A meshfree formulation for the simulation of mould filling processes in casting

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***Abstract*—The numerical simulation of the mould filling step in casting is crucial since it provides a complete set of detailed information. However, the mesh based methods usually used to model this processes have some drawbacks when dealing with this kind of problems. In order to overcome some of these limitations in this work the application of an innovative meshfree computational tool based on the Finite Pointset Method is proposed. The main features and details of its implementation are presented and finally, the accuracy and robustness of this scheme is assessed through the numerical simulations of three-dimensional test problems in mould filling processes.**

***Index Terms*—casting, meshless method, Finite Pointset Method, FPM**

I. Introduction

Many industrial applications require the production of aluminum alloy and metal matrix components with precise shapes, dimensions and surface fineness, which could be very complex in general. Shape casting processes as lost foam casting, die casting, stir casting and sand casting are among the most widely used procedures to manufacture aluminum alloy products. Such processes begin with a step in which a mould's cavity is filled with molten material followed by a cooling and solidification step. The features in the manufactured components and the number of defects are the result of the coupling of the physical phenomena involved in these steps. Therefore, in order to get homogeneous casting components with the desired characteristics and an acceptable low amount of defects, it is necessary to know and control all the physical phenomena involved in the selected process and to conduct a proper design procedure [1].

Currently the foundry industry is interested in the best possible performance at the lowest cost. The required performance can be achieved only when the desired microstructure and an acceptable low number of defects are obtained in the end product. For a specific alloy, this can be achieved only by knowing and understanding the selected casting process so that it can be optimized. Moreover, nowadays the industrial casting product development is shifting from traditional heuristic and experience-based trial-and-error design procedures to a deep scientific proof-of-concept design procedure.

Numerical simulation is commonly used to analyze and improve different casting processes since it provides a large amount of information that cannot be obtained through other techniques. It is the most technologically efficient, cost effective and powerful technology for the evaluation, analysis and prediction of the quality in the end products and the number of defects since it models the entire casting process and shows all the details and the dynamic behavior of the casting system in real working conditions. Therefore, the root causes of the quality in the end products and the casting defects are pinpointed and the possible solution routes to avoid them and to improve the overall quality could be determined, evaluated and analyzed with this tool [2].

Mesh-based methods such as the Finite Element Method (FEM), Finite Difference Method (FDM), Finite Volume Method (FVM), and more recently, meshless methods as Smoothed-particle hydrodynamics (SPH) have already been used to analyse mould filling processes [3]–[6]. The advantages of meshless methods over mesh-based methods are that they use a set of nodes to discretize the problem domain and its boundaries without requiring any information about the relationship between nodes such that they do not form an element mesh which lets to model deformations and discontinuities in the domain without the mesh-based methods drawbacks. Moreover, they have the flexibility to add or remove nodes wherever and whenever needed and it lets to easily develop adaptive schemes [7].

The so called Finite Pointset Method (FPM), member of the family of generalized finite difference methods (GFDM), is a meshfree method that has proven to be far superior to traditional mesh-based and some other meshfree methods to treat fluid dynamics problems involving complex geometries and heat transfer problems [8]–[12]. It has many advantages over other methods since it is able to naturally and easily incorporate any kind of boundary conditions without requiring any special treatment or stabilization and it is really simple to implement. Therefore, in this work we propose the application of this novel meshfree formulation for the numerical simulation of mould filling processes. The current paper is organized in the following manner: Section II shortly describes the governing equations and the numerical procedure used to solve them. Section III describes the basic ideas behind the meshfree formulation for the mould filling problem followed by the numerical test presented in Section IV with its corresponding results. Finally some conclusions are given in last section.

