterion (macro, nactive) |
|  | -DKTGF\_NO | f=0 | no KTGF scheme (macro, nactive) |
|  | -DKTGF\_EC2D | f=2 | KTGF scheme with possible 1-interface 2D erosion criterion (macro, inactive) |
| PD\_SOLID\_BODIES | -DSOLID\_BODIES | g=1 | Body transport (macro, inactive) |
|  | (blank space) | g=0 | No body transport |
| PD\_BTM | -DBTM\_SASPH | h=1 | BOUNDARY TREATMENT METHOD: SASPH (macro, inactive) |
|  | -DBTM\_DBSPH | h=2 | BOUNDARY TREATMENT METHOD: DBSPH (macro, inactive) |
| PD\_TIS | -DTIS\_LEAPFROG | i=3 | TIME\_INTEGRATION SCHEME: Leapfrog (macro, inactive) |
|  | -DTIS\_EULER | i=1 | TIME\_INTEGRATION SCHEME: Euler (macro, inactive) |
|  | -DTIS\_HEUN | i=2 | TIME\_INTEGRATION SCHEME Heun (macro, inactive) |

Table 13.1. Makefile variables; macros for the preprocessor directives; executable names (Makefile of SPHERA, [184]). The following constraints/incompatibilies are automatically corrected by the Makefile: “KTGF” needs “SASPH“; “SOLID\_BODIES” needs “SASPH” and “LEAPFROG”; DBSPH” needs “EULER”.

* 1. Commented template of the main input file of SPHERA v.9.0.0

Figure 13.1 reports the commented template of the main input file of SPHERA v.9.0.0.

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

|  |  |
| --- | --- |
| **Input file section** | **Synthetic Description** |
| Title | Test case title |
| Domain | Spatial resolution and choice of the boundary treatment scheme |
| Vertices | Vertices of the fluid domain boundaries |
| Lines/Faces | Vertex connections of the boundary lines/faces of the fluid domain in 2/3D |
| Boundaries | Features of the fluid domain bodies and boundaries (solid boundaries, open/inlet sections): initial conditions, boundary conditions, possible extrusions of water bodies from topography. |
| DBSPH | Quantities on the DB-SPH boundary treatment scheme, related to: spatial resolution at boundaries, MUSCL reconstruction scheme, geometry of semi-particles, slip conditions, limiters, monitors, number of files for the surface mesh (initial positions of the boundary elements), imposed kinematics (of the boundaries), inlet/outlet sections. |
| Bed-load transport | Input quantities for the following features: scheme for dense granular flows, erosion criterion, saturation scheme, monitors, liquefaction scheme. |
| Medium | Input physical quantities on the fluid and solid phase properties and the scheme for dense granular flows: bulk modulus, viscosity, saturation conditions, internal friction angle, limiting viscosity, maximum viscosity, initial effective porosity, mean diameter of the solid grains. |
| Body dynamics | Input physical quantities on the scheme for body transport in fluid flows: possible imposed kinematics; number of bodies; spatial resolution within the solid bodies; friction angle; limiters. For each body, the following quantities are requested: number of elements; mass; vectors of the initial position, velocity and angular velocity; tensor of the mass moment of inertia (if this is constant and not computed); initial orientation of the body with respect to the reference system. For each body element, the following quantities are requested: side lengths of the element; vector of the initial position; initial rotation of the element with respect to the reference system; Boolean operator to treat the element when configuring its reference body. |
| Run parameters | Final time, *CFL*, *C*and time integration scheme; weight of the partial smoothing; numerical quantities for memory management. |
| General physical properties | Gravity acceleration vector; reference pressure. |
| Restart | Frequency for writing the restart files |
| Output regulation / draw options | Frequency for writing SPHERA output files |
| Control points | Position of the monitoring points |
| Control lines | Position and discretization of the monitoring lines |
| Section flow rate | Geometry of the monitoring sections for the flow rate |
| Substations | Geometries of the electrical substations for the substation-flooding damage scheme and substation type (high-voltage transmission substation, medium-voltage distribution substation, low-voltage distribution substation). Each substation is described by a polygon. |

Table 13.2. Sections and relevant quantities of the main input file of SPHERA v.9.0.0 ([184]).

version.subversion.subsubversion !

! SPHERA main input file: template and

! comments

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

! SPHERA v.9.0.0 (Smoothed Particle Hydrodynamics research software; mesh-less

! Computational Fluid Dynamics code).

