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Surface tension problems solved with the particle finite element method using large time-steps☆

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ABSTRACT

In previous works [S. R. Idelsohn, J. Marti, P. Becker, E. Oñate, Analysis of multifluid flows with large time steps using the particle finite element method, International Journal for Numerical Methods in Fluids 75 (9) (2014) 621–644. doi:10.1002/fld.3908. URL http://dx.doi.org/10.1002/fld.3908, Juan M. Gimenez and Leo M. González, An extended validation of the last generation of particle finite element method for free surface flows, J Comput Phys 284 (0) (2015) 186–205. doi:http://dx.doi.org/10.1016/j.jcp.2014.12.025. URL http://www.sciencedirect.com/science/article/pii/S0021999114008420], the authors have presented a highly efficient extension of the Particle Finite Element Method, called PFEM-2, to solve two-phase flows. The methodology which uses X-IVS [S. Idelsohn, N. Nigro, A. Limache, E. Oñate, Large time-step explicit integration method for solving problems with dominant convection, Comp Methods in Appl Mech Eng 217–220 (2012) 168–185.] to treat convection terms allowing large time-steps was validated for problems where the gravity forces and/or the inertial forces dominate the flow. Although that is the target range of problems to solve with PFEM-2, most of real problems that fall in these categories also includes other flow regimes in certain regions of the domain. Maybe the most common secondary regime is when the surface tension dominates, as an example when drops or bubbles are released from the main flow, and this feature must be taken into account in any complete numerical strategy.

Attending to that, in this work the treatment of the surface tension to PFEM-2 is included. An implicit CSF methodology is employed together with a coupling between the marker function with a Level Set function to obtain a smooth representation of the normal of the interface which allows an accurate curvature calculation. Examples for curvature calculation and isolated bubbles and drops are presented where the accuracy and the computational efficiency are analyzed and contrasted with other numerical methodologies. Finally, a simulation of a jet atomization is analyzed. This case presents the above mentioned features: it is a inertia-dominant flow with a surface tension phenomena on drops and ligaments break up that can not be neglected.

1. Introduction

Solving efficiently multi-phase flows is still an open challenge. Although the dynamics of single phase flows are well understood and can be solved accurately without loss of efficiency, the computational modeling of two or more phases is an underdevelopment field with growing interest. In multi-phase flows the behavior of the fluid at each phase depends on the interface and its shape depends on the flow, then solving this complex coupling is a challenging task.

According to the framework used to derive the formulation, the numerical methods can be split into two main approaches, named Eulerian (fixed framework) and Lagrangian (mobile framework). Former formulations were the first ones to be developed and they provide a natural evolution from single-phase flows since most of Computational Fluid Dynamics (CFD) software are formulated within a fixed framework, while latter formulations offer a more natural choice for simulations in which deformations are not negligible, such as in multi-phase problems.

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In the Eulerian strategies, the Finite Element Method (FEM) is a standard tool to solve both structural and fluid problems. In the case of standard FEM, the exact solution cannot be represented in the space spanned by the shape functions, then they will not be able to capture it accurately, but an averaged solution will be obtained. This is particularly important for multi-phase models, since domains composed by different phases usually lead to discontinuities in the properties along the interface, which translates into discontinuities in the unknowns or in their gradients. An alternative to overcome this limitation is to use Enriched Finite Elements [4–7], which adds degrees of freedom to elements that are cut by the interface in order to capture the part of the solution that escapes from the standard shape function field. Coppola-Owen et al. [8] proposed a simple enrichment functions that is capable of capturing accurately gradient discontinuities (kinks) in the pressure field. Moreover, Ausas et al. [9] proposed a set of three enrichment functions that are able to capture both kinks and jumps in the pressure. Another option in the Eulerian framework is the Finite Volume Method (FVM), which has more followers than the FEM for fluid dynamics. The domain is discretized with cells, and the solution is obtained by calculating fluxes through the faces of each of them. This leads to a formulation that is automatically conservative on the fluxes, unlike FEM.

No matter which Eulerian strategy is used to solve the fluid dynamics, an accurate and efficient simulation of interface evolution is of fundamental importance. For example, in FEM, the use of enriched space is still insufficient to simulate multi-fluids unless it is coupled with a second tool to locate precisely the position of the interface, necessary to build the extra shape functions. It is possible to distinguish two broad classes of computational methods used to describe the evolution of interfaces, namely: interface capturing and interface tracking methods.

