Wall boundary condition for the unconditionally stable SPH

Jose Luis Cercos-Pita, Pablo Eleazar-Merino
CoreDigital department
CoreMarine AB
Stavanger, Norway
jlc@core-marine.com

Daniel Duque, Javier Calderon-Sanchez
Canal de Ensayos Hidrodinámicos (CEHINAV)
Universidad Politécnica de Madrid (UPM)
Madrid, SPain

I. Introduction

The SPH method, particularly in its weakly-compressible form (WCSPH), has often been considered an unstable numerical scheme, as supported by numerous critical publications (e.g., [1], [2]). Furthermore, the existence of the SPHERIC Grand Challenge GC#1, which focuses on "Consistency, Stability and Convergence", underscores the ongoing concerns regarding the stability of SPH.

However, this assumption may be attributed to misunderstandings and misconceptions. A closer examination of energy balance, as an extension of power balance (e.g., [3]), reveals that incorporating the time integration scheme is crucial for maintaining true energy balance [4]. This insight has led to two significant breakthroughs: a methodology for quantifying the artificial energy added to or removed from the system, and the development of a novel time integrator that intrinsically conserves energy. This time integrator is the Implicit Mid-Point (IMP) Euler scheme.

The resulting time-integration algorithm yields an unconditionally stable scheme, as long as the underlying fixed-point problem is solved accurately. In the original publication [4], a semi-implicit approach was adopted in practice, employing an iterative method to solve the fixed-point problem. Numerical experiments showed that the algorithm converged spectrally to the exact solution, producing residuals that were low enough to maintain stability, even with a relatively small number of iterations per time step. Furthermore, these simulations were performed using the Euler equations for ideal fluids, without any dissipative terms, supporting the robustness of the algorithm.

In light of these findings, we propose to revisit the SPHERIC Grand Challenge GC#1, reevaluating stability as a topic of concern. The work demonstrates that the WCSPH formulation is stable, and that other formulations can be reformulated to achieve unconditional stability as well.

However, unconditional stability is compromised by boundary conditions, except in the case of free surface boundaries, which can be modeled as compact support truncations. This limitation is acknowledged by the SPHERIC community, as reflected in the Grand Challenge GC#2: *Boundary Conditions*. In particular, the following question is posed on the challenge description:

> How to include BCs without losing intrinsic SPH conservation properties?

This paper addresses this question by formulating a boundary condition for solid walls that prioritizes energy conservation.

II. Solid walls model with exact energy conservation

Any SPH operator can be decomposed into two distinct terms,

$$\langle\cdot\rangle = \langle\cdot\rangle^{\Omega} + \langle\cdot\rangle^{\partial\Omega}, \tag{1}$$

representing the contributions from the fluid domain and the boundary, respectively. At first glance, it may seem intuitive to associate the first term with particle-particle interactions within the fluid and the second term with particle-boundary interactions. However, some formulations blur this distinction by incorporating particle-particle interactions into the second term, such as boundary formulations that require renormalization terms, like Boundary Integrals (BI) [5].

For simplicity, we consider an inviscid flow without conservative external forces. The total power, comprising the kinetic and compressibility energy variation rates, shall be equal to the power transferred from the boundary to the fluid:

$$\langle P_\mathrm{k}\rangle + \langle P_\mathrm{c}\rangle = -\langle P\rangle^{\partial\Omega}, \tag{2}$$

where the kinetic power and compressibility powers are defined as:

$$\langle P_\mathrm{k}\rangle := -\sum_{i\in\Omega}\frac{m_i}{\rho_i}\boldsymbol{u}_i\cdot\langle\nabla p\rangle_i^{\Omega} - \sum_{i\in\Omega}\frac{m_i}{\rho_i}\boldsymbol{u}_i\cdot\langle\nabla p\rangle_i^{\partial\Omega}, \tag{3}$$

$$\langle P_\mathrm{c}\rangle := -\sum_{i\in\Omega}\frac{m_i}{\rho_i}p_i\langle\nabla\cdot\boldsymbol{u}\rangle_i^{\Omega} - \sum_{i\in\Omega}\frac{m_i}{\rho_i}p_i\langle\nabla\cdot\boldsymbol{u}\rangle_i^{\partial\Omega}. \tag{4}$$

