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Particle finite element method applied to mould filling

Romain Aubry* — **Eugenio Oñate*** — **Sergio Rodolfo Idelsohn****
— **Facundo Del Pin ***

* *International Center for Numerical Methods in Engineering (CIMNE)*
Universidad Politecnica de Catalunya, Campus Norte UPC, 08034 Barcelona,
Spain

{romain, onate, fdelpin}@cimne.upc.edu

** *CIMEC, Universidad Nacional del Litoral, Güemes 3450, 3000 Santa Fe,*
Argentina
sergio@ceride.gov.ar

ABSTRACT. The Particle Finite Element Method (PFEM) is applied to the solution of three dimensional casting processes with solidification problems for a viscous incompressible fluid. One of the most salient features of the method is to treat the classical Navier-Stokes equations in a fully non-linear Lagrangian description, including the large deformations of the fluid during the filling process. The stabilisation of the convective term is then completely bypassed. A modified fractional step is presented to ensure mass conservation. A fully thermally coupled flow and the solidification strategy are also introduced.

RÉSUMÉ. La méthode des éléments finis particuliers (PFEM) est utilisée pour la résolution des procédés de mise en forme modélisés par des fluides visqueux incompressibles. L'utilisation de la formulation Lagrangienne appliquée aux équations de Navier-Stokes permet d'éviter la classique difficulté numérique due au terme convectif inclus dans la dérivée temporelle totale. Un schéma de pas fractionnaire modifié est présenté pour assurer la conservation de la masse. Le couplage thermique au travers de l'approximation de Boussinesq et le processus de solidification sont également présentés.

KEYWORDS: Lagrangian description, free surface problem, incompressibility, solidification, mass conservation.

MOTS-CLÉS : Description Lagrangienne, surface libre, incompressibilité, solidification, conservation de la masse.

1. Introduction

In casting processes, one of the biggest difficulties to be solved is created by the appearance of the free surface during the mould filling process, which has to be located. Various methods have already been studied with fixed grid like VOF, level set and pseudo-concentration. They all use a hyperbolic-like transport equation to solve the movement of the free surface as well as the Navier-Stokes equations. Various strategies have also been presented to track and smooth the free surface. Here, we take the choice to follow the free surface during its motion by following the movement of the particles in a Lagrangian manner, which implicitly gives the position and the evolution of the free surface. Furthermore, using the Lagrangian description allows to use total temporal derivatives and to circumvent the well-known difficulty of the stabilization of the convective term. However, due to the large motion of the fluid, which only produces deviatoric stresses through deformation rates, a complete remeshing has to be performed at each time step. Furthermore, the non linearity of the convective term is now present in all the spatial derivatives of the Navier-Stokes equation.

The Particle Finite Element Method (PFEM) (Idelsohn *et al.*, 2004, Oñate *et al.*, 2004) is a powerful method to solve free surfaces problems and is extended here to discontinuous pressure approximations and solidifications problems.

2. Numerical model of the fluid equations

2.1. The Navier-Stokes equations in a Lagrangian framework

We recall quickly the Lagrangian equations of motion for a Newtonian incompressible fluid flow and we refer to (Aubry *et al.*, 2004) for a complete presentation. The momentum conservation reads:

$$\rho_0 \frac{d\mathbf{V}}{dt} = -\mathbf{div}_x (Jp\mathbf{F}^{-T}) + 2\mu\mathbf{div}_x (J\mathbf{D}\mathbf{F}^{-T}) \quad [1]$$

$$\mathbf{F} = \mathbf{grad}_x(\mathbf{x}) \quad [2]$$

$$J = \det \mathbf{F} \quad [3]$$

where \mathbf{F} is the transformation gradient, J is the Jacobian of the transformation, \mathbf{D} the symmetric part of the strain rate, p the pressure, ρ_0 the density and μ the dynamic viscosity of the fluid. Incompressibility is expressed through the mass conservation as:

$$J = 1 \text{ or } \mathbf{grad}_x(\mathbf{V}) : \mathbf{F}^{-1} = 0 \quad [4]$$

We will see that this equation is particularly important for our application. Furthermore, as \mathbf{F} is a function of \mathbf{x} we see that the right hand side of [4] is highly non-linear respect to the displacement, which is the main unknown in a Lagrangian approach. Equations [1] and [4] must be completed with appropriate boundary and initial conditions.