II. GOVERNING EQUATIONS AND NUMERICAL PROCEDURE

The governing equations for mould filling processes are the incompressible Navier-Stokes equations which in Lagrangian form read

$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{v} + \mathbf{f}, \tag{1}$$

$$\nabla\cdot\mathbf{v} = 0, \tag{2}$$

where ρ is the density, p is the pressure, ν is the kinematic viscosity, $\mathbf{f}$ is the acceleration vector due to the body forces and $\mathbf{v}$ is the velocity. This system of equations is completed with the following initial and boundary conditions

$$\mathbf{v}|_{t=0} = \mathbf{v}_0, \tag{3}$$

$$\mathbf{v}|_{\partial\Omega_1} = \mathbf{0}, \tag{4}$$

$$\mathbf{v}\cdot\mathbf{n}|_{\partial\Omega_2} = 0, \tag{5}$$

$$\left.\frac{\partial(\mathbf{v}\cdot\mathbf{t}_i)}{\partial\mathbf{n}}\right|_{\partial\Omega_2} = 0, \tag{6}$$

$$(\tau - \mathbf{I}p)\,\mathbf{n}|_{\partial\Omega_3} = \sigma\kappa\mathbf{n}, \tag{7}$$

$$\mathbf{t}_i^T\tau\mathbf{n}|_{\partial\Omega_3} = 0, \tag{8}$$

where $\partial\Omega_1$ is a solid wall boundary with no-slip condition, $\partial\Omega_2$ is a solid wall boundary with free-slip condition, $\partial\Omega_3$ is a free surface, $\mathbf{v}_0$ is the initial velocity over the entire domain Ω, τ is the viscous stress tensor, σ is the surface tension, κ is the free surface boundary curvature, $\mathbf{n}$ is an outward orthonormal vector and $\mathbf{t}_i$ is a tangential unitary vector to the boundary, for $i = 1, 2$.

In order to solve the system of equations (1) and (2) with the boundary and initial conditions (3) - (8) in a natural and simple way, a semi-implicit Chorin-Uzawa's projection formulation of first order of accuracy will be used [13] which consists of the following steps [12]:

1) Explicitly update the nodes positions through

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \Delta t\mathbf{v}^n. \tag{9}$$

2) Implicitly solve for the intermediate velocities

$$\mathbf{v}^* - \Delta t\nu\nabla^2\mathbf{v}^* = \mathbf{v}^n + \Delta t\mathbf{f}^{n+1}, \tag{10}$$

with the boundary and initial conditions (3) - (8).

3) Implicitly solve for the artificial pressure

$$\nabla\varphi = \frac{\rho}{\Delta t}\nabla\cdot\mathbf{v}^*, \tag{11}$$

which must satisfy the following boundary conditions

$$\left.\frac{\partial\varphi}{\partial\mathbf{n}}\right|_{\partial\Omega_1,\partial\Omega_2} = 0, \tag{12}$$

$$\varphi|_{\partial\Omega_3} = 0. \tag{13}$$

4) Correct/Update the velocity field

$$\mathbf{v}^{n+1} = \mathbf{v}^* - \frac{\Delta t}{\rho}\nabla\varphi \tag{14}$$

5) Correct/Update the pressure field

$$p^{n+1} = \varphi - \rho\nu\nabla\cdot\mathbf{v}^*. \tag{15}$$

where $\mathbf{r}^n$ and $\mathbf{v}^n$ are initially given and they denote the nodes positions and its velocities at time t^n, respectively.

III. THE FINITE POINTSET METHOD (FPM)

In this section we describe the main ideas of the FPM method proposed by [14]. The FPM is a member of the family of the GFDM and it is based on the WLSM. Following [8]:

Let Ω be a given domain with boundary $\partial\Omega$ and suppose that the set of points $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N$ are distributed with corresponding function values $f(\mathbf{r}_1)$, $f(\mathbf{r}_2)$, $\ldots$, $f(\mathbf{r}_N)$. The problem is to find an approximate value of f at some arbitrary location $f(\mathbf{r})$ using its discrete values at particles positions inside a neighbourhood of $\mathbf{r}$. To define the set of nodes and the neighbourhood of $\mathbf{r}$, a weight function $w(\mathbf{r}-\mathbf{r}_i)$ is introduced

$$w_i = w(\mathbf{r}-\mathbf{r}_i) = \begin{cases} e^{-\gamma\|\mathbf{r}-\mathbf{r}_i\|^2/h^2}, & \text{if } \frac{\|\mathbf{r}-\mathbf{r}_i\|}{h} \le 1 \\ 0 & else \end{cases} \tag{16}$$

where h is the smoothing length, γ is a positive constant whose value is considered to be 6.5, and $\mathbf{r}_i$ is the position of the $i-$th point inside the neighbourhood. A Taylor's series expansion of $f(\mathbf{r}_i)$ around $\mathbf{r}$ reads

