A NEW CLASSIFICATION AND CONVERGENCE STUDY OF SPH-LIKE FIRST AND SECOND SPATIAL DERIVATIVES SCHEMES

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I. INTRODUCTION

Simulation of fluid flows using the Smoothed Particle Hydrodynamics (SPH) method relies on approximate forms of the first and second spatial derivatives. For example, calculating the velocity divergence and pressure gradient in the Navier-Stokes equations requires an approximation of the first derivative, while the second derivative is needed for the viscous term of thermal conduction. Despite its simplicity and ease of coding, the standard SPH originally introduced by Lucy [1] and Gingold and Monaghan [2] in 1977 suffers from a lack of consistency [3]. These schemes are not zeroth-order consistent, i.e., they do not yield the exact answer for a constant function. Now, after half a century, various schemes exist for estimating these spatial derivatives, and some of them are successful in resolving the consistency issue. For example, the anti-symmetric scheme [4], renormalization [5], [6] for the first derivative, as well as the difference scheme [7], [8] and renormalization [9] for the second derivative. There are also SPH-like methods presented to resolve the consistency challenge of SPH, e.g., the reproducing kernel particle method (RKPM) [10], moving least squares particle hydrodynamics [11], corrective smoothed particle method (CSPM) [12], [13], modified SPH (MSPH) [14], finite particle method (FPM) [15], [16], kernel gradient-free (KGF) SPH method [17], [18], and kernel derivative-free SPH [19]. In this study, I present a systematic classification of several widely used schemes, along with some novel approaches, and analyze their consistency and convergence rates within a one-dimensional framework. The objective is to establish a comprehensive framework that facilitates their application across diverse contexts in fluid dynamics.

II. NUMERICAL SCHEMES

In standared SPH, the approximation of an arbitrary field function u in terms of the values at neighboring particles u_j is found from

$$\langle u \rangle_i = \langle u(\mathbf{r}_i) \rangle = \sum_{j=1}^{n} \omega_j W_{ij} u_j, \tag{1}$$

where $W_{ij} = W_j(\mathbf{r}_i) = W(\mathbf{r}_i - \mathbf{r}_j; h)$ is the kernel or smoothing function with smoothing length h. By this simple definition, it is straight-forward to conclude thate the first derivatve (gradient) is

$$\langle \nabla u \rangle_i = \langle \nabla u(\mathbf{r}_i) \rangle = \sum_{j=1}^{n} \omega_j \nabla W_{ij} u_j, \tag{2}$$

where $\nabla W_{ij} = \frac{\partial W(r_{ij})}{\partial r_{ij}} \mathbf{e}_{ij}$ and $\mathbf{e}_{ij} = \frac{\mathbf{r}_{ij}}{r_{ij}}$, $r_{ij} = |\mathbf{r}_{ij}|$, and $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$.

A. *First derivatives*

To guarantee the zoeroth-order consistency (ZOC), this paper focuses on the gradient approximations of the form

$$\langle \nabla u \rangle_i = \sum_{j=1}^{n} \mathbf{G}_{ij} u_{ij}, \tag{3}$$

where $u_{ij} = u_j - u_i$. For first-order consistency (FOC) and second-order consistency (SOC), the term $\mathbf{G}_{ij}$ must satisfy the follwing conditions:

$$\sum_{j=1}^{n} \mathbf{G}_{ij} \mathbf{r}_i j = \mathbf{I}, \tag{4}$$

$$\sum_{j=1}^{n} \mathbf{G}_{ij} \mathbf{r}_i j \mathbf{r}_i j = \mathbf{0}, \tag{5}$$

where $\mathbf{I}$ is the unit second-order tensor. To satisfy the FOC condition (4), a second-order tensor parameter is required. Nevertheless, for SOC, both conditions (4) and (5) must be satisfied simultaneously. Thus, there will be a need for a second-order tensor and a third-order tensor as the corrective parameters.

