Analysis of two-phase flows using position-based PFEM formulation

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Abstract. The numerical simulation of flows with topological changes is quite challenging, being approached in the literature by different techniques, highlighting fixed mesh methods, generally based on immersed boundary techniques, and the particle-based methods, generally based on a Lagrangian description of the flow. One approach that has proven to be efficient is the particle finite element method (PFEM), which combines the concepts of particle methods with the finite element method. In this context, this work presents the development of methodology for simulating two-phase flows with free surface and topological changes within an alternative formulation of PFEM, where instead of velocities as nodal parameters, particle positions are used. Initially, the domains of the two fluids are represented by a cloud of particles to which the physical characteristics of the fluid that they represent are attributed, as well as the initial conditions. A mesh of finite elements is built on this particle cloud to solve the equation of motion in the Lagrangian description, with the physical characteristics, as well as velocity and pressure fields, being interpolated by the shape functions of the finite elements. To avoid large mesh distortions, and also mesh entanglement, at each step the mesh is destroyed and a new one is built using Delaunay triangulation together with the α-shape method to define the boundaries, together with a particle relocation technique that must ensure the quality of the mesh (avoid extremely small element edges or elements with very small volume), as well as ensuring the conservation of the number of particles of each fluid. This formulation is tested by numerical examples with results compared to the literature.

Keywords: Finite element, Particle methods, Free surface flows, Two-phase flows.

1 Introduction

There are few cases in the field of fluid mechanics where an analytical solution can be found, with the majority of cases being static or steady state. Moreover, such analytical solutions tend to be restricted to a limited set of geometries and boundary conditions. In this way, the study of numerical formulations contributes to Engineering advances in the analysis of physical and geometrically complex fluid mechanics problems.

Several studies have been conducted to simulate free-surface flows problems with topological changes; however, there is still no consensus on the most appropriate computational techniques for modeling these problems. One way of doing this, is with the fixed mesh methods, employing an Eulerian description for the fluid. Based on immersed boundary, or interface capture techniques, such methods allow the free surface to move within a fixed mesh. Although being considered a robust way to simulate problems with topological changes, fixed-mesh methods present difficulties to keepa refined adaptive discretization close to the structure boundary to capture boundary layer effects.

Particle-based methods, such as Smoothed Particle Hydrodynamics (SPH) and Moving Particle Semi-Implicit (MPS) emerge as numerical alternatives for modeling flows with topological changes as in Gingold and Monaghan [1], Koshizuka and Oka [2], Kondo and Koshizuka [3]. Such methods are based on Lagrangian descriptions of the flow and consider the fluid as a set of particles that interact according to specific numerical models that aim to represent the mechanics of a continuous medium.

More recently, Idelsohn et al. [4] proposed the Particle Finite Element Method (PFEM) that combines the advantages of FEM with the concept of particle methods. This method considers the domain represented by a cloud of particles that carry the physical properties of the fluid, such as density, viscosity, and unknown fields, such as velocity and pressure, however, a finite element mesh is built over this cloud to solve the motion equation. This mesh is constantly reconstructed to allow the representation of large distortions and topological changes. This unites the versatility of particle methods with the FEM facilities regarding unstructured discretization and the boundary conditions enforcement, as can one can see in Idelsohn et al. [4], Idelsohn et al. [5] and Aubry et al. [6], Avancini et al. [7]. The traditional PFEM formulation uses particle velocities as the main variables, demanding an additional numerical integration to update particle positions. However, when dealing with particles, it makes sense to consider the position of each material point as the main variable.

In the research group in which this work is inserted, Avancini and Sanches [8] proposes a total Lagrangian finite element formulation based on positions, for free surface flows with finite distortions. In Avancini et al. [7] this formulation is extended to the PFEM context, enabling any distortion scale, including topological changes. This formulation has shown robust and precise, and, at same time has a more compact description. In this context, this work aims to develop and implement numerical techniques to model two-phase flows with multiple interfaces.

