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SPH-FDM boundary for the analysis of thermal process in homogeneous media with a discontinuous interface

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ABSTRACT

A SPH-FDM boundary method is proposed for the analysis of thermal process in homogeneous media with a discontinuous interface in this study, in which the smoothed particle hydrodynamics (SPH) method is used in the inner computational domain; and the finite difference method (FDM) is used as the function approximation near the boundary. This mixed method not only can improve the calculation accuracy under the first-type boundary conditions (i.e., Dirichlet), but also can convert the second- and third-type boundary conditions (i.e., Neumann and Robin) into the first-type boundary conditions in solving heat conduction problems of homogeneous media. As a result, a second-order accuracy can be achieved in the entire solution domain. The proposed SPH-FDM boundary method is applicable to the analysis of heat conduction in various media, including the problems with discontinuous interface in the computational domain and the solidification of materials with a moving phase transition boundary. Numerical results show that the proposed SPH-FDM boundary method overcomes the difficulties of the conventional SPH method in dealing with the second- and third-type boundary conditions and has a very high calculation accuracy.

1. Introduction

Smoothed particle hydrodynamics (SPH) is a Lagrangian mesh-free particle method consisting of two steps of approximation: the kernel approximation and the particle approximation [1–3]. In the kernel approximation, the function and its derivatives are represented as integrations over the support domain; while in the particle approximation, the support domain is divided into discrete particles with their own masses, densities, velocities and pressures [4,5]. SPH was initially developed to solve astrophysical problems in unbounded domains [6], where the governing equation could be expressed by the classical Newtonian fluid dynamics. Subsequently, this method was also successfully applied in other fields, such as fluid dynamics and free surface flows [7,8] and non-Newtonian multiphase flows [9–11].

A major concern in the application of SPH method is the physical type of boundary conditions (BCs), such as the solid BC, open BC, inflow/outflow BC and periodic condition [12–14]. Fang et al. [15] simulated transient viscoelastic free surface flows and introduced the artificial pressure between particles to stabilize the SPH system avoiding the tensile instability. Ataie-Ashtiani et al. [16] proposed an incompressible SPH method to simulate free surface incompressible fluid problems. Liu and Liu [17] proposed an improved SPH method for resolving discontinuous interface of shock waves in aerodynamics based on the Taylor series expansion. Fourtakas et al. [18] presented a method to impose 2-D solid wall boundary conditions in SPH, by which arbitrary complex domains could be readily discretised ensuring approximate zeroth and first-order consistency. These findings provide an effective approach for the calculation of SPH boundary problems. Also, the SPH method is well suited for thermal processes of some complicated surface flows due to its Lagrangian nature [4,19]. Jeong et al. [19] developed an algorithm for the boundary condition implementation by decomposing a second order partial differential equation (PDE) into two first order PDEs, which was applicable to complex geometries and nanoscale heat transfer. Schwaiger [20] established a SPH formulation of the Laplacian operator that could greatly improve the accuracy near free boundaries based on a gradient approximation commonly used in thermal problems. In addition, Alshaer et al. [21] investigated the SPH modelling of transient heat transfer in pulsed-laser ablation of aluminium where the laser was applied directly to the free-surface boundary of a specimen.

It is important to note that the compact support domain can be truncated by the solution domain boundary in the kernel approximation. As a consequence, the conventional SPH function may not

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be applicable to the entire solution domain, and a first-order or even zero-order accuracy can hardly be achieved. Libersky et al. [22] introduced virtual particles to reflect a symmetrical surface boundary condition and simulated the dynamic characteristics of materials in hypervelocity impact. The Corrective Smoothed Particle Method (CSPM) combining the kernel estimate with the Taylor series expansion [23] can improve the stability of the conventional SPH method, and it is of second-order accuracy in the solution domain and first-order accuracy near the boundary, respectively. Chen et al., [24] proposed Reproducing Kernel Particle Method (RKPM) in which the reconstruction of the kernel function made it possible for the SPH method to achieve high accuracy, albeit at an increased computational expense to determine the kernel function for each particle and the risk of singular matrices. Zhang and Batra [25] proposed Modified Smoothed Particle Hydrodynamics (MSPH) method to obtain high accuracy. However, this method requires solving a large set of equations, thereby resulting in an expensive computational cost. Some virtual particles can be placed at the boundary to produce a highly repulsive force to the particles near the boundary, and thus to prevent these particles from unphysical penetration through the boundary. Randles and Libersky [26] proposed a more general treatment of the boundary conditions by assigning the same boundary value of a field variable to all virtual particles, and then interpolating smoothly the specified boundary virtual particle values and the calculated values of the interior particles. However, this approach was only applicable to some special problems. Esmaili Sikarudi and Nikseresht [27] proposed an approach to facilitate the implementation of Neumann and Robin boundary conditions based on the smoothing directional derivatives and the manipulated Taylor series.

