

On Discretization of Second-order Derivatives in Smoothed Particle Hydrodynamics

R. Fatehi, M.A. Fayazbakhsh, M.T. Manzari

Abstract—Discretization of spatial derivatives is an important issue in meshfree methods especially when the derivative terms contain non-linear coefficients. In this paper, various methods used for discretization of second-order spatial derivatives are investigated in the context of Smoothed Particle Hydrodynamics. Three popular forms (i.e. "double summation", "second-order kernel derivation", and "difference scheme") are studied using one-dimensional unsteady heat conduction equation. To assess these schemes, transient response to a step function initial condition is considered. Due to parabolic nature of the heat equation, one can expect smooth and monotone solutions. It is shown, however in this paper, that regardless of the type of kernel function used and the size of smoothing radius, the double summation discretization form leads to non-physical oscillations which persist in the solution. Also, results show that when a second-order kernel derivative is used, a high-order kernel function shall be employed in such a way that the distance of inflection point from origin in the kernel function be less than the nearest particle distance. Otherwise, solutions may exhibit oscillations near discontinuities unlike the "difference scheme" which unconditionally produces monotone results.

Keywords—Heat conduction, Meshfree methods, Smoothed Particle Hydrodynamics (SPH), Second-order derivatives.

I. INTRODUCTION

SECOND-order spatial derivatives frequently arise in transport equations representing thermal, mass, and momentum diffusions. To solve these equations numerically, it is required to discretize these terms on some spatial points. This process is almost standard in numerical methods that are based on computational grids, such as finite difference, finite volume, and finite element methods. In some other computational methods, called meshfree or meshless methods, since the computational points are not connected through a grid, discretization of spatial derivatives needs special treatments.

One of major successful meshfree methods in fluid dynamics is the Smoothed Particle Hydrodynamics (SPH) that is based on the Lagrangian approach. In this method, each computational point carries field variables (such as velocity, pressure, temperature, and etc) and moves with the fluid in time. SPH was first presented by Lucy [1] and Gingold and Monaghan [2] simultaneously in 1977 to simulate astrophysical problems. In 1982, Gingold and Monaghan [3] used it for non-dissipative compressible flows. In 1994 Monaghan [4] extended the SPH method to incompressible free surface flows and it was successfully applied to low-Reynolds viscous flow [5], [6] and other problems in fluid dynamics, heat transfer,

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and solid mechanics. For a concise review of the method, see [7].

To evaluate first-order spatial derivative in SPH, a kernel interpolation is used. For second-order derivatives, three different schemes are frequently used; "double summation scheme", "second-order kernel derivation scheme", and "difference scheme". In the following section, these schemes are introduced and their usage, pros and cons are described. In the next section, using one-dimensional unsteady heat conduction equation, the ability of each scheme to handle a stiff initial condition is tested. Through this study, capabilities of each method is shown. Finally, the conclusions are summarized.

II. SPH FORMULATION

Smoothed Particle Hydrodynamics (SPH) is a meshfree particle method. The word "particle" does not mean a physical mass, instead, it refers to a region in space. Field variables are associated with these particles and at any other point in space are found by averaging or smoothing the particle values over the region of interest. This is fulfilled by an interpolation or weight function which is often called the interpolation kernel. In practice, it means summation of quantities over neighbouring particles. For a typical field variable u at point i , the SPH interpolation becomes

$$u_i = \frac{1}{\psi_i} \sum_j^N u_j W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (1)$$

in which W is the kernel function with the mutual particle distance $\mathbf{r}_i - \mathbf{r}_j$ and the smoothing radius h as its parameters. The kernel function is a smoothed version of the Dirac delta function. W is positive for $|\mathbf{r}_i - \mathbf{r}_j| < h$ and vanishes outside the radius h . Also ψ is particle number density defined as

$$\psi_i = \sum_j^N W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (2)$$

and N is the number of neighbouring particles. In the following, $W(\mathbf{r}_i - \mathbf{r}_j, h)$ is summarized to W_{ij} . Although eqn. (1) looks different from the standard form [7], for our purpose, they are the same.