2 Lagrangian description of incompressible flows

Taking the equilibrium configuration of the fluid Ω_n in the instant t_n as reference, the partially updated Lagrangian description of the linear momentum equation is given by:

$$\rho\ddot{\mathbf{x}}_{n+1} - \nabla_n \cdot (\mathbf{S} \cdot \mathbf{F}_n^T) - \mathbf{b}_n = \mathbf{0}. \tag{1}$$

for more details on the deduction of this partial differential equation, it is recommended to consult [7, 9]. Where ρ refers to density; $\ddot{\mathbf{x}}_{n+1}$ refers to current acceleration; $\mathbf{F}_n$ refers to the deformation gradient tensor from the reference configuration Ω_n to the current configuration Ω_{n+1}; $\mathbf{b}_n$ refers to the volume forces with respect to the reference volume; and $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor with respect to the reference configuration.

The mass conservation in the updated Lagrangian description can be expressed locally as:

$$\rho_{n+1} J = \rho_n, \tag{2}$$

where J denotes the scalar Jacobian of the deformation from the reference configuration Ω_n (the determinant of $\mathbf{F}_n$) to the current configuration Ω_{n+1}; ρ_{n+1} is the current density and ρ_n is the reference density. Note that for incompressible materials we have $\rho_{n+1} = \rho_n$, so that mass conservation resumes to $J - 1 = 0$.

2.1 Constitutive model

Stress in incompressible Newtonian flows are not dependent from the deformation history, so that the constitutive relationship for incompressible Newtonian flows in terms of second Piola-Kirchhoff stress tensor and Green strain rate tensor may be written as $\dot{\mathbf{E}}$ (see [8]):

$$\mathbf{S} = \mathfrak{D}_n : \dot{\mathbf{E}} - pJ\mathbf{C}^{-1}. \tag{3}$$

where p denotes the pressure; $\mathbf{C}$ is the right Cauchy-Green stretch tensor from Ω_n to Ω_{n+1} and $\mathfrak{D}_n$ is the fourth order constitutive tensor given by:

$$(\mathfrak{D}_n)_{ijkl} = J_n (F_n^{-1})_{ia} (F_n^{-1})_{jb} (F_n^{-1})_{kc} (F_n^{-1})_{ld} (\mathfrak{D}_{n+1})_{abcd}, \tag{4}$$

$\mathfrak{D}_n$ is the constitutive tensor in the reference configuration, $(\mathfrak{D}_{n+1})_{abcd} = \mu\,(\delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc})$ is the constitutive tensor in the current configuration, with μ being the dynamic viscosity.

3 Position-based PFEM for two-phase flow

The basic idea of PFEM is to represent the fluid domain by cloud of particles, with a finite element mesh being built, taking the particles as nodes, to solve the motion equations and update the particle positions. At the end of each time step the FEM mesh is erased and reconstructed for the next step solution. The process of mesh reconstruction is associated to geometric criteria to deffine the fluid subdomains and boundaries [4–7].

3.1 Finite element formulation for one finite step

A weak form of the governing equations presented in section 2 suitable for finite element discretization can be obtained by applying the stationary energy principle according to Avancini and Sanches [8] taking nodal (particle) current positions and pressure as variational parameters. By applying the stationary energy principle regarding current positions, combined with the finite element technique, results the weak form of momentum equation:

$$\int_{\Omega_n} \rho\boldsymbol{\phi}_a\cdot\ddot{\mathbf{x}}^h_{n+1}d\Omega_n+\int_{\Omega_n}\dot{\mathbf{E}}^h:\mathfrak{D}^h_n:\frac{\partial\mathbf{E}^h_n}{\partial(\mathbf{x}_{n+1})_a}d\Omega_n-\int_{\Omega_n}p^h\frac{\partial J^h_n}{\partial(\mathbf{x}_{n+1})_a}d\Omega_n-\int_{\Omega_n}\boldsymbol{\phi}_a\cdot\mathbf{b}_n d\Omega_n-\int_{\Gamma_n}\boldsymbol{\phi}_a\cdot\mathbf{f}^{sup}_n d\Gamma_n=\mathbf{0}, \tag{5}$$