If the discrete gradient and divergence operators are properly chosen to be skew-adjoint, then, for fixed walls, the last term of Eq. (2) cancels the sum of the last terms in Eqs. (3 & 4). Indeed, for the popular symmetric gradient and antisymmetric divergence, the balance can be written as

$$\langle P\rangle^{\partial\Omega} = \sum_{i\in\Omega}\sum_{j\in\bar{\Omega}}\frac{m_i}{\rho_i}\frac{m_j}{\rho_j}\left(p_j\boldsymbol{u}_i + p_i\boldsymbol{u}_j\right)\cdot\nabla W_{ij}. \tag{5}$$

with $\bar{\Omega}$ being the complementary domain (the "outside" of the simulation cell), where the field values must be defined. In particular, the fields of the form

$$\begin{cases} \boldsymbol{u}_j = -k\boldsymbol{u}_i \\ p_j = kp_i, \end{cases} \tag{6}$$

are solutions to Eq. (5). The constant k can be used to model different boundary conditions. For solid walls, $k = 1$ is the sensible option, resulting in a local symmetric extension.

Therefore, fixed walls may be modeled with boundary terms

$$\langle \nabla p \rangle_i^{\partial\Omega} = -2p_i \sum_{j\in\bar{\Omega}} \nabla W_{ij} \frac{m_j}{\rho_j}, \tag{7}$$

$$\langle \nabla \cdot \boldsymbol{u} \rangle_i^{\partial\Omega} = 2\boldsymbol{u}_i \cdot \sum_{j\in\bar{\Omega}} \nabla W_{ij} \frac{m_j}{\rho_j}, \tag{8}$$

which are fully compatible with a BI description,

$$\langle \nabla p \rangle_i^{\partial\Omega} = 2p_i \sum_{j\in\partial\Omega} \boldsymbol{n}_j W_{ij} s_j, \tag{9}$$

$$\langle \nabla \cdot \boldsymbol{u} \rangle_i^{\partial\Omega} = -2\boldsymbol{u}_i \cdot \sum_{j\in\partial\Omega} \boldsymbol{n}_j W_{ij} s_j, \tag{10}$$

where s_j is the area of a generic j-th boundary element and $\boldsymbol{n}_j$ its outward-facing normal vector. Note that this BI formulation does not require a renormalization factor.

In order to extend the previous expressions to moving walls, let $\boldsymbol{U}_j$ be the velocity of the j-th boundary element. The energy transfer rate due to the interaction of particle i with boundary element j can be expected to be

$$\langle P \rangle_{ij}^{\partial\Omega} = \frac{m_i}{\rho_i} (s_j p_j \boldsymbol{n}_j) \cdot \boldsymbol{U}_j W_{ij}, \tag{11}$$

leading to these final expressions for the differential operators:

$$\langle \nabla p \rangle_i^{\partial\Omega} = 2p_i \sum_{j\in\partial\Omega} \boldsymbol{n_j} W_{ij} s_j, \tag{12}$$

$$\langle \nabla \cdot \boldsymbol{u} \rangle_i^{\partial\Omega} = 2 \sum_{j\in\partial\Omega} (\boldsymbol{U}_j - \boldsymbol{u}_i) \cdot \boldsymbol{n_j} W_{ij} s_j. \tag{13}$$

III. Practical applications

Four practical applications are considered: First, the normal impact of a fluid jet upon a surface, which mimics one of the simulations carried out in Ref. [4]. Second, a moving piston, a quite challenging simulation that, to our knowledge, cannot be carried out with any other current formulation. Third, a canonical dam-break, with different formulations. Finally, a 3D spacecraft landing on water, in order to assess the capability of the new formulation to deal with complex geometries and severe impacts.

Except when stated otherwise, all simulations are carried out with the IMP [4] and the boundary condition treatment proposed in Eqs. (12 & 13). No boundary force or any other methodology is applied to grant that the boundary is not trespassed. (In fact, some particles do indeed trespass the walls, but they always remain attached to the boundary and eventually move back to the fluid domain.)

