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Neumann and Robin boundary conditions for heat conduction modeling using smoothed particle hydrodynamics

M.A. Esmaili Sikarudi, A.H. Nikseresht *

Mechanical and Aerospace Engineering Department, Shiraz University of Technology, Shiraz, Iran

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ABSTRACT

Smoothed particle hydrodynamics is a robust Lagrangian particle method which is widely used in various applications, from astrophysics to hydrodynamics and heat conduction. It has intrinsic capabilities for simulating large deformation, composites, multiphysics events, and multiphase fluid flows. It is vital to use reliable boundary conditions when boundary value problems like heat conduction or Poisson equation for incompressible flows are solved. Since smoothed particle hydrodynamics is not a boundary fitted grids method, implementation of boundary conditions can be problematic. Many methods have been proposed for enhancing the accuracy of implementation of boundary conditions. In the present study a new approach for facilitating the implementation of Robin and Neumann boundary conditions is proposed and proven to give accurate results. Also there is no need to use complicated preprocessing as in virtual particle method. The new method is compared to an equivalent one dimensional moving least square scheme and it is shown that the present method is less sensitive to particle disorder.

1. Introduction

Smoothed particle hydrodynamics method was introduced by Lucy and Gingold in 1977 [1,2]. It was first used for astrophysical simulations, but soon its application extended to compressible and incompressible fluid flow simulations [3,4]. As SPH[1] is a particle method, it has a Lagrangian nature. When it comes to moving boundaries, such as free surface flows, impact or even explosion problems, this nature is very useful [5]. In particle methods, finite numbers of particles substitute the continuum domain. These particles have some or all of continuum's domain properties. SPH is completely a meshless method and meshless methods have several advantages due to the fact that they do not need any grid systems. Remeshing is inevitable when Lagrangian approaches are used in grid based methods. This remeshing needs interpolations between the old and new grid systems; thus, errors may be encountered and simulation time prolongs. Meshless methods are capable of modeling multiphysics simulations easily, so that different materials and phases can have different particles [6,7]. Since particles can be added into the computational domain with ease, meshless methods are more flexible for adaptation, and they are easily extendible to three dimensions.

Meshless methods usually have trouble with the implementation of boundary conditions. Many approaches have been proposed to improve boundary condition implementation in SPH method. There are methods which can eliminate consistency deficiency and improve simulation accuracy throughout the domain, especially near boundaries. Liu et al. proposed reproducing kernel particle method in 1995 [8] and moving least square method was proposed by Dilts et al. in 1999 [9]. These methods are used for correcting the interpolation kernels and their derivatives for first order consistency and second order accuracy; however, moving least square method is favored for higher orders of consistency and accuracy. It is efficient only if the derivatives of interpolation kernels are corrected. Belytschko et al. proposed CSPH[2] method in which the first derivatives of interpolating function are corrected [10,11]; however, correction of kernel functions or their derivatives throughout the domain, may violate conservation laws and prolongs simulation time [12,13]. In 1999, Cleary and Monaghan proposed a method for correcting errors through corrections of density near boundaries; moreover, they showed that how SPH formulation can naturally conserve heat flux at material discontinuities [14]. Jeong used extrapolations to enhance accuracy near boundaries [15]. In

* Corresponding author.
E-mail addresses: m.esmaili@sutech.ac.ir (M.A. Esmaili Sikarudi), nikser@sutech.ac.ir (A.H. Nikseresht).

[1] Smoothed Particle Hydrodynamics.

[2] Corrected Smoothed Particle Hydrodynamics.

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this method, heat equation is solved in two separate steps. Vishwakarma proposed using virtual particles out of domain boundaries. He simulated one dimensional and two dimensional heat transfer cases [16,17]. This method needs a cumbersome preprocessing. Ryan modeled Neumann and Robin boundary conditions with a novel method in two dimensional cases [18]. In this method, the entire solid and fluid domain are included in the simulation. This method is simpler.

Using virtual boundary particles is not a robust choice in particular engineering cases. As, SPH kernel functions are approximate Dirac delta functions, Dirichlet boundary conditions can be modeled easily. However, it would be more challenging to implement Neumann and mixed boundary conditions. In the present study, new methods are proposed, so that Neumann and Robin boundary conditions are implemented easily, preprocessing is simple, and there is no need for positioning virtual boundary particles.

2. Governing equations and discretization

Like other discretizing methods, both governing equations and computational domain are discretized with the SPH method. Computational domain is discretized into some particles. Each particle has its own mass, and carries kinematic and thermodynamic properties such as temperature, pressure or velocity. Number of particles should be enough in order to have a good approximate of continuous fluids or solids. In problems with large gradients, using finer particles produces more accurate results.

Interpolation is the basis of most meshless methods, such as RBF[3] [19], MPS[4] [20], EFG[5] [21], and SPH. Even in grid based methods, like FEM,[6] the interpolation accuracy is very important.

