Influence of Smoothing Length and Virtual Particles on SPH Accuracy

T. El-Gammal, E. E. Khalil, H. Haridy, and E. Abo-Serie

Abstract—Using a well known 2-D transient heat conduction benchmark, a parametric study is conducted to identify the best values for the smoothing length (h) as function of particles spacing in order to minimize the error in the temperature distribution particularly at the center of the domain when applying the Smooth Particle Hydrodynamics (SPH) algorithm. Also the effect of the virtual particles on the numerical solution has been investigated. The results showed that the predefined smoothing length can have significant influence on the accuracy of the prediction and using the optimum value leads to minimum error in temperature prediction values. The results obtained with and without virtual particles has been presented and compared with the analytical solution.

Index Terms—Meshless, smoothing length, SPH, virtual particles.

I. INTRODUCTION

One of the most popular numerical meshless methods for solving the physical problems is the Smoothing Particle Hydrodynamics (SPH). It's a Lagrangian adaptive method that doesn't need to grid/mesh for solving the discretized domain. In this method the physical domain is discretized into unconnected particles that have physical properties (i.e. volume, mass, velocity....etc) of the domain [1]. Unlike the conventional numerical methods such as Finite Difference (F.D.) the meshless method uses field functions and their derivatives at different points (particles) whose values are approximately calculated using weighting (smoothing) kernel function. SPH is one of the recently developed meshless methods which have acquired the reliability and trustworthy in the last years such as the meshless element-free Galerkin (EFG) method [2]– [4], moving least-square methods [5], [6] and the diffuse approximation method [7].

The Lagrangian nature of SPH makes it more suitable for simulations involving fluid free surfaces, interfaces between different material, multiphase flow and highly deformable geometries. Simulating such applications by mesh based methods is challenging and required large memory and long computational time due to the continuous change in the computational mesh in space and time to fit the domain. After being developed for simulating the cosmological

phenomenon [8], [9], SPH has been used in solving fluid and solid mechanics problems.

The main advantages of SPH are the easiness to model complex material surface behavior and complicated physics, such as solidification [10], [11] and multiphase flows [12].

In SPH, The field function (Temperature, pressure, velocity....etc.) is calculated for a discrete particle from the field functions of the all surrounding particles weighted by the smoothing function. The smoothing (weighting) kernel function takes into account the effect of the neighboring particles within a predefined radius called smoothing length (h). Many famous kernel functions use a dependent factor (K) to multiply with the smoothing length (h).

In this work the value of smooth length has been varied to investigate its effect on the final result. The problem chosen for this investigation is a 2-D diffusion transient case which has been simulated previously using SPH technique with a constant predefined smooth length [13]. This previous study showed significant error particularly at the location where low temperature gradient exist (at the center of the plate). The current study developed the technique to minimize the error by varying the smooth length and introducing virtual ghost particle to improve the boundary conditions representation. The results have been compared with previous investigation and the analytical solution of the conduction equation.

II. PROBLEM DEFINITION

The problem used here is the famous benchmark 2-D rectangular plate of lengths $L \times H$ undergoing heat conduction process. The process will be mainly cooling due to isothermal cooling boundaries. The plate temperature will cool from initial temperature (T_i) to final temperature (T_f) which depends on the final state required to be stopped at.

For 2-D heat diffusion in Cartesian coordinates, the equation for the temperature field $T = T(x, y, t)$ is

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \quad (1)$$

where (α) is the thermal diffusivity in (m^2/s).

An analytical solution based on separation of variables and substitution of specified boundary conditions can be written in symbolic form to identify the temperature of the interior of the plate $T(x,y,t)$ as follows:

$$T(x, y, t) = \frac{16 T_i}{\pi^2} \sum_{k=1,3,\dots}^{\infty} \sum_{l=1,3,\dots}^{\infty} \frac{e^{[-\alpha\pi^2(k^2/L^2 + l^2/H^2)t]}}{kl} \sin\left(\frac{k\pi x}{L}\right) \sin\left(\frac{l\pi y}{H}\right) \quad (2)$$

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III. METHODOLOGY

SPH formulation starts from the integral representation of field function using the Dirac delta function $\delta(x_{ij})$. The following relation states the one dimensional mathematical concept:

$$f(x_i) = \int f(x_j) \delta(x_{ij}) dx \delta(x_{ij}) = \begin{cases} 1 & i = j \\ 0 & \text{else} \end{cases} \quad (3)$$

The main step of the derivation of SPH is substituting the Dirac delta function with even, limited-zone, kernel function $W(x_{ij}, h)$. Then we can write the function approximation in SPH formulation as:

$$f(x_i) \approx \langle f(x_i) \rangle = \int f(x_j) W(x_{ij}, h) dx \quad (4)$$

where $\langle f(x_i) \rangle$ is the kernel approximation of the scalar field $f(x)$ at particle (i) .