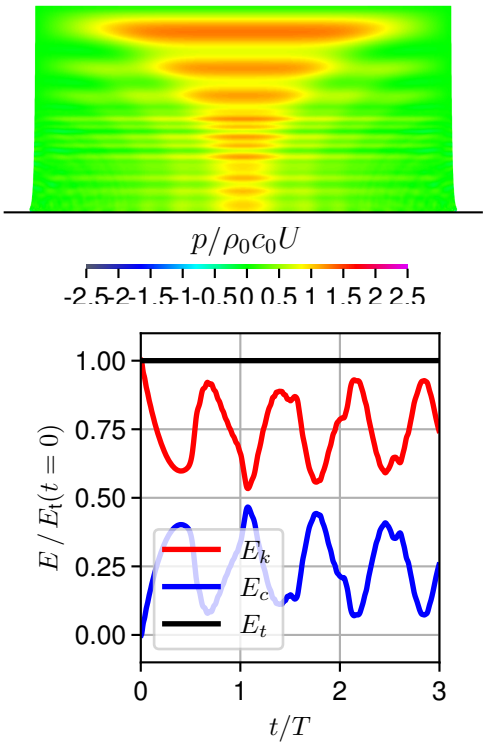

Fig. 1. Normal impact simulation. Top: Snapshot of the simulation at $t = T/4$. Bottom: Energy profile

A snapshot of the normal fluid jet impact simulation, as well as its energy profile, is depicted in Fig. 1. As expected, the simulation results resemble those obtained with the normal impact of two fluid jets [4].

Much more interesting is the simulation of the adiabatic expansion and contraction of a piston. A compressible fluid is enclosed in a box with an initial pressure that is higher than that outside. The fluid is left to expand pushing the piston wall outward, until it stops and compresses back, with a resulting oscillatory motion. Again, inviscid flow is considered, so the energy should be exactly conserved as the piston moves periodically. The simulation is particularly challenging because pressure waves are constantly introduced into the fluid by the moving wall, but no dissipation occurs, or else the motion would cease to be periodic.

Fig. 2 shows a snapshot of the piston simulation, together with the energy profile during three cycles. The snapshot clearly shows the expected pressure waves — nevertheless, as shown by the energy profile, the simulation remained stable and the energy is well conserved.

Regarding the dam-break case, it has been simulated with the current formulation as well as the traditional BI [5]. These are carried out with either no dissipative terms, or with a δ-SPH treatment [3].

On Fig. 3 the pressure register at a probe is depicted, for

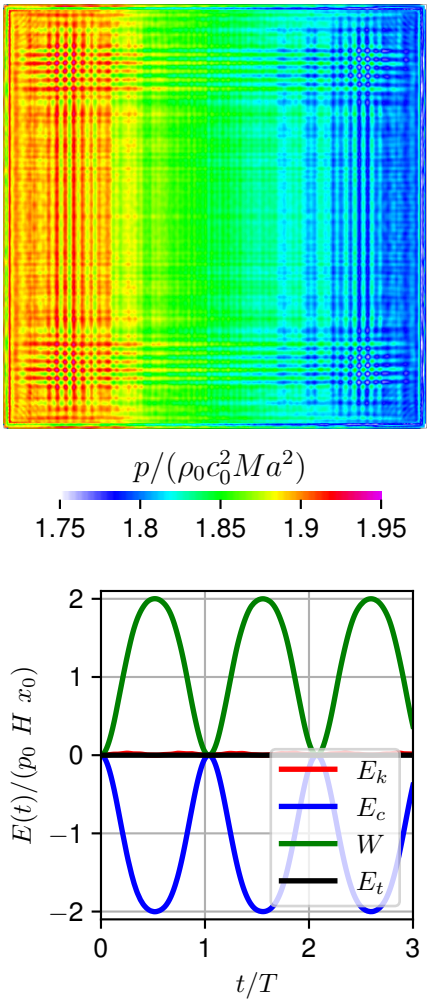

Fig. 2. Piston simulation. Top: Snapshot of the simulation at $t/T = 0.2$. Bottom: Energy profile