A function is approximated by Eq. (1), in the SPH method.

$$f(\overrightarrow{r_i}) \approx \int_{\Omega_i} f(\overrightarrow{r})\, W(\vec{r} - \vec{r}_i, h)\, dr. \tag{1}$$

W is a radial weight function which is called the kernel function, and the integration is done over a subdomain Ω_i which is called the support domain. Radius of the support domain is a multiplication of the smoothing length parameter h.

The kernel function is an approximate Dirac delta function; Eq. (1) is, in fact, an approximation to the following equation:

$$f(\overrightarrow{r_i}) = \int_{\Omega_i} f(\overrightarrow{r})\, \delta(\overrightarrow{r} - \overrightarrow{r_i})\, dr. \tag{2}$$

This approximation is called integral approximation. Eq. (2) is a well-known characteristic of Dirac delta function.

Having done the integral approximation, Eq. (1) should be discretized over neighboring particles. This discretization is called particle approximation and it is shown in Eq. (3) [12].

$$\int_{\Omega_i} f(\overrightarrow{r})\, W(\overrightarrow{r} - \overrightarrow{r_i}, h)\, dr \approx \sum_{j=1}^{N} f_j\, W(\overrightarrow{r_j} - \overrightarrow{r_i}, h)\, \Delta\Omega_j. \tag{3}$$

Integration over a subdomain Ω_i changes to summation over neighboring particles j, so that the value of function f at particle i is interpolated using the value of its adjacent particles j.

Since every particle has its own mass and density, the differential volume of each particle is replaced with its equivalent expression, as it is shown in Eq. (4).

$$\sum_{j=1}^{N} f_j\, W(\overrightarrow{r_j} - \overrightarrow{r_i}, h)\, \Delta\Omega_j = \sum_{j=1}^{N} f_j\, W(\overrightarrow{r_j} - \overrightarrow{r_i}, h)\, \frac{m_j}{\rho_j}. \tag{4}$$

In Eq. (4), interpolation is done over a specified subdomain Ω_i around particle i, which is called the support domain. Nodal integration is dependent on accuracy of kernel type and integration points. Support domains with small radii, contain fewer particles; thus, less integration points are available, and accuracy deteriorates. A Larger radius of support domains causes results to smooth out.

As mentioned before, kernel functions are an approximation of the Dirac delta function; this means they have the following characteristics [12]:

1- Kernel functions are non-negative throughout the support domain.

2- Kernels change from their maximum value to zero at the borders of the support domain smoothly, so that kernel functions have compact support domains. Compactness reduces the computation expense.

3- Integral of kernel functions is unity over the support domain, as it is shown in Eq. (5):

$$\int_{\Omega_i} W(\overrightarrow{r}, h)\, dr = 1. \tag{5}$$

4- Kernel functions are even and radial, so that the discretization error is second order, and symmetry is assured.

Any function with the above characteristics can be used as a kernel function in the SPH method. Some of them are quadratic, quintic and spline kernels. Spline functions are more favorable, because their sensitivity to particle disorder is less than other functions; moreover, they show better accuracy in nodal integration [22]. Cubic spline kernel is shown in the following equation.

$$W(\vec{r}, h) = \kappa \begin{cases} 1 - \frac{3}{2}q^2 + \frac{3}{4}q^3 & 0 \le q \le 1 \\ \frac{1}{4}(2-q)^3 & 1 \le q \le 2 \\ 0 & q \ge 2. \end{cases} \tag{6}$$

The parameter q is the distance between particle i and particle j, divided by the smoothing length h as in Eq. (7).

$$q_{ij} = |\overrightarrow{r_i} - \overrightarrow{r_j}|/h. \tag{7}$$

As the integration of the kernel function should be unity over the support domain, the parameter κ is dependent on the dimension of the problem. It is $2/3h$ in one dimensional, $10/7\pi h^2$ in two dimensional and $1/\pi h^3$ in three dimensional problems. A graph of a 2D cubic spline kernel is sketched in Fig. 1.

In order to solve heat conduction Eq. (8) with Neumann and Robin boundary conditions, gradient and Laplacian operators should be discretized.

$$\frac{\partial T}{\partial t} = \alpha\, \nabla^2 T \tag{8}$$

where α is the heat diffusion coefficient.

The gradient of a function can be discretized by manipulating its integral approximation. The integral approximation of the gradient is as follows:

$$\nabla f(\overrightarrow{r_i}) = \int_{\Omega_i} \nabla f(\overrightarrow{r})\, W(\overrightarrow{r} - \overrightarrow{r_i}, h)\, dr. \tag{9}$$

[3] Radial Basis Function.
[4] Moving Particle Semi-implicit.
[5] Element Free Galerkin.
[6] Finite Element Method.