! Copyright 2005-2018 (RSE SpA -formerly ERSE SpA, formerly CESI RICERCA,

! formerly CESI-Ricerca di Sistema)

!

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

!

! This file is part of SPHERA.

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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),bsph(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,

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

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

! ... ! (other vertices; no gaps on vertex

! IDs)

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 "fictitious 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 (no gaps on line

! IDs)

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 "fictitious reservoirs".

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

! the actual 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 1/2/3 vertex IDs are 0 in case of pentagonal/quadrilateral/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 clockwise to keep coherence with SA-SPH walls).

! Faces can only be triangles or rectangles (generic quadrilaterals are not

! permitted), but only "perimeter" faces can also be generic quadrilaterals (not

! only rectangles), pentagons and hexagons.

1 face\_1\_vertex\_1 ... face\_1\_vertex\_6 face\_1\_Boundary\_ID

! first face data ("-1" is mandatory

! for meaningless vertex IDs (e.g.,

! 5th and 6th vertices of a

! quadrilateral)

... ! other records; no gaps on face IDs)

face\_last\_ID face\_last\_vertex\_1 ... face\_last\_vertex\_6 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(only

! removal of the particles crossing the boundary),

! tapis (not recommended)

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

Shear\_stress\_coefficient laminar\_flag\_check ! Shear\_stress\_coefficient=1.0

! (no-slip, under assessment in 3D

! with SA-SPH),0.(free-slip,

! default choice in 3D with SA-SPH);

! laminar\_no-slip\_check=.true.(check

! on laminar regime to activate

! shear stress terms at boundaries

! in case of no-slip conditions;

! laminar regime check has no

! effect in the inner domain),

! .false.(no check: always apply

! no-slip conditions in case

! Shear\_stress\_coefficient=1.0)

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 DBSPH\_fictitious\_reservoir\_flag

! 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);

! DBSPH\_fictitious\_reservoir\_flag = .true.(DB-SPH

! fictitious fluid particles to complete the kernel

! support at the free-surface, in pre-processing),

! .false.(no fictitious fluid particles)

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

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

! topography; dx\_CartTopog>=dx); 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 ! n\_circum(number of vertices circumscribing

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

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

! horizontal projection of the reservoir. Admitted

! figures: triangles and convex non-degenerate

! quadrilateral (otherwise the subroutine call for

! point\_inout\_convex\_non\_degenerate\_polygon must be

! replaced with other calls to subroutines such as

! point\_inout\_quadrilateral).

... ! 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. Admitted

! figures: triangles and convex non-degenerate

! quadrilateral (otherwise the subroutine call for

! point\_inout\_convex\_non\_degenerate\_polygon must be

! replaced with other calls to subroutines such as

! point\_inout\_quadrilateral). From a plan view, the

! vertices are provided anticlockwise.

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

fluid\_ID

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 slip\_ID Gamma\_limiter\_flag

! 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)

! slip\_ID (ID for slip conditions) = 0 (free-slip), 1 (no-slip),

! 2 (run-time choice depending on the inner shear viscosity terms in SPH-NS

! balance equations)

! Gamma\_limiter\_flag: logical variable to activate or deactivate Gamma upper

! limiter (.true.)

negative\_wall\_p\_allowed FS\_allowed ! negative\_wall\_p\_allowed: pressure of wall

! elements can be negative (logical);

! FS\_allowed: free surface detection can be

! avoided (logical).

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

surface\_mesh\_files flag\_in-built\_monitors ! surface\_mesh\_files: number of files

! of the DBSPH surface meshes;

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

! flag for in-built motion of control

! lines and DB-SPH frontiers

! do i=1,surface\_mesh\_file

imposed\_kinematics\_i\_records rotation\_centre\_i\_x rotation\_centre\_i\_y rotation\_centre\_i\_z

! imposed\_kinematics\_i\_records(number of

! records, which describe a possible imposed

! kinematics for the i-th DBSPH surface

! mesh file);

! rotation\_centre\_1 (centre of rotation for

! DB-SPH frontiers for the i-th DBSPH

! surface mesh file)

! if (imposed\_kinematics\_i\_records>0): start

i\_time\_1 i\_velocity\_x\_1 i\_velocity\_y\_1 i\_velocity\_z\_1 i\_omega\_x\_1 i\_omega\_y\_1 i\_omega\_z\_1

! ... ! other possible records

i\_time\_last i\_velocity\_x\_last i\_velocity\_y\_last i\_velocity\_z\_last i\_omega\_x\_last i\_omega\_y\_last i\_omega\_z\_last

! (records for the imposed

! kinematics to frontiers for the i-th

! DBSPH surface mesh file); time of the last

! record should be slightly higher than time

! at the end of the simulation.