Purely Eulerian algorithms, which solve the fluid in a fixed underlying mesh, use capturing methods. In this approach the interface is determined by an implicit function that is advected in the computational domain. Popular methods of this type are the Level Set Method (LSM) [10], which has become widely used when the interface undergoes extreme topological changes, e.g., merging or pinching off; and the Volume of Fluid (VOF) technique [11], which is naturally employed with FVM.

The LSM consists in using a distance function that is convected according to the fluid velocity. This function represents the distance from a point to the interface. By definition, the interface will be located where its value is zero. This level function is variable in the space, but if it has large variations in time, after some time steps it does not represent the distance to the interface anymore, leading to diffusion of the interface and mainly loss of mass. For this reason a reinitialization of the level set must be done to recover a distance function which guarantees that the properties are better conserved. Moreover, an Eulerian advection of the level set function produces large diffusion and requires small time-steps to achieve accurate solutions.

On the other hand, VOF is based on the conservative nature of the FVM, where instead of tracking an interface, it is more natural to save the content of different phases at each cell and define the shape and position from this data later on. The method defines a function that is the fraction occupied by one of the phases in each cell of the domain. Therefore the interface position is not tracked, but the fraction of fluid instead. Once fluids have been convected among cells, the interface position can be reconstructed (accepting some accuracy loss). This exchange between cells, inherited from the conservative nature of the FVM, allows to guarantee mass conservation. This is an important advantage respect to the LSM, in which mass loss is a critical topic which must be addressed and treated. Moreover, the FVM is very robust and is likely to be the most used one in commercial/widespread codes. As an example of application, OpenFOAM® [12] uses this strategy to solve multi-fluid problems.

Formulations clustered in the Lagrangian framework are a more natural choice for simulations where there are large deformations. The original idea, proposed by Monaghan et al. [13] and later works applied to fluid mechanics [14], was a meshless method named Smoothed Particle Hidrodynamics (SPH). Using particles that are advected carrying its own properties over the domain, they are able to almost avoid the numerical diffusion. In the context of incompressible flow, the Lagrangian perspective makes it possible to use a material derivative formulation where the absence of the non-linear convective terms transform the Navier–Stokes system into a transformed linear coupled problem between points and velocities. In the case of multi-phase problems, the calculation of the interface evolution is naturally done using particles [15,16]. However most of Lagrangian formulations have the uncomfortable drawback of requiring a particle position treatment. In the case of meshless methods a constant track of all the moving points must be kept where searching algorithms have to be used to speed up the computational time to calculate the interaction forces. On the other hand, the mesh-based methods must lead with the necessity of constructing or controlling the mesh quality during each time-step of the simulation if the accuracy of the solution has to be maintained. Searching algorithms, evaluation of the mesh distortions or the re-meshing processes are always computationally expensive and it would be interesting to explore the possibility of avoiding those steps.

Alternatives, that combines both Eulerian and Lagrangian tools, have provided to be a good alternative to pure methods. In [17] a pure Eulerian solver for the fluid is used, but Lagrangian marker particles are used to improve the LSM, then the interface tracking. This method proves to be more accurate than the pure Eulerian or pure Lagrangian counterpart in the tracking of the interface. Another option is the named Particle Finite Element Method (PFEM) [18] which consists of using a set of particles that define the nodes of a finite element mesh. Since fluids have no deformation limit, remeshing must be done at each time step. As all Lagrangian methods, the PFEM offers a more natural solution to problems where the particles of the domain can move freely. Unlike LSM, there is no need to recalculate the surface since the location of the interface is obtained trivially; since each particle is associated with a material no extra function is needed. Combining the original idea of Particle in Cell (PIC) [19] where a fixed mesh is used to calculate forces and pressures and moving particles to convect properties, the PFEM method was extended leading to a novel strategy so-called PFEM-2 [3,20]. Among the advantages of the method, the Lagrangian formulation employed allows to convect material properties such as density, viscosity, etc., eliminating the need of the non-linear convective term. Also, using an improved explicit integration named X-IVS (eXplicit Integration following the Velocity Streamlines) added to an implicit correction of diffusive terms, there is no limitation in the time step, being the required precision the only bound for the time-step [21]. The enhanced PFEM-2 version to solve multiphase problems, presented in [1] and validated in [2], preserves the large time-step goodnesses of the single-phase strategy, also includes enrichment strategies to capture discontinuities in the pressure gradient, i.e., pressure kinks. However, the range of application of this strategy does not cover an important group of two-phase problems such as those where the surface tension is dominant.

In those problems, a surface tension model must be implemented at the interface being a validated strategy the Continuous Surface Force model (CSF) [22] which is based on an approximation of the interface curvature from the gradient of the marker function. In the case of VOF function, the gradient cannot be calculated accurately since it is a discontinuous step function, and its

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