The SPH discretization of the spatial derivative of u is constructed using the derivative of kernel as

$$\left\langle \frac{\partial u}{\partial x_p} \right\rangle_i = \frac{1}{\psi_i} \sum_j^N (u_j - u_i) \frac{\partial W_{ij}}{\partial x_p} \quad (3)$$

This is called symmetric form and is widely used in literature [7]. For second-order derivatives, there are different ways to

reach the discretization form. Here three popular forms are introduced.

A. Double summation scheme

Assuming that the value of u and its derivative have already been calculated and stored for all particles, one can extend the formulation for the first derivative (eqn. (3)) to

$$\left\langle \frac{\partial}{\partial x_q} \left(K \frac{\partial u}{\partial x_p} \right) \right\rangle_i = \frac{1}{\psi_i} \sum_j^N \left(\left\langle K \frac{\partial u}{\partial x_p} \right\rangle_j - \left\langle K \frac{\partial u}{\partial x_p} \right\rangle_i \right) \frac{\partial W_{ij}}{\partial x_q} \quad (4)$$

where K is a diffusion coefficient. This formulation is used by Flebbe *et al.* [8] and Watkins *et al.* [9] to include physical viscosity in astrophysical problems and by Jeong *et al.* [10] for two-dimensional heat conduction problem. Also [11], [12], [13], [14], [15] used it to handle viscous term in low-Reynolds number incompressible flows. Since double summation scheme uses the value of first derivatives, it is fairly simple to handle Neumann-type boundary conditions and non-homogeneous coefficients. The results show good behaviour when the solution are smooth. For stiff problems, however, it leads to non-physical oscillations [8], [9]. Although several authors attended to reduce the oscillations in the results of this scheme. It is shown in this paper that oscillations originate from the nature of this scheme.

B. Second-order kernel derivation scheme

In this scheme, the second-order derivative of the kernel function is used to calculate the second-order derivative of the main quantity. The form that was used by Chaniotis *et al* [16] with variable coefficients can be written as

$$\left\langle \frac{\partial}{\partial x_q} \left(K \frac{\partial u}{\partial x_p} \right) \right\rangle_i = \frac{K_i}{\psi_i} \sum_j^N (u_j - u_i) \frac{\partial^2 W_{ij}}{\partial x_q \partial x_p} + \left\langle \frac{\partial K}{\partial x_q} \right\rangle_i \left\langle \frac{\partial u}{\partial x_p} \right\rangle_i \quad (5)$$

where the first-order derivatives in the last term are evaluated from eqn. (3). They used this scheme to simulate viscous and heat conducting flows in one and two dimensions. Since the kernel is a known function, this provides a convenient way to find the second-order derivative of a variable.

C. Difference scheme

A popular scheme used in many problems involving second-order derivatives, such as heat conduction and mass diffusion, is the difference scheme [7]. The idea was first presented by Cleary [17] to treat viscosity and heat conduction by a single scheme. For a typical variable u this scheme is written as

$$\left\langle \frac{\partial}{\partial x_q} \left(K \frac{\partial u}{\partial x_p} \right) \right\rangle_i = \frac{1}{\psi_i} \sum_j^N \left(4 \frac{\Delta x_q \Delta x_p}{\Delta r^2} - \delta_{pq} \right) K_{ij} \frac{(u_j - u_i)}{\Delta r^2} \nabla W_{ij} \cdot \Delta \mathbf{r} \quad (6)$$

where K_{ij} is an average of K_i and K_j . In eqn. (6), the summation is computed on an estimate of first-order derivative contribution of each neighbouring particle in the form of $\frac{(u_j - u_i)}{\Delta r}$. Since it is similar to finite difference method, we named it as "difference scheme". Monaghan [7] presented a proof in the context of kernel interpolation.

Unlike double summation scheme which needs value of the first-order derivative at each point, the two latter schemes evaluate the second-order derivative directly and seem to be computationally more efficient. This is not, however, an advantage at all. Many second-order derivative terms, involve coefficients that are not constant and may be functions of either the variable itself or its first-order derivative. A non-Newtonian viscous flow is an example. For problems in which the first-order derivative must be calculated anyway, the computational overhead associated with the double summation scheme can be overlooked. Furthermore, when the problem includes Neumann-type boundary conditions, two latter schemes cannot be implemented in a straightforward.