For two or three dimensions, the kernel function $W(x_{ij}, h)$ can be replaced by $W(r_{ij}, h)$ such that (r_{ij}) is the vectorial distance between (i) and (j) . Also the differential length (dx) is updated to differential area (ds) or volume (dv) .

The gradient $(\partial f(x_i)/\partial x)$ and Laplacian $(\partial^2 f(x_i)/\partial x^2)$ of the field function are evaluated in integral representation [13] to be:

$$\partial f(x_i)/\partial x \approx \langle \nabla f(x) \rangle = \int f(x_j) \nabla_i W(x_{ij}, h) dx \quad (5)$$

$$\begin{aligned} \partial^2 f(x_i)/\partial x^2 &\approx \langle f_{xx} \rangle \\ &= 2 \int \frac{[f(x_i) - f(x_j)]}{r_{ij}^2} \cdot x_{ij} \cdot \nabla_i W(x_{ij}, h) dx \end{aligned} \quad (6)$$

The second main step of SPH is after the integral representation is the particle approximation. The field functions in (4), (5) and (6) are discretized in spaced, differential particles representing the domain, so the integrations approximate to summations of functions weighted by the kernel function.

$$\langle f(x_i) \rangle = \sum \frac{m_j}{\rho_i} f(x_j) W(r_{ij}, h) \quad (7)$$

$$\langle \nabla_i f(x) \rangle = \sum \frac{m_j}{\rho_i} f(x_j) \nabla_i W(r_{ij}, h) \quad (8)$$

$$\langle f_{xx} \rangle = 2 \sum \frac{m_j}{\rho_i} \frac{[f(x_i) - f(x_j)]}{r_{ij}^2} \cdot x_{ij} \cdot \nabla_i W(r_{ij}, h) \quad (9)$$

SPH formulation mentioned above can be substituted into the heat diffusion equation (1). Accordingly, the SPH representation of pure heat conduction case in 2-D can be written as follows:

$$\begin{aligned} \frac{\partial T}{\partial t} = 2\alpha \left(\sum \frac{m_j}{\rho_i} \frac{[T(x_i) - T(x_j)]}{r_{ij}^2} \cdot x_{ij} \cdot \nabla_i W \right. \\ \left. + \sum \frac{m_j}{\rho_i} \frac{[T(x_i) - T(x_j)]}{r_{ij}^2} \cdot y_{ij} \cdot \nabla_i W_{ij} \right) \end{aligned} \quad (10)$$

The compact cubic spline kernel function has been used in this study. It was firstly proposed by Monaghan and

Lattanzio [14].

The formulations of the cubic spline kernel function (W_{ij}) and its spatial derivative can be shown in (11) and (12).

$$W(r_{ij}, h) = W_{ij} = a_n * \begin{cases} \frac{2}{3} - R^2 + \frac{1}{2}R^3 & 0 \leq R < 1 \\ \frac{1}{6}(2 - R)^3 & 1 \leq R < 2 \\ 0 & R > 2 \end{cases} \quad (11)$$

$$\nabla_i W_{ij} = \frac{dW_{ij}}{dR} \times \frac{dR}{dr_{ij}} \times \frac{(x_i - x_j)}{r_{ij}} \quad (12)$$

where $(R=r_{ij}/h)$ is the ratio between the magnitude of the distance between two neighboring particles (r_{ij}) and the smoothing length (h) . In Eq. (11), (n) is the dimension of the space, and the coefficient (a_n) is dependent on the smoothing length (h) and has values:

$$a_1 = \frac{1}{h} \quad a_2 = \frac{15}{7\pi h^2} \quad a_3 = \frac{3}{2\pi h^3}$$

In one, two, and three dimensions, respectively.

IV. NUMERICAL ANALYSIS

A. Domain Particles Distribution

Using Matlab®, the plate domain $(L = H)$ is discretized into 41×41 particles which are classified into interior and boundary particles.

The initial temperature (T_i) is set to all the particles. Particle differential area will be calculated from its spacings in x and y coordinates (i.e. $m/\rho = ds = dx \times dy$). The plate starts at $T_i = T(x, y, 0) = 100^\circ \text{C}$ with isothermal cooling boundaries $T_b = T(0, y, T) = T(L, y, T) = T(x, 0, T) = T(x, H, T) = 0^\circ \text{C}$.

B. Virtual (ghost) Particles

The virtual or ghost particles [15], [16] are generated in every time step as an image for the medium particles near the boundary (i.e. lie within the kernel domain of the wall/boundary particle) as in Fig. 1.

Fig. 1. Real and virtual particles within the supporting zone of the boundary particle

The virtual particle gains its physical properties from its real particle and the boundary condition of the wall. The artificially existed particles play an important role in completing the kernels of the particles to give accurate

physical properties for all particles. Also they facilitate the applying of the boundary conditions as in F.D. especially for Neumann boundary condition.