$$f(\mathbf{r}_i) = f(\mathbf{r}) + \sum_{k=1}^{3} f_k\left(r_{k_i} - r_k\right) + \frac{1}{2}\sum_{k,l=1}^{3} f_{kl}\left(r_{k_i} - r_k\right)\left(r_{l_i} - r_l\right) + \epsilon_i, \tag{17}$$

where ϵ_i is the truncation error of the Taylor's series expansion, r_{ki} and r_k represent the $k-$th components of the position vectors $\mathbf{r}_i$ and $\mathbf{r}$, respectively. f_k and f_{kl} ($f_{kl} = f_{kl}$) represent the set of first and second spatial derivatives at node position $\mathbf{r}$. The values of f_k and f_{kl} can be computed minimizing the error ϵ_i for the n_p Taylor's series expansion of $f(\mathbf{r}_i)$ corresponding to the n_p nodes inside the neighbourhood of $\mathbf{r}$. This system of equations can be written in matrix form as $\mathbf{e} = M\mathbf{a} - \mathbf{b}$, where $\mathbf{e} = [e_1, e_2, e_3, \cdots, e_{n_p}]^t$, $\mathbf{a} = [f, f_1, f_2, f_3, f_{11}, f_{12}, f_{13}, f_{22}, f_{23}, f_{33}]^t$, $\mathbf{b} = [f(\mathbf{r}_1), f(\mathbf{r}_2), \cdots, f(\mathbf{r}_{n_p})]^t$, $M = [\mathbf{s}_1, \mathbf{s}_2, \cdots, \mathbf{s}_{n_p}]t$, $\mathbf{s}_i = [1,\ \Delta r_{1_i},\ \Delta r_{2_i},\ \Delta r_{3_i},\ \Delta r_{11_i},\ \Delta r_{12_i},\ \Delta r_{13_i},\ \Delta r_{22_i},\ \Delta r_{23_i},\ \Delta r_{33_i}]^t$, $\Delta r_{k_i} = r_{k_i} - r_k$, $\Delta r_{kl_i} = (r_{k_i} - r_k)(r_{l_i} - r_l)$ and $\Delta r_{kk_i} = 0.5(r_{k_i} - r_k)(r_{k_i} - r_k)$, for $k, l = 1, 2, 3$ and $k \neq l$. The unknown vector $\mathbf{a}$ is obtained through WLSM by minimizing the quadratic form

$$J = \sum_{i=1}^{n_p} w_i\epsilon_i^2, \tag{18}$$

which reads $(M^tWM)\mathbf{a} = (M^tW)\mathbf{b}$, where $W = \mathrm{diag}(w_1, w_2, \cdots, w_{n_p})$. Therefore, $\mathbf{a} = (M^tWM)^{-1}(M^tW)\mathbf{b}$. In this way we automatically get the values of f and its derivatives at points $\mathbf{r}$.

A. FPM formulation for the semi-implicit Chorin-Uzawa's scheme

Poisson equations as (11) and coupled vector boundary value problems as (10) have been already studied in [12], [15]. Following such works we present, for completeness, the corresponding FPM formulation to solve the equations (9 -