III. ANALYSIS AND RESULTS

In this section, a partial differential equation is considered representing heat conduction in a 1D domain. To have a simple form, all coefficients are taken as unity.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad (7)$$

A unit step function is considered as the initial condition for u i.e.

$$u(x, t = 0) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases} \quad (8)$$

The above heat conduction problem has an analytic solution involving the Error function as shown in eqn. (9).

$$u(x, t) = \frac{1}{2} \left(1 + \operatorname{erf} \left(\frac{x}{\sqrt{4t}} \right) \right) \quad (9)$$

For the numerical solution, time marching can be done using Euler's explicit method. Considering a constant time-step Δt we have

$$u_i^{t+\Delta t} = u_i^t + \Delta t \left\langle \frac{\partial^2 u}{\partial x^2} \right\rangle_i^t \quad (10)$$

The analytic solution of eqn. (9) is monotone, i.e., u constantly increases with x . To obtain such results from the numerical method, in the first time-step $t = 0$, the calculated value of $\frac{\partial^2 u}{\partial x^2}$ should also be monotone.

Assuming equally distributed particles, the value of particle number density becomes equal for all particles, say Ψ . In general, we consider an arbitrary kernel function W and an ordinary smoothing radius $h = n\Delta x$. Thus eqn. (3) reduces to

$$\Psi \left\langle \frac{\partial u}{\partial x} \right\rangle_i = [(u_{i+1} - u_i) - (u_{i-1} - u_i)] W' \left(\frac{1}{n} \right) + [(u_{i+2} - u_i) - (u_{i-2} - u_i)] W' \left(\frac{2}{n} \right) + \dots + [(u_{i+(n-1)} - u_i) - (u_{i-1} - u_i)] W' \left(\frac{n-1}{n} \right) + [(u_{i+n} - u_i) - (u_{i-n} - u_i)] W' \left(\frac{n}{n} \right) \quad (11)$$

TABLE I
 SECOND-ORDER DERIVATIVE VALUES OF u ESTIMATED BY DOUBLE SUMMATION SCHEME WITH $h = 2\Delta x$

x	-3	-2	-1	0	1	2	3	4
$\Psi^2 \frac{\partial^2 u}{\partial x^2}$	0	0	$W'(\frac{1}{2})^2$	$W'(\frac{1}{2})^2$	$-W'(\frac{1}{2})^2$	$-W'(\frac{1}{2})^2$	0	0

TABLE II
 SECOND-ORDER DERIVATIVE VALUES OF u ESTIMATED BY DOUBLE SUMMATION SCHEME WITH $h = 3\Delta x$ WHERE $A = W(\frac{2}{3})^2$, $B = 2W'(\frac{1}{3})W'(\frac{2}{3})$, AND $C = W'(\frac{1}{3})^2$.

x	-3	-2	-1	0	1	2	3	4
$\Psi^2 \frac{\partial^2 u}{\partial x^2}$	A	$A+B$	$A+B+C$	$A+C$	$-A-C$	$-A-B-C$	$-A-B$	$-A$

in which $W(R)$ stands for $W(\Delta r, h)$ where $R = \frac{\Delta r}{h}$ and $W'(R) = \frac{dW(R)}{dR}$. Therefore, the last term vanishes because $W'(1) = 0$.

In the following, the performance of each of the three aforementioned schemes for calculating the second derivative of u is compared.

A. Double summation scheme

Assuming $h = 2\Delta x$ the second derivative takes the values shown in table I.

It is observed here that from $x = -1$ to $x = 0$ and from $x = 1$ to $x = 2$ the second derivative of u is constant. This is in contrast to the fact that the second-order derivative should be monotone.

Taking $h = 3\Delta x$, there is even more deviation from the trend of the analytic solution. As shown in table II the absolute value of the second derivative first increases by a term of $2W'(\frac{1}{3})W'(\frac{2}{3})$ and then decreases near the jump region.

By going on with $h = n\Delta x$ where $n = 4, 5, \dots$ we see that terms with the same effect exist in the numerical solution. These terms generate oscillations in the vicinity of the initial discontinuity. These oscillations may decrease by taking longer smoothing radii, but they cannot be totally eliminated. This makes the double summation scheme unconditionally oscillating near sharp variations.

B. Second-order kernel derivation scheme

As implied earlier, when the coefficient is constant, it is not necessary to calculate the first-order derivative in order to achieve the second-order derivative of a quantity in this scheme. For the current problem, table III shows values of the second-order derivative for $h = 3\Delta x$.