In the problem domain, the virtual particles were applied to the four boundaries as shown in Fig. 2.

Fig. 2. Plate domain discretization into real, boundary and virtual particles

C. Time Marching

Depending on implicit second order Leapfrog method, the temperature at the mid of the current time step is calculated using the value of mid of the previous time step and the temperature rate of change based on the values of the time step preceding.

$$\text{At } t = dt \text{ (i.e. } n=1) \\ T_{\frac{1}{2}} = T_0 + \left(\frac{dt}{2}\right) * \frac{\partial T}{\partial t} \Big|_{n=1} \quad (13)$$

where $\frac{\partial T}{\partial t} \Big|_{n=0}$ are evaluated by initial values T_0 from the heat conduction equation.

For $n > 1$

$$T_{(n-1)+\frac{1}{2}} = T_{(n-1)-\frac{1}{2}} + dt * \frac{\partial T}{\partial t} \Big|_n \quad (14)$$

where $\frac{\partial T}{\partial t} \Big|_n$ are evaluated by T_{n-1} from the heat conduction equation.

The time step has been chosen to satisfy the Monaghan and Cleary [17] criterion for pure heat conduction problems,

$$dt \leq 0.15 \frac{h^2}{\alpha} \quad (15)$$

In this case, the thermal diffusivity and time step were considered as ($\alpha = 1 \text{ cm}^2/\text{s}$, $dt = 0.001 \text{ s}$) respectively. The value of (h) was then optimized to minimize the error.

In a second step, the optimized SPH algorithm was compared with no-virtual SPH to study the error due to the incomplete kernels near the boundary. Both results were taken at the same (h_{opt}) and the time step ($dt = 0.001 \text{ s}$).

V. RESULTS

A. Optimum Smoothing Length

Fig. 3 lists the percentage errors ($\frac{T_{analytical} - T_{SPH}}{T_i}$) after

$t=8\text{s}$ for different smoothing lengths. The error varies throughout the plate and its maximum value is located in the center of the plate. The table shows clearly that there is an optimum value for smoothing length ($h_{opt}=1.28dx$) for best accuracy and the accuracy drops down for further increase or decrease in the value. This means that (h_{opt}) generates the best shape of kernel function to the temperature profile for the most of points (especially points close to the center). However, at the same time, the points near the boundary lose its accuracy if the virtual particles are not taken into considerations.

Fig. 3. The effect of changing the smoothing length on the accuracy of the SPH solution

After the choice of (h_{opt}), the results produced by the code are compared with conventional SPH results introduced by R. Rook [13] to determine the effect of the virtual particles at $t=1, 4, 8 \text{ s}$, the results have been compared with the reference obtained from the analytical solutions. The comparison is illustrated in isothermal contour lines shown in figures 4, 5, and 6. The optimized smoothing length achieves better accuracy than the conventional SPH. This is obvious when time marches to the steady state. The conventional SPH error increases and spreads over the whole contour lines in a noticeable way. The main reason for that is the high gradient exists near the boundaries and diminishes towards the centers, so the increase or decrease of smoothing on particles of high gradients distorts the weighting kernel function and consequently the supporting area of a particle nearby boundary becomes greatly inaccurate.

Fig. 4. Isothermal contour lines at $t=1\text{s}$

Needless to say that adding the virtual particles to the conventional SPH leads to an increase in computational time. Including the virtual particles shows computational time of 31.82 s while the no-virtual SPH generates its results in 23.53 s. However, with the optimized smoothing length the computation time was less than that of the conventional SPH which took 87 s.

Fig. 5. Isothermal contour lines at $t=4s$

Fig. 6. Isothermal contour lines at $t=8s$

B. Virtual Particles

Fig. 7. Isothermal contour lines at $t=8s$ (no-virtual SPH with optimized SPH)

After the determination of (h_{opt}) , the effect of virtual particles is compared with no-virtual SPH and the results are presented in Figs. 7 and 8 which show the contours lines of no-virtual SPH outfitting the analytical lines at the center but in lower behavior than conventional SPH because of optimized smoothing length used in it. No-virtual SPH missed the accuracy except in corners. In later times of

cooling (i.e. $t > 8s$), the results of no-virtual SPH lose their accuracy as well as the conventional SPH. This is because the error of incomplete kernels is transmitted and increased among particles towards the center to reach a maximum value.

Fig. 9. Isothermal contour lines at $t=8s$ (no-virtual SPH with conventional SPH)

VI. CONCLUSION

Optimizing the smoothing length in SPH achieves the merits of high accuracy, consistent contours with the analytical solution, and less computation time. Any increase or decrease in the smoothing length will change the kernel weighting function (W_{ij}) in (shape and value) and disorients it from the actual temperature profile. Although the smoothing length has been considered constant throughout the domain it is believed that having special distribution for the smoothing length can lead to more accurate results but that will be on the account of computation time.

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