! if (imposed\_kinematics\_i\_records>0): end

! enddo

n\_inlet n\_outlet ply\_n\_face\_vert ! n\_inlet(number of inlet sections)

! n\_outlet(number of outlet sections)

! ply\_n\_face\_vert(maximum number of vertices

! of the DB-SPH faces as represented in the

! ".ply" input files(3/4/5/6 in 3D, 4 in 2D)

! if (n\_inlet>0): 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>0): end

! if (n\_outlet>0): 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>0): end

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

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

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

erosion\_criterion\_ID ID\_main\_fluid

! 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).

saturation\_scheme time\_minimum\_saturation time\_maximum\_saturation

! saturation\_scheme=0(dry soil),1(fully

! saturated soil),2(saturation zones

! depepending on time\_minimum\_saturation and

! time\_maximum\_saturation),3(Lagrangian

! scheme for saturation conditions; mixture

! particles are either fully saturated or

! dry).

! time\_minimum\_saturation: time related to

! a relative minimum saturation of the

! granular material.

! time\_maximum\_saturation: time related to

! a relative maximum saturation of the

! granular material. So far,

! time\_minimum\_saturation has to be smaller

! than (or equal to)

! time\_maximum\_saturation. When t<=t\_min\_sat

! , there is always phreatic zone below the

! free surface and dry soil elsewhere. When

! t>=t\_max\_sat, the saturation zones are

! freezed at t\_max\_sat.

! 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)

deposition\_at\_frontiers Gamma\_slope\_flag

! 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)

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

t\_q0 t\_liq ! t\_q0: quake start time; t\_liq:

! liquefaction time

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(only if

! erosion\_criterion\_ID>0)

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 ! >0.

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

! parameter)

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

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

phi saturated\_medium\_flag ! phi(internal friction angle in degrees,

! even if the code works in radians);

! saturated\_medium\_flag=.true.(fully

! saturated medium),.false.(dry medium).

cohesion viscosity\_max tuned\_viscosity limiting\_viscosity

! cohesion (draft parameter); viscosity\_max

! (threshold for the dynamic mixture

! viscosity to held particles fixed in

! the elastic-plastic strain regime);

! tuned\_viscosity (tuned dynamic viscosity -

! only for Manenti et al., 2012)

! limiting dynamic viscosity

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

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

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

roughness\_coefficient d\_50

! roughness\_coefficient; d\_50

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

! Bodies with imposed kinematics are listed after all the bodies with computed

! kinematics

n\_bodies dx/dx\_body friction\_angle time\_max\_no\_gravity\_force time\_max\_no\_body\_frontier\_impingements body\_minimum\_pressure\_limiter body\_maximum\_pressure\_limiter FSI\_free\_slip\_conditions

! n\_bodies(number of transported solid

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

! particle size and body particle size);

! friction\_angle(in radians; non-negative

! value: friction angle for body-frontier

! interactions; negative value: sliding

! friction depends on the local slope angle

! instead of the friction angle);

! time\_max\_no\_gravity\_force(gravity

! force is deactivated until this time, no

! deactivation in case of negative value);

! time\_max\_no\_body\_frontier\_impingements

! (body-frontier impingements are

! deactivated until this time, no

! deactivation in case of negative value);

! body\_minimum\_pressure\_limiter=

! .true.(no negative pressure on the body

! surface),.false.(no limiter);

! body\_maximum\_pressure\_limiter=

! .true.(maximum pressure on the body

! surface is limited by physical

! constraints),.false.(no limiter);

! FSI\_free\_slip\_conditions=.true.(free-slip

! conditions for FSI),.false.(no-slip

! conditions for FSI)

! 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

n\_R\_IO\_x n\_R\_IO\_y n\_R\_IO\_z teta\_R\_IO

! n\_R\_IO(rotation axis -unit vector-);

! teta\_R\_IO(rotation angle). Rotation of

! the body with respect to the reference

! system at t=0. This rotation is

! cumulative with respect to the element

! initial rotation. This rotation is

! relevant only for IC and I/O purposes.