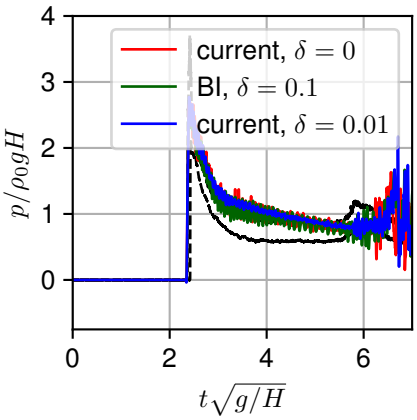

Fig. 3. Pressure at sensor 1 for different formulations.

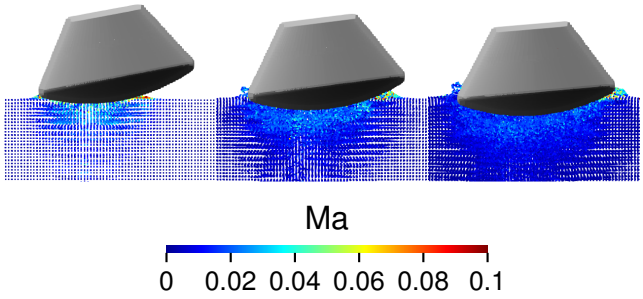

Fig. 4. Snapshots of the spacecraft landing

several formulations — but for the traditional BI without δ-SPH, which quickly becomes unstable. The new formulation is seen to produce results similar to BI when a fairly large δ parameter is considered for the latter. Along the same line, the current formulation results in significantly less noisy fields when a very small δ dissipation is set.

Finally, snapshots of the spacecraft landing are depicted in Fig. 4. The new formulation is able to effectively deal with complex 3D geometries, keeping the simulation stable without dissipative terms even for rather violent impact phenomena.

IV. Conclusions

A novel boundary condition formulation for solid walls has been introduced, offering exact energy conservation and consistent mechanical energy transfer between the solid and fluid.

When combined with the IMP, this formulation results in an unconditionally stable scheme. This stability allows for smooth SPH simulations of highly dynamic and challenging cases, without the need for dissipative terms to ensure stability. For instance, this advancement enables the simulation of the adiabatic expansion and contraction, a task previously impossible with existing methods in the literature. Additionally, the new formulation has shown superior performance in the dam-break scenario, outperforming other available approaches.

Furthermore, the formulation is easy to implement and, due to its boundary-integral (BI) nature, as opposed to traditional fluid extensions, it is particularly well-suited for simulations involving complex geometries.

Bibliography

[1] J. Vila, "On particle weighted methods and Smooth Particle Hydrodynamics," *Mathematical Models & Methods in Applied Sciences*, vol. 9, no. 2, pp. 161–209, 1999.

[2] D. Meringolo, A. Colagrossi, S. Marrone, and F. Aristodemo, "On the filtering of acoustic components in weakly-compressible SPH simulations," *Journal of Fluids and Structures*, vol. 70, pp. 1–23, 2017.

[3] M. Antuono, S. Marrone, A. Colagrossi, and B. Bouscasse, "Energy balance in the δ-SPH scheme," *Computer Methods in Applied Mechanics and Engineering*, vol. 289, pp. 209–226, 2015.

[4] J. L. Cercos-Pita, P. E. Merino-Alonso, J. Calderon-Sanchez, and D. Duque, "The role of time integration in energy conservation in smoothed particle hydrodynamics fluid dynamics simulations," *European Journal of Mechanics-B/Fluids*, vol. 97, pp. 78–92, 2023.

[5] M. Ferrand, D. R. Laurence, B. D. Rogers, D. Violeau, and C. Kassiotis, "Unified semi-analytical wall boundary conditions for inviscid, laminar or turbulent flows in the meshless SPH method," *International Journal for Numerical Methods in Fluids*, vol. 71, no. 4, pp. 446–472, 2013.