By assuming that the second derivative of W is positive for $x \geq \frac{1}{3}$, we can see that $\frac{\partial^2 u}{\partial x^2}$ remains monotone in both sides of $x = 0$. But some kernel functions are used for which the second derivative changes sign somewhere in their smoothing

TABLE III
 SECOND-ORDER DERIVATIVE VALUES OF u ESTIMATED BY SECOND-ORDER KERNEL DERIVATION SCHEME WITH $h = 3\Delta x$ WHERE $D = W''(\frac{2}{3})$ AND $E = W''(\frac{1}{3})$.

x	-3	-2	-1	0	1	2	3	4
$\Psi \frac{\partial^2 u}{\partial x^2}$	0	0	D	$D+E$	$-D-E$	$-D$	0	0

TABLE IV
 THE POSITION OF INFLECTION POINT FOR SOME POPULAR KERNEL FUNCTIONS.

Kernel function	Position of inflection point
Lucy [1]	$\frac{1}{4}h$
Cubic spline [18]	$\frac{1}{3}h$
Quartic spline [19]	$0.28h$
Quintic spline [19]	$0.25h$

radius. Using such a kernel, the same oscillations may happen from $x = 1$ to $x = 2$ as was seen in the double summation scheme. In other words, $W''(\frac{1}{3})$ becomes negative and as a result $\frac{\partial^2 u}{\partial x^2}$ is no more monotone.

To avoid this non-physical oscillation, the kernel function must be chosen in such a manner that the distance of the inflection point from the origin becomes less than Δx . Thus, under specific conditions, the second-order kernel derivation scheme can show oscillations. These can be eliminated by using appropriate kernel functions. Increasing the number of neighbouring particles (i.e. greater h and n) needs smoother kernels that means more computational cost. To have an overview, table IV shows some popular kernel functions and the position of their inflection points as a ratio of h . For example, maximum values of n (number of neighbouring particles at one side of i) for quartic spline kernel is 3.6. This means that if one uses $h = 4\Delta x$ the result would no longer be monotone.

C. Difference scheme

Table V shows the values obtained by the difference scheme, eqn. (6). Since W is monotone, W' never changes sign. So the value of $\frac{\partial^2 u}{\partial x^2}$ is always increasing. So we can conclude that the difference scheme which is widely used in the literature is unconditionally non-oscillating.

IV. CONCLUSIONS

In this paper, the process of discretizations of the second-order spatial derivatives were reviewed in the context of

TABLE V
 SECOND-ORDER DERIVATIVE VALUES OF u ESTIMATED BY DIFFERENCE SCHEME WITH $h = 3\Delta x$ WHERE $F = \frac{1}{\Delta x}W'(\frac{2}{3})$ AND $G = \frac{2}{\Delta x}W'(\frac{1}{3})$

x	-3	-2	-1	0	1	2	3	4
$\Psi \frac{\partial^2 u}{\partial x^2}$	0	0	F	$F+G$	$-F-G$	$-F$	0	0

the Smoothed Particle Hydrodynamics (SPH) method. Three methods that are used in literature to discretize the second derivative, namely the double summation scheme, the second-order kernel derivation scheme, and the difference scheme were studied.

By using the step function as an initial condition in a simple one dimensional heat equation as a stiff problem, it was concluded that:

- The double summation scheme presents non-physical oscillations near the discontinuity. It was also shown that the nature of the scheme causes such oscillations which cannot be eliminated, though they can be reduced by time-marching or larger smoothing radii.
- The second-order kernel derivation scheme also showed oscillations for particular kernel functions. It was inferred that to totally eliminate the non-physical oscillation phenomena, the second derivative of the kernel function should be positive at all neighbouring particles, i.e. the inflection point of the kernel function should take place before the nearest contributing neighbour. Thus for greater smoothing lengths, there are fewer kernels which do not show non-physical oscillations.
- The difference scheme does not have the difficulty of the first two schemes and shows no non-physical oscillations unconditionally.

The last two schemes can be less resource-consuming than the double summation scheme, but they have some problems in implementation of Neumann-type boundary conditions. Finally, the double summation scheme, if fixed for the non-physical oscillations of the second derivative, can be more convenient for problems involving Neumann boundary conditions. Different kernel functions may be used for the first and second derivative calculation to circumvent the oscillation problem.

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