Table I summarizes 9 first derivative schemes into three categories. The first category, namely "Direct Derivative," presents the corrections to the standard SPH scheme (2). They use the kernel gradient ∇W in $\mathbf{G}$, and to restore FOC, the renormalization tensor $\mathbf{B}_i = \left(\sum_j \omega_j \nabla W_{ij} r_{ij} \right)^{-1}$ should be used. For SOC, here it is suggected to $\mathbf{C}_j(\mathbf{r}_i) = \mathbf{C}_{0,i} + \mathbf{C}_{1,i} \cdot \mathbf{r}_{ij}$ which $\mathbf{C}_{0,i}$ and $\mathbf{C}_{1,i}$ should be found by solving

$$\mathbf{C}_{0,i} \cdot \sum_{j=1}^{n} \omega_j \nabla W_{ij} \mathbf{r}_{ij} + \mathbf{C}_{1,i} \cdot \sum_{j=1}^{n} \omega_j \nabla W_{ij} \mathbf{r}_{ij} \mathbf{r}_{ij} = \mathbf{I}, \tag{6}$$

and

$$\mathbf{C}_{0,i} \cdot \sum_{j=1}^{n} \omega_j \nabla W_{ij} \mathbf{r}_{ij} \mathbf{r}_{ij} + \mathbf{C}_{1,i} \cdot \sum_{j=1}^{n} \omega_j \nabla W_{ij} \mathbf{r}_{ij} \mathbf{r}_{ij} \mathbf{r}_{ij} = \mathbf{0}. \quad (7)$$

The next two categories do not use the kernel gradient, so they are called ”Diffuse Derivatives” [20]. This idea is also used in kernel gradient-free (KGF) SPH [17], [18] and kernel derivative-free SPH [19] in a different manner. The term ”Non-Singular (NS)” in the third category refers to replacing the term $\frac{W_{ij}}{r_{ij}}$ with W_{ij}, which always gives finite values even at $r_{ij} = 0$. However, it should be noted that in both ”Diffuse Derivatives” and ”Diffuse Derivatives NS,” the particle i should be omitted in the summation in (3), i.e., $\sum_{j \neq i} \mathbf{G}_{ij} u_{ij}$.

TABLE I
SUMMARY OF FIRST DERIVATIVE APPROXIMATION OF THE FORM (3)

Method (Consistency)	$\mathbf{G}_{ij}$
Direct Derivative (ZOC) (Conventional SPH)	$\omega_j \nabla W_{ij}$
Direct Derivative (FOC) (Corrected Gradient)	$\omega_j \mathbf{B}_i \cdot \nabla W_{ij}$
Direct Derivative (SOC) (Corrected Gradient)	$\omega_j \mathbf{C}_j(\mathbf{r}_i) \cdot \nabla W_{ij}$
Diffuse Derivative (ZOC) (Uncorrected)	$\omega_j \frac{W_{ij}}{r_{ij}} \mathbf{e}_{ij}$
Diffuse Derivative (FOC) (Corrected)	$\omega_j \mathbf{B'}_i \cdot \frac{W_{ij}}{r_{ij}} e_{ij}$
Diffuse Derivative (SOC) (Corrected)	$\omega_j \mathbf{C'}_j(\mathbf{r}_i) \cdot \frac{W_{ij}}{r_{ij}} \mathbf{e}_{ij}$
Diffuse Derivative NS[1](ZOC) (Uncorrected)	$\omega_j W_{ij} \mathbf{e}_{ij}$
Diffuse Derivative NS (FOC) (Corrected)	$\omega_j \mathbf{B''}_i \cdot W_{ij} e_{ij}$
Diffuse Derivative NS (SOC) (Corrected)	$\omega_j \mathbf{C''}_j(\mathbf{r}_i) \cdot W_{ij} \mathbf{e}_{ij}$

[1] NS: Non-singular.

B. Second derivatives

The general form of the second derivative approximation categorized in this paper is

$$\left\langle \nabla^2 u \right\rangle_i = \sum_{j=1}^{n} \psi_{ij} u_{ij}, \quad (8)$$

where ψ_{ij} is given in table II for four categories. The consistency conditions for SOC are

$$\sum_{j=1}^{n} \psi_{ij} \mathbf{r}_i j = \mathbf{0}, \quad (9)$$

$$\sum_{j=1}^{n} \psi_{ij} \mathbf{r}_i j \mathbf{r}_i j = 2\mathbf{I}. \quad (10)$$

Since the condition (9) is homogeneous, the FOC gives a trivial solution. Therefore, only ZOC and SOC schemes are reported in table II. In this table, there is a fourth category, namely ”Mixed,” which refers to the idea first suggested by Brookshaw [7], whose uncorrected form is now conventional in the SPH community. The corrected scheme of the ”Mixed” approach in table II is different from what was suggested by Fatehi and Manzari [9].