where $\boldsymbol{\phi}_a$ denotes the vector of position shape functions associated to node a; $\ddot{\mathbf{x}}^h_{n+1}$ is the current acceleration; $\dot{\mathbf{E}}^h$ is the Green's strain rate tensor; $\mathbf{E}^h$ refers to Green's strain tensor; $(\mathbf{x}_{n+1})_a$ is the current position of node a; $\mathbf{f}^{sup}_n$ refers to surface forces; p^h denotes the pressure.

PFEM requires pressure and positions to be both interpolated by linear shape functions, however ,it can lead to a spurious pressure field and to numerical instabilities as a result of violating the the inf-sup conditions for incompressible flows [10]. Thus, the application of the stationary energy principle regarding pressure need be be followed by the introduction of a pressure stabilizeing technique. Following Avancini et al. [7], we use the Petrov-Galerking Pressure Stabilization (PSPG), introduced by Tezduyar [11], leading to the stabilized weak form of incompressibility condition:

$$-\int_{\Omega_n}\phi_a(J^h_n-1)d\Omega_n+\int_{\Omega_n}\tau_{PSPG}\frac{1}{\rho}((\mathbf{F}^h_n)^{-T}\cdot\nabla_n\phi_a)d\Omega_n\cdot[\rho\ddot{\mathbf{x}}^h_{n+1}-\nabla_n\cdot(\mathbf{S}^h\cdot(\mathbf{F}^h_n)^T)-\mathbf{b}_n]d\Omega_n=\mathbf{0}, \tag{6}$$

where τ_{PSPG} refers to the stabilizing parameter (see Avancini et al. [7]) and ϕ_a is the pressure shape function associated to node a.

To get the fully discrete equations, we use the time-marching Alpha-Generalized method, leading to a non-linear system that is solved by Newton-Raphson technique, as shown in [7].

3.2 PFEM solution of two-phase flows

In our formulation, the particles carry the physical properties of the fluid (viscosity and density), as well as the nodal values of position and pressure for the continuum media. Thus, the strategy the two-phase flow PFEM model consists of identifying the particles belonging to each fluid domain during pre-processing, establishing a label that identifies the type of fluid, and assigning the appropriate physical parameters.

After solving the nonlinear system of equations by the FEM in a given time step and reaching the current configuration for the particles, the mesh is erased and reconstructed by Delaunar triangulation. At the remeshing step, the α-shape method [4]is employed to define the fluid domain boundaries. However the combination α-shape-Delaunay triangulation can lead to unsuitable meshes, so that a particles relocation technique (see Avancini [9]) is associated to control mesh quality.

As Newtonian fluids can distort indefinitely, some particles can get very close to each other, leading to mesh entanglement risk. In this case, one of the particles is are relocated to the largest element edge linked to particles of the same fluid as the relocated particle and the Delaunay triangulation is performed again, followed by the α-shape boundary deffinition. This implies that the mesh control need to be carried separately to each phase in two-phase flows instead of globally.

At fluid-solid interfaces, ghost fluid particles are kept fixed to prevent leaking. Such ghost particles allow the authomatic fluid-solid contact detection by the Delaunay-α shape procedure [7]. In the case of two phase flows, we allow the ghost particles to assume the physical properties of both fluids.

The physical properties of the ghost particles are deffined after the Delaunay-α shape procedure, when we assigne to the ghost particle the properties of the closest node conected to it.

The resultin strategy is monolithic and the fluid-fluid interface configuration is authomatically updated, being defined by the center of the edges that are linked to particles of different fluids. In this way, for a closed domain filled with two fluids, the α-shape technique is dispensable, as there is no interface with any empty domain to be defined.