2.2. Space discretization

Applying the finite element Galerkin method to equations [1] and [4], we obtain:

$$\mathbf{M} \frac{d\mathbf{V}}{dt} + \mathbf{K}(\mathbf{U})\mathbf{V} + \mathbf{B}(\mathbf{U})\mathbf{P} = \mathbf{F} \quad [5]$$

$$\mathbf{B}(\mathbf{U})\mathbf{V} = 0$$

where \mathbf{V} and \mathbf{U} are the velocity and displacement vectors, and the matrix follow the classical notations for the finite element solution of the Navier-Stokes equations. Once more the non linear dependence of the displacement of all the matrices has been emphasized. Furthermore, it should be noted that the incompressibility condition [4] has been changed for:

$$-\mathbf{div}_x(\mathbf{V}) = 0 \quad [6]$$

which is the time derivative of [4]. Evidently, [4] and [6] are equivalent at the continuum level. We will see that the time integration of [6] will play a major role in the mass conservation.

2.3. Fractional step, preconditioned Uzawa method and mixed elements

The time discretization is performed with a θ -scheme and through a classical fractional step, designed at the algebraic level following (Codina, 2001). After the introduction of an auxiliary velocity variable and a few algebraic manipulations, the scheme reads:

$$\begin{aligned} \frac{\mathbf{M}}{dt}(\tilde{\mathbf{V}}^{n+1} - \mathbf{V}^n) + \mathbf{K}(\mathbf{U}^{n+\theta})\tilde{\mathbf{V}}^{n+\theta} + \gamma\mathbf{G}(\mathbf{U}^{n+\theta})\mathbf{P}^n &= \mathbf{F}^{n+\theta} \\ dt\mathbf{D}\mathbf{M}^{-1}\mathbf{G}(\mathbf{U}^{n+\theta})(\mathbf{P}^{n+1} - \gamma\mathbf{P}^n) &= \mathbf{D}(\mathbf{U}^{n+\theta})\tilde{\mathbf{V}}^{n+1} \end{aligned}$$

$$\frac{\mathbf{M}}{dt}(\mathbf{V}^{n+1} - \tilde{\mathbf{V}}^{n+1}) + \mathbf{G}(\mathbf{U}^{n+\theta})(\mathbf{P}^{n+1} - \gamma\mathbf{P}^n) = \mathbf{0}$$

where dt is the time increment and γ is a numerical parameter varying from 0 to 1. As noted in (Codina, 2001), the two pairs of interesting values for (γ, θ) are (0,1) which is first order in time, and (1,1/2), which is second order in time. At this point, a classical approximation is usually made:

$$\mathbf{DM}^{-1}\mathbf{G} \approx \mathbf{L} \quad [7]$$

where \mathbf{L} is the Laplace operator for continuous pressure. Writing the previous fractional step in terms of \mathbf{V}^{n+1} , a natural stabilization term of the form $dt(\mathbf{DM}^{-1}\mathbf{G} - \mathbf{L})(\mathbf{P}^{n+1} - \gamma\mathbf{P}^n)$ then appears. This term is efficient only for first order schemes and other strategies have to be designed for second order in time and equal order interpolation (Codina, Idelsohn *et al.*, Oñate *et al.*). Furthermore, this induces a wrong boundary condition for the pressure and produces a non-discrete divergence free end-of-step velocity.