pos\_rotC\_x pos\_rotC\_y pos\_rotC\_z ! pos\_rotC(centre of rotation for the

! vector alfa 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)

! do i=1,n\_records

time\_i velocity\_x\_i velocity\_y\_i velocity\_z\_i omega\_x\_i omega\_y\_i omega\_z\_i

! i-th record for the imposed

! kinematics of the body (the time of the

! last record should be slightly higher

! than time at the end of the simulation)

! enddo

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)

n\_R\_IO\_elem\_x n\_R\_IO\_elem\_y n\_R\_IO\_elem\_z teta\_R\_IO\_elem

! n\_R\_IO\_elem(rotation axis -unit vector-);

! teta\_R\_IO\_elem(rotation angle). Rotation

! of the body element with respect to the

! reference system at t=0. This rotation is

! cumulative with respect to the body

! IC rotation. This rotation is relevant

! only for IC and I/O purposes.

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; in

! case of a restarted simulation, these

! values are reported in the log file, but

! they are actually overwritten by the

! values read from the input restart file);

! this line has no influence in case of

! restart

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

! CFL;

! vsc\_coeff(viscous stability condition

! coefficient, default value: 0.05);

! 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,

! COEFNMAXPARTI considers that the number of

! particles inside the domain can be higher

! than the first assessment of the number of

! SPH particles (initial particles or

! reservoir particles -in case reservoir is

! derived from topography-): COEFNMAXPARTI

! takes into account contributions from

! inlet sections and, in case of reservoir

! derived from topography, also the

! particles of the mixture dam/reservoir

! (beyond the main water reservoir);

! COEFNMAXPARTJ:maxb(max number of

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

! same number applies both for fluid

! neighbours and DB-SPH wall element

! neighbours;

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

! frontiers),1(mobile frontiers)

nag\_aux MAXCLOSEBOUNDFACES MAXNUMCONVEXEDGES GCBFVecDim

! nag\_aux(rough overestimation of the

! number of fluid particles in the

! domain, it is only related to the very

! first allocation of the particle array,

! it is influential only in case of

! reservoir extruded from topography);

! MAXCLOSEBOUNDFACES(max number of

! neighbouring boundary face per fluid

! particle); MAXNUMCONVEXEDGES(max number

! of edges); GCBFVecDim (rough

! overestimation of the number of Grid Cell

! - Boundary Face intersections (SA-SPH;

! in case of restart, this value is only

! read, not used; in case its value is too

! little, crashes occur without code

! warnings/errors; GCBFVecDim only occupies

! 4B times the number of elements, thus, it

! is sufficient to overestimate this number

! as the number of faces times the number

! of the positioning grid cells, further,

! reducing GCBFVecDim does not imply any

! appreciable variation in the computational

! time).

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

! density limiters),1(density limiters for

! debug)- Density limiters do not apply to

! the mixture particles which are held

! fixed (elasto-plastic strain rate

! regime)

##### 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 #####

restart\_mode restart\_time\_value ! restart\_mode("time" or "step");

! restart\_time\_value(positive time value in

! seconds or step number, according to

! restart\_mode; this value has to be lower

! than the time value of the last restart

! output; default value: 2.\*dt\_out\_PV)

restart\_file ! restart\_file(restart file name -with

! file extension-)

##### 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 for the water

! front: output file ".fro")

restart time dt\_restart ! dt\_restart(restart time frequency)

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\_reservoir\_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\_reservoir\_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 ! The edge order is not arbitrary to detect the

! free surface. Edge 1 is the farest from the

! free surface.

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. These sections must

! be convex non-degenerate quadrilaterals. Otherwise, the subroutine call for

! point\_inout\_convex\_non\_degenerate\_polygon must be replaced with other

! calls (to subroutines such as point\_inout\_quadrilateral).

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 ! to be omitted in case of triangles

! vertices of the first section (

! anti-clockwise viewing the section face

! from the outside of the fluid domain)

... ! other possible section records

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

##### substations #####

! Input variables for monitoring the electrical substations (both high-voltage

! transmission substations, medium-voltage distribution substations and

! low-voltage distribution substations). From a plan view, each substation is

! described by a polygon (either triangle, quadrilateral, pentagon or hexagon).

n\_sub dt\_out\_sub ! n\_sub(number of the substations);

! dt\_out\_sub(writing time step duration for

! monitoring the substations)

first\_substation\_ID ! first\_substation\_ID=1

type\_ID n\_vertices ! type\_ID(substation type ID)=1

! (high-voltage),2(medium-voltage),3

! (low-voltage);