4 Numerical examples

In this section we present numerical examples to verify the proposed formulation.

4.1 Fluid layers inversion

This example consists of the analysis of two fluids: water and glycerin. First, the static case is analyzed in order to verify the numerical pressure field with the analytical one. In the second case, the decantation problem is analyzed with the same fluids, but now in inverse positions. Due to the action of gravity, the layers are inverted and at the end the pressure field can be verified again.

Figure 1 (a) shows the two-phase fluid model used for a static pressure field check. Discontinuities in the applied properties were also verified, such as density and viscosity. Figure 1 (b) presents the scheme used for the dynamic analysis of a two-phase fluid. Note that in case (b), the densest fluid starts at the top, so this is a decantation problem, the final solution of which is achieved by inverting the layers.

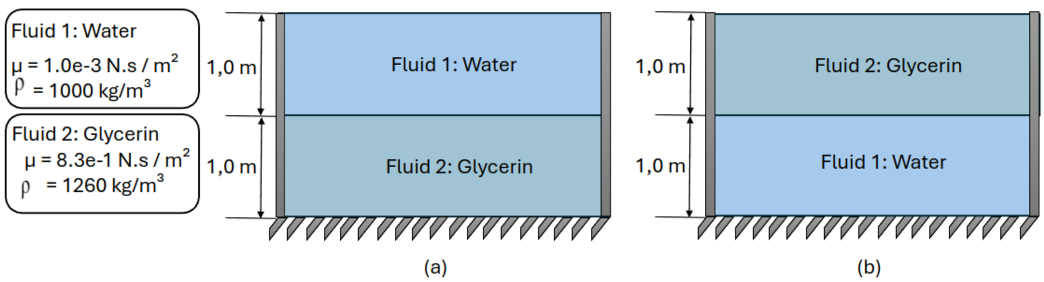

Figure 1. Models for verification and analysis of two-phase fluids with positional PFEM.

Figure 2 presents the results for the pressure field in case (a). It is noted that the results correspond to the analytical ones.

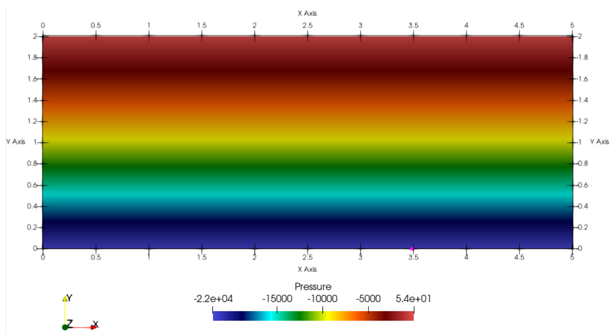

Figure 2. Pressure field - static problem.

Figure 3 shows configurations of a two-phase fluid over time for the case (b). It is noted that due to the density gradient, the phenomenon of decantation occurs. It is observed that the final configuration is given by the inversion of the fluids, as observed in nature.

Figure 4 presents the result of the pressure field for the quasi-stationary result of the dynamic analysis of case (b). This pressure field refers to the time step t = 40.75 s and is 95% compatible with the analytical one referring to the stationary solution after complete inversion of the fluids.

4.2 Water dam break

This example presents the rupture of a water dam. Note that this is a free surface flow, however, due to the simulation of both air and water, it is not necessary to apply the alpha-shape geometric criterion to define the

