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EDITORIAL

Latest developments and application of SPH using DualSPHysics

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The meshless method smoothed particle hydrodynamics (SPH) experienced major developments over the past 20 years. Due to its Lagrangian nature, SPH is being proven to be a robust and accurate computational method suited for scientific applications specifically characterised by complex and violent hydrodynamics, multi-physics, highly deforming interfaces, high nonlinearity and fragmentation. Recent developments of SPH embrace a wide range of different physical phenomena and application fields, including coastal and offshore engineering, astrophysics, mixing and multiphase problems in process engineering, flexible or deformable structures, hydraulics engineering, wave breaking and fluid–structure interaction, processes in waste water treatment, wave energy and naval engineering.

The typical bottleneck of such approach is its computational cost. In particular, for weakly compressible SPH (WCSPH), due to the large number of neighbouring particles (i.e. computational nodes) and the explicit time integration which results in small timesteps, researchers and developers have striven towards hardware acceleration using message passing interface (MPI) and more recently, graphic processing units (GPUs).

Among the WCSPH-based solvers developed worldwide, the DualSPHysics solver (https://dual.sphysics.org/) is possibly the most downloaded (recently achieved the 100,000 downloads) and most advanced open-source SPH-based code worldwide. DualSPHysics is developed as a collaboration between the Universidade de Vigo, University of Manchester, University of Lisbon, Università di Parma, Universitat Politécnica de Catalunya, and New Jersey Institute of Technology. DualSPHysics use is intended to enable simulations of real engineering problems using a standard desktop PC using the computational power of modern GPUs.

The present Special Issue "*Latest Developments and Application of SPH using DualSPHysics*" in Computation Particle Mechanics collects a variety of articles with relevant advances in implementation and/or application of the SPH-based DualSPHysics solver. The research papers published in the present Special Issue are highlighted hereafter with a brief overview of the major advancements.

The first paper presents the latest developments included in the DualSPHysics solver. The DualSPHysics solver was initially focused on coastal engineering problems using high-performance computing techniques to deal with the high computational cost of the SPH method. This manuscript describes the improvements added to DualSPHysics that allowed the solver to evolve from a pure fluid dynamics solver to a complete multiphysics framework. Significant formulation advances such as the new density diffusion term or the improved mDBC boundary conditions are included. The coupling with wave generation and propagation models such as SWASH and OceanWave3D was incorporated into the SPH solver to minimise the size of the study area and optimise the use of SPH. The incorporation of the discrete element method allows modelling complex debris flows. Other coupling methodologies that enable multiphysics simulations are the coupling with the MoorDyn library to simulate floating objects with a variety of moorings and the coupling with the Project Chrono multiphysics library to model complex articulated mechanisms with joints, hinges and springs. The latest hardware acceleration enhancements are also included to exploit the computing power of current GPUs. The manuscript also presents the different DualSPHysics approaches for multiphase gas–liquid simulations and the combination of Newtonian and non-Newtonian fluids. The combination of the above enables DualSPHysics to address a wide range of applications, the most challing and novel ones are highlighted.

While the first paper focuses on the DualSPHysics solver, the second paper describes an open-source tool that allows

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the user to render realistic images and animations for DualSPHysics simulations. This post-processing tool named VisualSPHysics is integrated into Blender suite (https://www.blender.org/). As multi-platform 3D animation software, VisualSPHysics has been distributed as open source. VisualSPHysics allows to load the results of SPH simulations performed by DualSPHysics into the Blender environment, and then add the numerous professional visualisation effects available in Blender. This provides SPH users with quick and easy access to realistic visualisation of their application cases with DualSPHysics for dissemination and outreach activities.

The third paper presents a significant advance in boundary conditions (BCs) for DualSPHysics solver and the SPH method in general. DualSPHysics employs dynamic boundary conditions (DBC) that are simple, robust, efficient and relatively accurate with complex 2D and 3D geometries. However, the DBC methodology presented some problems such as the creation of a non-physical gap between the fluid and the boundary or the presence of noise in the pressure near the boundary. Reducing these inaccuracies usually requires increasing the resolution which results in a significant increase in execution times. This manuscript describes the new mDBC boundary conditions included in DualSPHysics (modified dynamic boundary conditions). The mDBC wall boundary is able to solve the main issues of DBC even for complex 3D geometries. The use of mDBC does not increase the computation time significantly and also allows more accurate results to be obtained using lower resolution, which means a major reduction in the execution time. The capabilities of the mDBC are demonstrated through various academic tests and by validation using a complex 3D flow in a fish pass with experimental data.