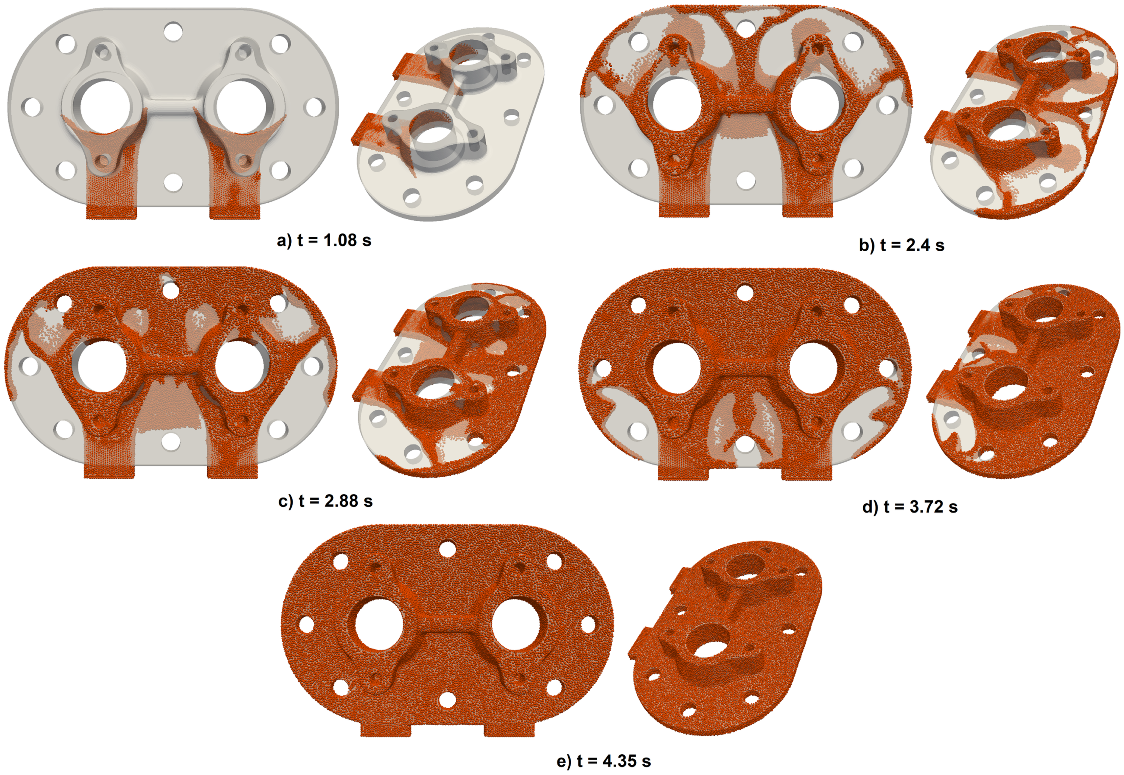

Fig. 1. Numerical filling patterns at different time steps.

15). Equation (11) is an elliptic partial differential equation, which can be written in the following general form

$$Af + \mathbf{B} \cdot \nabla f + C\nabla^2 f = D \tag{19}$$

and the boundary conditions take the general form

$$Ef + G\nabla f \cdot \mathbf{n} = H. \tag{20}$$

In the FPM representation of the above problem, equation (19) must be taken together with the system of n_p Taylor's series expansion of $f(\mathbf{r}_i)$ around $\mathbf{r}$. In this case, the matrices we need to compute by each particle in Ω take the following form: $\mathbf{b} = [f(\mathbf{r}_1), f(\mathbf{r}_2), \cdots, f(\mathbf{r}_{n_p}), D]^t$, $M = [\mathbf{s}_1, \mathbf{s}_2, \cdots, \mathbf{s}_{n_p}, \mathbf{s}_E]t$ and $W = \mathrm{diag}(w_1, w_2, \cdots, w_{n_p}, 1)$, where $\mathbf{s}_E = [A, B_1, B_2, B_3, C, 0, 0, C, 0, C]^t$ and $\mathbf{B} = [B1, B2, B3]t$. If $\mathbf{r}_i \in \partial\Omega$, additionally we have to add the general boundary condition (20). Therefore, in this case, the matrices we need to compute by each particle in $\partial\Omega$ take the following form: $\mathbf{b} = [f(\mathbf{r}_1), f(\mathbf{r}_2), \cdots, f(\mathbf{r}_{n_p}), D, F]^t$, $M = [\mathbf{s}_1, \mathbf{s}_2, \cdots, \mathbf{s}_{n_p}, \mathbf{s}_E, \mathbf{s}_B]t$ and $W = \mathrm{diag}(w_1, w_2, \cdots, w_{n_p}, 1, 1)$, where $\mathbf{s}_B = [E, n_1, n_2, n_3, 0, 0, 0, 0, 0, 0]^t$.