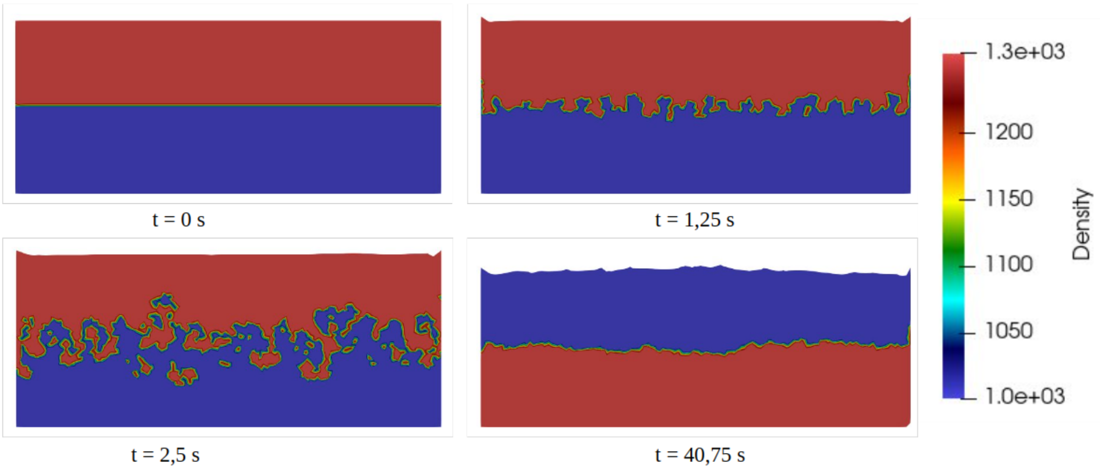

Figure 3. Dynamic analysis of a two-phase fluid with multiple interfaces.

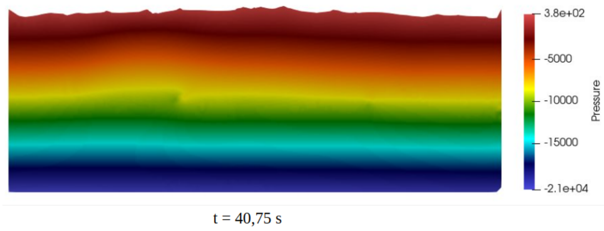

Figure 4. Pressure field - dynamic case.

fluid-fluid interface. Problems were simulated with meshes of 2 and 5 mm average characteristic size. Figure 5 presents a third example for the analysis of two-phase fluids. In this example, both air and water are simulated and the results are compared with experimental results of flow over time.

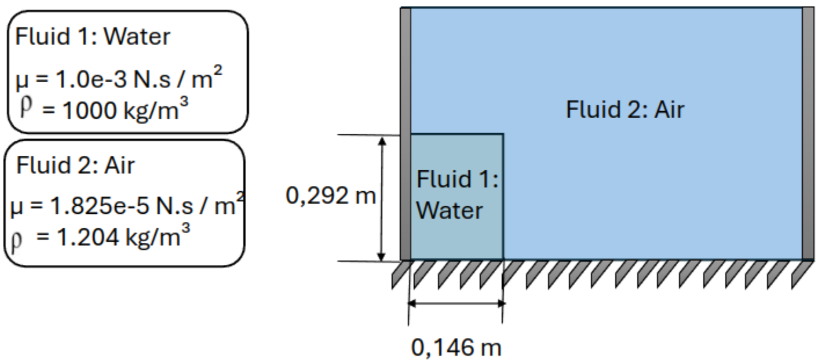

Figure 5. Dam break - Geometry and data.

The analysis of the dynamics of the water of the dam flow over some time steps is presented in Figure 6. This sequence of frames allows us to summarize the temporal development of the analyzed flow.

This example is also important to simulate, as it has several experimental results as presented by Martin and Moyce [12], Koshizuka et al. [13] and some numerical results with other methods as presented by Avancini et al. [7], Avancini [9], Hirt and Nichols [14], Koshizuka and Oka [15]. Figure 7 illustrates the experimental validation of the implementations made for modeling a two-phase program with positional PFEM. The parameter t* refers to the dimensionless time given by $t* = t\sqrt{2g/L}$. Where $g = 9.81m/s$ denotes gravity and $L = 0.146m$ refers to the initial length of the fluid base.