The authors of the fourth paper performed a numerical investigation into a rough bed in combination with body near the bed in the presence of a free-surface flow. The body considered is a sphere in close proximity to the rough bed. The aim is to examine the hydrodynamics near the vicinity of natural sediment in fluvial beds, fish habitat structures or even architectural structures. The results are validated qualitatively and quantitatively against experimental data using the velocity profile and forces measurements and show good overall agreement to the experiments. This work demonstrates how SPH can be applied to environmental flows especially fluvial beds.

The work in the fifth paper describes a numerical campaign on fish passages, more specifically on the vertical slot fishway (VSF). The hydraulic parameters of the free-surface flow in the Igarapava HPP fishway, in Brazil, were studied. The numerical results were compared to available experimental data. Open boundary conditions applied in inlet and outlet zones allowed reproducing discharges, velocity profiles, and water elevation accurately. Authors focused on examining the effectiveness of diffusion terms for the momentum and continuity equation in SPH. Results demonstrated that the numerical model accuracy benefits from the artificial diffusion terms (i.e. combining delta-SPH and artificial viscosity) that allow to remove that the numerical noise and improve the accuracy of the numerical results.

The sixth paper presents a novel application of the DualSPHysics in the field of coastal engineering and coastal protection. To employ a meshless approach allowed elucidating the scattering process of the armour blocks on the additional rubble mound behind a breakwater during tsunami overflow events and providing further knowhow for the design of resilient coastal defences. Numerical analysis was performed using a block model with its shape adjusted to account for the artificial gap created by the Dynamic Boundary Conditions. The displacement of armour units under tsunamis flows was reproduced and validated with experimental data. In addition, by means of numerical modelling, the hydrodynamic forces that caused the instability of the armour blocks were assessed accurately. This further knowledge might help to optimize shape and interlocking of the proposed armour units in future designs. Besides the mere technical aspect, the work is an elegant example where some of the functionalities available in DualSPHysics code were satisfactory employed for the scope: i) Dynamic Boundary Conditions, ii) Periodic Boundary Conditions to impose fluid recirculation in the numerical domain, iii) sponge layers to prevent undesired reflected waves, iv) relaxation zone for imposing hydrodynamic boundary conditions and v) coupling with Discrete Element Method to simulate the interaction between solid–solid interaction.

The work presented in the seventh paper describes a novel approach to modelling flexible beams in DualSPHysics by using the extra capabilities provided by the Project Chrono multiphysics library. This technique is based on the Euler–Bernoulli beam theory to define a robust lumped elasticity formulation. Flexible structures were modelled by means of several solid elements connected to each other by rotational hinges with damping and stiffness according to the elastic properties of the structure. One of the advantages of this method was the ease of implementation using the functionality already available in the coupling of DualSPHysics with Project Chrono. The accuracy and stability of this approach were validated by reproducing the static displacement function of an elastic cantilever beam under gravity. The dynamic response was verified with a free-oscillating cantilever plate benchmark. The fluid–structure interaction capability was then assessed by reproducing a column of water breaking and impacting against a flexible plate.

The authors of the eighth paper examined the anisotropic dispersion of a Gaussian contaminant plume in porous media demonstrating an approximately consistent SPH simulations. The approximation consistency was demonstrated by increasing the support size of the smoothing kernel along with the spatial resolution. Of interest is the convergence characteristics of the numerical solution. Indeed, the artificial negative concentrations which are usually present due to numerical oscillations are shown to be minimised. These negative concentrations arisen from the diffusion coefficient tensor and its non-zero off-diagonal components. It is shown that larger supports and therefore smoothing of the concentrations away from the maximum concentrations limit the oscillations and thus unphysical negative values.

The ninth paper deals with the simulation of flow-object-structure interaction for a post overtopping case. The authors proposed a calibration-based methodology based on one-way coupling approach for the incident waves at the offshore boundary of the domain, which results computationally efficient to apply for 3D simulation. Of interest is the understanding of potential risks during extreme storm events, for which detailed post-overtopping processes are investigated using DualSPHysics coupled with the nonlinear shallow water equation-based model SWASH. This is potentially useful for users of SPH methods. The paper shows very interesting results in simulating the flow in a house invested by an overtopping flow and, thanks to visualization tools, it shows the evolution of the flooding and transport of objects in a very effective way for lay observers, being potentially very useful for public engagement. Finally, this work showed how furniture can be moved by a storm wave in a seaside apartment and, although the object/furniture motion is not validated with experiment or other numerical method, demonstrated extended functionalities and applications of the DualSPHysics solver.