! n\_vertices(number of vertices describing

! the substation)=3,4,5,6

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 ! to be omitted in case of triangles

vertex\_5\_x vertex\_5\_y vertex\_5\_z ! to be omitted in case of

! ! triangles/quadrilaterals

vertex\_6\_x vertex\_6\_y vertex\_6\_z ! to be omitted in case of

! ! triangles/quadrilaterals/pentagons

! vertices of the first section (

! anti-clockwise viewing the substation from

! the outside of the fluid domain:

! clockwise in plan view)

... ! other possible section records

##### end substations #####

Figure 13.1. Commented template of the main input file of SPHERA v.9.0.0.

* 1. Tutorials

SPHERA v.9.0.0 is validated on 34 test cases (following sub-sections), each one having possible variants. Some of the tutorials 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.

* + 1. “body\_body\_impacts”

This tutorial is completely described in Amicarelli et al. (2015). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “body\_boundary\_impacts”

This tutorial is completely described in Amicarelli et al. (2015). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “dam\_breach\_ICOLD\_trunks”

This tutorial is described in Amicarelli & Agate (2014, SPHERIC) and Amicarelli & Agate (2015, SPHERIC). Here, the tutorial is represented by means of the mixture model for dense granular flows of Amicarelli et al. (2017).

* + 1. “db\_2bodies”

This tutorial is completely described in Amicarelli et al. (2015). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “db\_2D\_demo”

This is a very simple and very fast tutorial representing a 2D dam break (over a flat bottom) at a rough spatial resolution. Amicarelli et al. (2013, RdS) completely describes this test case. This project report is Open-Access and also includes a synthetic English version.

* + 1. “db\_Alpe\_Gera”

This tutorial is completely described in Amicarelli & Agate (2017). This project report is Open-Access and also includes a synthetic English version.

* + 1. “db\_Alpe\_Gera\_Lanzada\_substations”

This tutorial is completely described in Amicarelli (2018). This project report is Open-Access and also includes a synthetic English version.

* + 1. “db\_body\_exp\_UniBas”

This tutorial is completely described in Amicarelli et al. (2015). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “db\_ICOLD”

This tutorial is described in Amicarelli & Agate (2014, SPHERIC).

* + 1. “db\_multi\_body”

This tutorial is completely described in Amicarelli et al. (2015). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “db\_squat\_obstacle”

This tutorial is described in Amicarelli et al. (2013). The paper version available on ResearchGate might help in case the published version is unavailable. Here, the surface mesh is generated by SnappyHexMesh (2018) and SPHERA source code improvements for the DB-SPH treatment (Amicarelli et al., 2015, SPHERIC) apply.

* + 1. “db\_tall\_obstacle”

This tutorial is described in Amicarelli et al. (2013). The paper version available on ResearchGate might help in case the published version is unavailable. Here, the surface mesh is generated by SnappyHexMesh (2018) and SPHERA source code improvements for the DB-SPH treatment (Amicarelli et al., 2015, SPHERIC) apply.

* + 1. “dike\_breach\_2D\_expSchHag12JHR\_ID22”

This tutorial is completely described in Amicarelli & Agate (2017, RdS). This project report is Open-Access and also includes a synthetic English version.

* + 1. “edb\_2D\_demo”

This tutorial of SPHERA v.9.0.0 (2015) was used as a reference test case to carry out a sensitivity analysis in Manenti et al. (2018). This paper is Open-Access and also describes in detail the present test case.

* + 1. “edb\_2D\_FraCap02”

This tutorial is described in Amicarelli et al. (2017). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “edb\_2D\_FraCap02\_Taipei”

This tutorial is described in Amicarelli et al. (2017). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “edb\_2D\_Spi05”

This tutorial is described in Amicarelli et al. (2017). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “edb\_ICOLD”

This tutorial is described in Amicarelli et al. (2017). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “edb\_KarlSand”

This tutorial is described in Amicarelli et al. (2017). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “edb\_Pon10”

This tutorial is described in Amicarelli et al. (2017). The paper version available on ResearchGate might help in case the published version is unavailable.

* + 1. “floating\_cube\_stability”

This is a very simple and demonstrative tutorial: a solid cube is leaned on still water (rough resolution). Amicarelli et al. (2014, SPHERIC) completely describes this test case, which is also available on Amicarelli et al. (2014, RdS). This project report is Open-Access and also includes a synthetic English version.