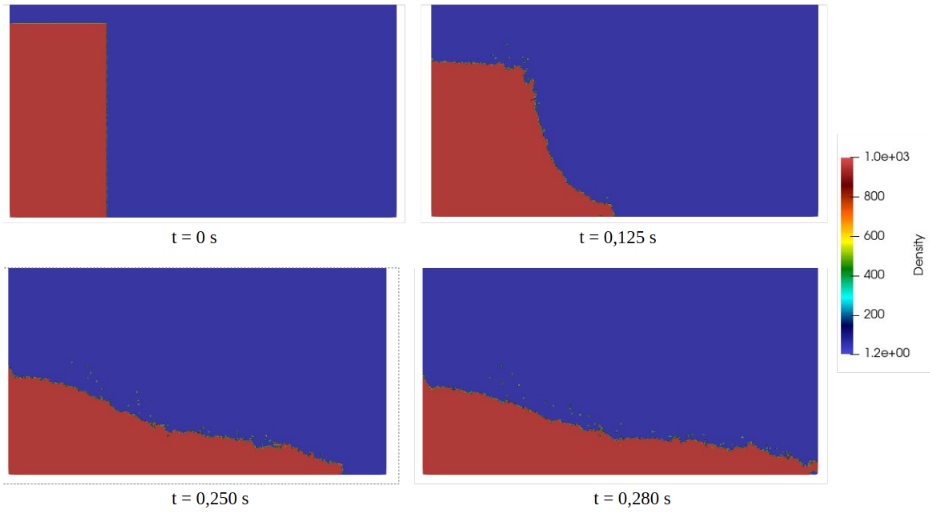

Figure 6. Dam break - Fluid/water interface.

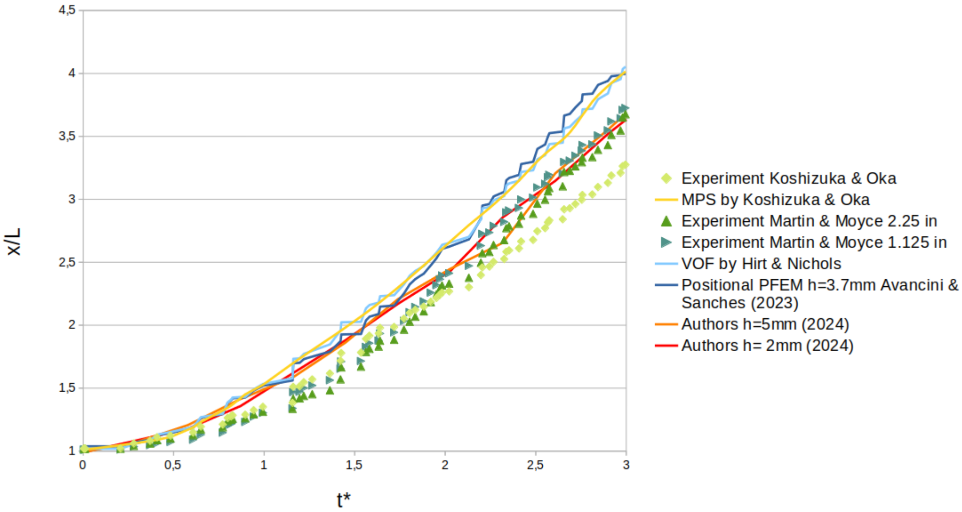

Figure 7. Dam-Break - Maximum horizontal position of water.

5 Conclusion

In this work we presented a methodology to the simulation of two-phase incompressible flows with topological changes in the individual fluid domains. The methodology is based on a position-based formulation of the PFEM. This methodology has been tested by numerical examples and compared to analytical and experimental results from the literature showing good agreement, revealing a robust tool for this type of complex fluid mechanics phenomena. Future works shall study focus on understanding the mass and momentum conservation within the individual fluid phasis, application to fluid-structure interaction and the simulation of problems with slip conditions at the interfaces.

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