The authors of the tenth paper applied the SPH method combined with a microbial kinetic model to evaluate the effects of hydrodynamics on biomass distribution in a stirred bioreactor using different proximity impellers. This manuscript presents an implementation of the DualSPHysics solver extended with: i) a Monod model to describe the growth of microorganisms according to nutrient concentration; ii) a diffusion–advection equation integrated into the fluid dynamic equations to model solute transport due to fluid motion and molecular diffusion due to solute concentration gradients. The microbial and hydrodynamic process were validated with analytical solutions. The mixing time and biomass distribution has then been analysed using different impellers models at different rotational speeds to determine the performance of each impeller design. The robust results provided by this modified version of DualSPHysics opened up a new field of application of this SPH model in important industrial bioprocesses.

The eleventh article presents an analysis of the sensitivity of SPH simulation for highly directionally spreaded and crossing breaking waves to the variation of the value of smoothing length h normalised by initial inter-particle distance dp simulations. Physical model tests from multi-directional wave basin experiments were employed for numerical model validation. Formation, shape, plunging, re-attachment of the plunging jet, position of the forward face of the breaking wave, duration of the breaking, mass of the breaking jet seemed to be accurately reproduced if $h/dp = 1.7 \div 2.0$. For lower values (i.e. $h/dp = 1.4$) the spatial and temporal extent of breaking was considerably underestimated, where large discretisation errors might depend on the low number of particles in the kernel's support for low values of the smoothing length. Values of h/dp larger than 2.0 seemed, instead, to lead to overestimation of the duration and spatial extent of the wave breaking. This work led actually to further understanding of the breaking process and its simulation on particle based schemes: a clear dependence of the spatial extent and the duration of wave breaking on the smoothing length was proven. Although lacking on further analysis on the influence of different kernel functions or diffusive schemes on wave breaking processes, the work is perhaps the first one to look to complex three-dimensional wave breaking, extending further previous works mostly based on 2D modelling.

With the popularity of emerging technologies in discretisation schemes and numerical simulations advancing rapidly, the authors of the twelfth paper portrayed a detail comparison on two of the most popular emerging schemes, smoothed particle hydrodynamics and lattice Boltzmann method (LBM). The work provides a direct comparison on the scheme, the implementation of the physics and the accuracy of such schemes. The numerical methods have similarities on the assumption of weak compressibility through an equation of state for barotropic flows and an explicit time integration. Nevertheless, the origins are different with SPH using a continuum Naver-Stokes discretisation whereas LBM has origins from the meso-scale. Test cases such as the Poiseuille flow, a lid-driven cavity, and oscillatory viscous flows test cases are used to demonstrate the accuracy and convergence characteristics. Conclusions are drawn to the performance of each method with the SPH lacking accurate wall boundary representation and the LBM showing over diffusive numerical characteristics.

The thirteenth paper covers a numerical campaign in an anaerobic digester tank of a wastewater treatment plant aiming to understand the hydrodynamics and most importantly the mixing characteristics using the finite time Lyapunov exponent (FTLE) as a measure of mixing in the tank. Two geometries have been used in this work, a simplified digester geometry which does not include a free-surface and a more realistic geometry from an engineering perspective which reassembles the physical tank closely in the presence of a free surface. In the latter, the inlet in the form of a draft tube generated splashing in the free surface. The authors performed a comparison of the free-surface profile with volume of fluids method and demonstrated the applicability and advantages of SPH and the DualSPHysics solver in such flows. In addition, the FTLE, vorticity and Q-criterion have been used to visualise and quantify mixing.

The fourteenth paper investigates the heat transfer of nuclear reactors for multiphase flows which are usually encountered in such complex applications. As well known, nuclear energy is becoming an emerging topic as a clean energy alternative to fossil fuels. The authors implemented a comprehensive heat transfer model in a single and multiphase setting to examine the suitability of the SPH scheme and the DualSPHysics solver for nuclear applications. Several test cases demonstrated the suitability of the method to such flows, especially in the presence of multiphase flows and conclude positively on the suitability of the scheme in nuclear safety analysis.

Concluding, fourteen scientific journal publications have been collected and published in the present Special Issue "*Latest Developments and Application of SPH using DualSPHysics*" in Computation Particle Mechanics: seven of them proposing novel schemes and numerical model implementations, four contributions tackling novel and challenging model applications in engineering, one rather focused on basics and fundamentals of the proposed SPH scheme in comparison with LBM, and two works on post-processing tool development and applications. Overall, the published works prove evidence of the advances attained over the year by DualSPHysics solver and of the growing scientific community that worldwide is contributing to extend successfully the model applicability beyond its original fields of application.