If we define $\mathbf{q} = [q_1, q_2, \cdots, q_{10}]^t$ as the first row of $(M^tWM)^{-1}$ and the terms in the moving least squares solution $\mathbf{a} = (M^tWM)^{-1}(M^tW)\mathbf{b}$ are worked out, we can see that the following linear equations arises

$$\begin{aligned} f(\mathbf{r}_j) - \sum_{i=1}^{n(j)} w_i \,(q_1 + q_2\Delta r_{1_i} + q_3\Delta r_{2_i} + q_4\Delta r_{3_i} + q_5\Delta r_{11_i} \\ + q_6\Delta r_{12_i} + q_7\Delta r_{13_i} + q_8\Delta r_{22_i} + q_9\Delta r_{23_i} + q_{10}\Delta r_{33_i})\, f(\mathbf{r}_i) \\ = [Aq_1 + B_1q_2 + B_2q_3 + B_3q_4 + (q_5 + q_8 + q_{10})\, C]\, D \\ + (n_1q_2 + n_2q_3 + n_3q_4)\, E, \end{aligned}$$

where $f(\mathbf{r}_j)$ denotes the unknown function value at particle j and $n(j)$ the number of $j-$th particle neighbours. Since equation (III-A) is valid for $j = 1, 2, \cdots, N$, this can be arranged in a full sparse system of linear equations $L\mathbf{F} = \mathbf{P}$ which can be solved by iterative methods. In the same way, coupled vector boundary value problems as (10) are treated similarly. For further information on this kind of problems, we refer to [12]. Therefore, all kind of problems as (9 - 15) can be solved with this formulation, just adding appropriate entries in the corresponding systems of equations [12], [15].

IV. Numerical Example

In this section the suitability and feasibility of this FPM formulation in order to simulate 3D mould filling processes in metal casting will be evaluated considering the filling of a pump cover. In this example, the problem domain was discretized with approximately 180000 points with a mean spacing of 0.0015 m. The inlet velocity was taken as $\mathbf{v} = [-0.1, 0, 0]^t$ m/s. The pressure in all particles as well as the atmospheric pressure were considered as zero. The surface tension forces and the gravitational acceleration vector were neglected. The density and viscosity of the fluid were considered as $\rho = 6964$ kg/m^3 and $\mu = 0.0143$ Pa$*$s, respectively. These parameters corresponds to the physical parameters of the molten cast iron. Finally, the smoothing length used in the simulation was $h = 0.0045$ m, a slip boundary condition was used at solid walls and the time step was chosen as $\Delta t = 0.004$ s.

Two perspective views of the filling patterns at different time steps are depicted in Figure 1. There, the picture on the left shows the view exactly from the top whilst the second one shows the view from the top at some angle to the right. As it is shown in this figure, the leading material is divided in four liquid fronts when it impacts the two annular central sections of the die. Two central jets partially merge forming a single liquid front which is split again when it impacts the central cylindrical obstacle. The emerging jets move backwards and starts filling the rear part of the mould. Splashing droplets and liquid fragmentations are visible in this part. The remaining two jets flow around the curved outsides of the die until they collide with the fronts coming from the rear and central parts of the mould. In the two annular central sections of the mould, the liquid flow up into the upper extensions. At this point the rear part of the mould is substantially filled and the fluid flow is towards the front part of the mould. Afterwards, almost all the mould cavity is filled and the biggest voids are principally behind two of the cylindrical obstacles near the inflow jets. They are uniformly filled until the filling process finishes.

These pictures show the robustness of this FPM formulation for the simulation of complex 3D mould filling processes since the splashing into droplets, the fluid fragmentation into jets and the fronts collisions observed in this example are well reproduced and predicted by this approach.

V. Conclusions

Based on the numerical performance shown in the numerical example we can conclude that the current approach is suitable and feasible for the simulation of 3D mould filling processes. It is stable and it has enough accuracy in order to capture the splashing into droplets, the fluid fragmentation into jets and fronts collisions which are observed in this kind of processes. Since this formulation is a truly meshfree method it could be used for the study and analysis of complex problems involving high deformations and domain fragmentations with a great computational advantage since it does not need to compute any numerical quadrature and it does not need remeshing approaches. Further, it is able to naturally and easily handle any kind of boundary conditions without requiring any special treatment or stabilization and it is really simple to implement. Therefore, it could be a promising numerical tool for the simulation of industrial processes involving complex flows and other phenomena described by elliptic partial differential equations as heat transfer. Consequently, it depicts a rich source of research opportunities.

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