* + 1. “flushing\_2D”

This tutorial is described in Amicarelli & Agate (2014, SPHERIC). Here, the tutorial is represented by means of the mixture model for dense granular flows of Amicarelli et al. (2017).

* + 1. “flushing\_3D”

As a 3D version of the previous tutorial, this test case is available on Amicarelli et al. (2014, RdS). This project report is Open-Access and also includes a synthetic English version.

* + 1. “jet\_plate”

The 7 variants of this tutorial are described in Amicarelli et al. (2013) and Amicarelli et al. (2015). Here the DBSPH boundary scheme is treated with automated procedures (Amicarelli & Agate, 2015, SPHERIC) and the scheme for body transport is corrected in terms of no-slip conditions for fluid-body interactions (Amicarelli, 2018, SPHERIC).

* + 1. “rectangular\_side\_weir\_Fr\_0\_491”

This tutorial is described in Amicarelli (2018, SPHERIC) and is also available in Amicarelli & Agate (2017, RdS). This project report is Open-Access and also includes a synthetic English version.

* + 1. “San\_Fernando\_Lower\_van\_Norman\_dam\_liquefaction”

This tutorial is described in Amicarelli (2016, SPHERIC). Here, the tutorial is represented by means of the mixture model for dense granular flows of Amicarelli et al. (2017).

* + 1. “sloshing\_tank\_TbyTn\_0\_78”

This tutorial is described in Amicarelli et al. (2013). The paper version available on ResearchGate might help in case the published version is unavailable. Here, the surface mesh is generated by SnappyHexMesh (2018) and SPHERA source code improvements for the DB-SPH treatment (Amicarelli et al., 2015, SPHERIC) apply.

* + 1. “sloshing\_tank\_TbyTn\_1\_07”

This tutorial is described in Amicarelli et al. (2013). The paper version available on ResearchGate might help in case the published version is unavailable. Here, the surface mesh is generated by SnappyHexMesh (2018) and SPHERA source code improvements for the DB-SPH treatment (Amicarelli et al., 2015, SPHERIC) apply.

* + 1. “spherical\_Couette\_flows”

This tutorial is described in Amicarelli (2016, SPHERIC). The tutorial is also available on Amicarelli & Agate (2016, RdS). This project report is Open-Access and also includes a synthetic English version.

* + 1. “SPH\_udb\_exp\_Kim2015HYDROL”

This tutorial is described in Amicarelli (2018, SPHERIC). The tutorial is also available on Amicarelli (2017, RdS). This project report is Open-Access and also includes a synthetic English version.

* + 1. “submerged\_landslide”

This tutorial is described in Amicarelli & Agate (2014, SPHERIC). Here, the tutorial is represented by means of the mixture model for dense granular flows of Amicarelli et al. (2017).

* + 1. “still\_water\_tank”

This tutorial is a very simple and rough-resolution 2D test case on hydrostatic conditions.

* + 1. “wave\_motion\_for\_WaveSAX”

This tutorial is described in Peviani et al. (2017, RdS). This project report is Open-Access and also includes a synthetic English version.

* + 1. “wedges\_falls\_on\_still\_water”

This tutorial is completely described in Amicarelli et al. (2015). The paper version available on ResearchGate might help in case the published version is unavailable.

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* HPCEFM15 - High Performance Computing for Environmental Fluid Mechanics 2015 (Italian National HPC Research Project); instrumental funding based on competitive calls (ISCRA-C project at CINECA, Italy); 2015 - in progress; Amicarelli A., A. Balzarini, S. Sibilla, G. Agate, G. Leuzzi, P. Monti, G. Pirovano, G.M. Riva, A. Toppetti, E. Persi, G. Petaccia, L. Ziane, M.C. Khellaf.
* HSPHMI14 - High performance computing for Lagrangian numerical models to simulate free surface and multi-phase flows (SPH) and the scalar transport in turbulent flows (MIcromixing); June 2014 - March 2015; Amicarelli A., G. Agate, G. Leuzzi, P. Monti, R. Guandalini, S. Sibilla; HPC Italian National Research Project (ISCRA-C2); competitive call for instrumental funds.

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# SPHERA registration

SPHERA v.8.0 Copyright is registered (“Registro pubblico speciale per i programmi per elaboratore, SIAE”, Italy). Since SPHERA v.8.0, the code has been developed on a public GitHub repository.

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