In this study, a SPH-FDM boundary method is proposed for the analysis of thermal process in homogeneous media with a discontinuous interface, in which SPH is used in the inner computational domain and finite difference method (FDM) is used in the function approximation near the boundary. This approach allows for the achievement of second-order accuracy in the entire solution domain, and overcomes the difficulties in dealing with the second-type (Neumann) and the third-type (Robin) boundary conditions. In this preliminary study, the SPH-FDM boundary method is used to solve heat conduction problems in homogeneous media, including the problems with discontinuous interface in the computational domain and the solidification of materials with moving phase transition boundary. This method should be applicable for many complex engineering problems such as highly nonlinear deformation and fluid dynamics.

2. The SPH method and a new boundary treatment

2.1. Particle approximation

In SPH, the field function to be solved can be expressed in an integral form (kernel approximation), and then discretized into the summation of series (particle approximation). In this study, it is illustrated using a one-dimensional function, where the kernel approximation of $f(x_i)$ at x_i in the domain is [17,28]

$$f(x_i) = \int_{\Omega} f(x_j) W(x_i - x_j, h) dx_j \tag{1}$$

where $W(x_i\text{-}x_j, h)$ is the kernel function, h is the smoothing length of the kernel function, and Ω is the integral domain, respectively.

The replacement of the field function at both sides of Eq. (1) with $f'(x)$ and $f''(x)$ yields the kernel approximation of the first and the second derivative, respectively. It should be stated that the effect of boundary terms is neglected in deducing the first order kernel approximation with an integration by part formula. In Eq. (1), the mass in the Ω domain is assumed to be divided into n particles with a mass of m_1, m_2, m_3, ... and m_n, and a density of ρ_1, ρ_2, ρ_3, ... and ρ_n, respectively. Then, the field function for particle i can be approximated as

$$f(x_i) = \sum_{j=1}^{n} f(x_j) W(x_i - x_j, h) \frac{m_j}{\rho_j} \tag{2}$$

where x_i and x_j are the coordinate of particle i and j, and m_j and ρ_j are the mass and density of particle j, respectively.

The particle approximation of the first derivative at particle x_i can be obtained based on the antisymmetry of the derivative of the kernel function:

$$f'(x_i) = \sum_{j=1}^{n} [f(x_j) - f(x_i)] \frac{\partial W(x_i - x_j, h)}{\partial x_i} \frac{m_j}{\rho_j} \tag{3}$$

Similarly, the particle approximation of the second derivative at particle x_i is [17,28,29]

$$f''(x_i) = \sum_{j=1}^{n} f(x_j) \frac{\partial^2 W(x_i - x_j, h)}{\partial x_i^2} \frac{m_j}{\rho_j} \tag{4}$$

However, the particle approximation of the second derivative in Eq. (4) is sensitive to particle disorder, and thus a confused distribution of particles around particle i can result in very low accuracy. For those thermal problems of interest in this study, the heat transferred from particle j to particle i depends only on the distance between the two particles, which is contrary to the thermodynamics law. Thus, the following equation is used [17,28,29]:

$$f''(x_i) = \sum_{j=1}^{n} \frac{2m_j}{\rho_j} \frac{x_i - x_j}{r_{ij}^2} [f(x_i) - f(x_j)] \frac{\partial W(x_i - x_j, h)}{\partial x_i} \tag{5}$$

In fact, Eq. (5) is the so-called Morris operation for the second kernel derivative [29]. The selection of the kernel function $W(R, h)$ is of critical importance for SPH, which can have an effect on the efficiency and stability of numerical algorithm. Note $R = r/h$, where r is the inter particle distance. Various kernel functions were used such as Gaussian, quadratic, quintic and spline kernel functions [6,17,27,29]. Recently, Ferrand et al. [13] proposed an analytical formulation for the 2-D and 3-D cases using the Wendland kernel function. For simplicity, a B-spline function is used here [4,23,28]:

$$W(R, h) = \alpha_d \times \begin{cases} \frac{2}{3} - R^2 + \frac{1}{2}R^3 & 0 \leqslant R < 1 \\ \frac{1}{6}(2 - R)^3 & 1 \leqslant R < 2 \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

where α_d is the normalized constant, which is $1/h$ and $15/7\pi h^2$ in one- and two-dimensional spaces, respectively.

2.2. SPH-FDM boundary

A SPH-FDM boundary is proposed in this study, where the function $u(x)$ near the boundary is expressed in a polynomial form (e.g., quadratic function):

$$u(x) = a + bx + cx^2 \tag{7}$$

where u is the field variable, and a, b and c are the parameters to be determined, respectively.

The $u(x)$ for point i (Fig. 1, i = 1, 2, 3, 4 ...) near the boundary can be expressed as:

$$\begin{cases} u_i = a \\ u_{i+1} = a + b\Delta x + c(\Delta x)^2 \\ u_{i+2} = a + 2b\Delta x + 4c(\Delta x)^2 \end{cases} \tag{8}$$

where Δx is the point distance.