Instead of using the precedent approximation, we replace the velocity mass matrix in $\mathbf{DM}^{-1}\mathbf{G}$ by its lumped mass matrix version in the fractional step so that the same boundary conditions as the monolithic approach are applied, and an exactly discrete divergence-free solution is obtained by also replacing the consistent velocity mass matrix by its lumped counterpart in the projection step of the fractional step. Furthermore, discontinuous approximations of the pressure are now available as well as a second order in time for a mixed finite element satisfying the inf-sup condition.

2.4. Mass conservation

A classical difficulty of free surface problems is the conservation of mass during the computation. Incompressibility is enforced only weakly through the pressure acting as the Lagrangian multiplier of this condition. A valuable property of discontinuous pressure elements is the enforcement of mass conservation at the element level. In solid mechanics with incompressible media, condition [4] is usually weakly enforced and linearized through a Newton-like method. In fluid mechanics, equation [6] is usually preferred due to its Eulerian form. So we see that for a Lagrangian fluid, mass conservation will depend crucially of two factors, namely a good approximation of the incompressibility and a good integration of the velocity in time, which is confirmed through numerical results. We therefore use a second order fractional step with a P1++/P1 element with discontinuous linear pressure satisfying the inf-sup condition. With the discontinuous pressure, a better mass conservation is obtained, but more than else allows using a second order scheme which provides a much better integration of condition [6].

3. The thermal problem

3.1. The energy conservation

In a Lagrangian description, the energy conservation and its weak form read:

$$\rho_0 C \frac{dT}{dt} = \mathbf{div}_x (\kappa J \mathbf{F}^{-1} \mathbf{F}^{-T} \mathbf{grad}_x (T)) \quad [8]$$

$$\frac{\mathbf{M}_T}{dt} (\mathbf{T}^{n+\theta} - \mathbf{T}^n) + \mathbf{K}_T (\mathbf{U}^{n+\theta}) \mathbf{T}^{n+\theta} = 0 \quad [9]$$

where C is the heat capacity and κ the conductivity of the media considered. The non linearity is also reflected in the spatial operators of the right hand side.

3.2. Thermo-mechanical coupling

The equations of motion of the fluid are coupled with the heat equation through the Boussinesq approximation by introducing a dependence on the density of the temperature in the gravity forces. On the other side, the temperature is implicitly coupled with the displacement as the spatial operators related to the temperature equation are function of the displacement. The system is then fully coupled.

3.3. Solidification

We introduce solidification effects through the latent heat release and the solid fraction function. The mushy zone is modelled as a variable viscosity zone until the solid fraction of the zone becomes 1.

4. Meshing and boundary recognition

4.1. Remeshing

As previously mentioned, the large deformations of the fluid produce severe distortion in the mesh so that a remeshing is performed every time step. This remeshing, due to its frequency must be fast and robust, particularly in a three-dimensional context. There we have chosen to use the revisited Delaunay based mesh generator, as described in (Frey *et al*, 1999). It allows eliminating slivers during the generation process. Furthermore, as the Delaunay kernel connects points,

the cloud of nodes of the last time step could be used to create the new mesh, which minimizes the interpolation error.

4.2 Boundary recognition

The α -shape method (Edelsbrunner *et al*, 1994) is used to determine the free surface, whereas the solid surfaces are explicitly known. Mainly, the α -shape method tries to reconstruct the shape of a cloud of points by relying on a distance argument. In practice, it determines if a given tetrahedron must be taken as a fluid element if its radius is not larger than a local value corresponding to a given size map. The α -shape can be used in a constrained isotropic context, and tests are currently being performed in an anisotropic context.

5. Conclusions

An efficient and robust solution is presented for the incompressible Navier-Stokes equations coupled with thermal effects and solidification. The Lagrangian description provides a natural framework to treat free surface problems appearing in casting processes. The modified fractional step allows uncoupling the velocity and the pressure computation, the use of discontinuous pressure elements and second order time discretization. This appears to be of utmost importance in the mass conservation process in a moving grid strategy.

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