TABLE II
SUMMARY OF SECOND DERIVATIVE APPROXIMATION OF THE FORM (8)

Method (Consistency)	ψ_{ij}
Direct Derivative (ZOC) (Conventional SPH)	$\omega_j \nabla^2 W_{ij}$
Direct Derivative (SOC) (Corrected Laplacian)	$\omega_j C_j(\mathbf{r}_i) \nabla^2 W_{ij}$
Diffuse Derivative (ZOC) (Uncorrected)	$2\omega_j \frac{W_{ij}}{r_{ij}^2}$
Diffuse Derivative (SOC) (Corrected)	$2\omega_j C'_j(\mathbf{r}_i) \frac{W_{ij}}{r_{ij}^2}$
Diffuse Derivative NS (ZOC) (Uncorrected)	$2\omega_j \frac{W_{ij}}{r_{ij}}$
Diffuse Derivative NS (SOC) (Corrected)	$2\omega_j C''_j(\mathbf{r}_i) \frac{W_{ij}}{r_{ij}}$
Mixed (ZOC) (Conventional)	$2\omega_j \nabla W_{ij} \cdot \frac{\mathbf{e}_i}{r_{ij}}$
Mixed (SOC) (Corrected)	$2\omega_j C'_j(\mathbf{r}_i) \nabla W_{ij} \cdot \frac{\mathbf{e}_i}{r_{ij}}$

III. RESULTS AND DISCUSSION

To analyze the performance of the schemes in tables I and II, a simple 1D domain was considered, and the derivatives of the function $u(x) = 1 + \cos(\pi x)$ were numerically evaluated. The kernel function for all the schemes was the quintic Wendland function [21], with a cut-off length equal to the smoothing length h. The results were obtained for different particle spacing Δx and different $h/\Delta x$ values on regular and irregular particle arrangements. Then, the L_2 norm was employed to quantify the errors associated with each derivative scheme. The results from the computational experiments are illustrated in Fig. 1 and Fig. 2 for the first and second derivative schemes, respectively.

IV. CONCLUSIONS

It was observed that although ZOC schemes offer rapid and straightforward implementation, the results lack convergence, and there is a risk of increasing errors. In contrast, all FOC first derivative schemes exhibit convergence rates ranging from 1.0 to 2.0, accompanied by a reasonable computational cost. Furthermore, while SOC schemes for the first derivative achieve a convergence rate of 2.0, the convergence of SOC second derivative schemes may face challenges especially in very small particle spacing due to the ill-conditioned nature of the matrix involved in solving for the corrective parameters.

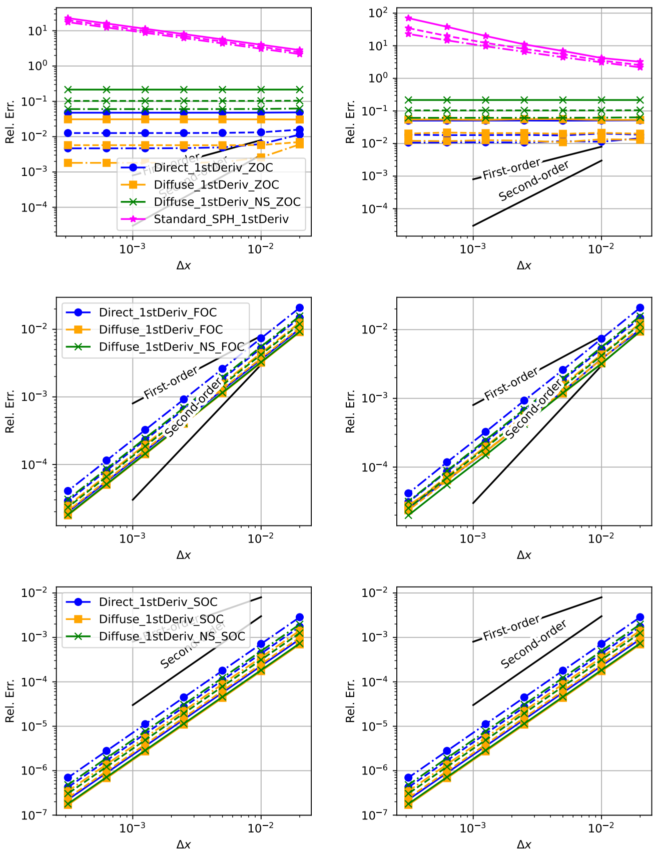

Fig. 1. Convergence of different zeroth-order consistent (ZOC) schemes (top), first-order consistent (FOC) schemes (middle), and second-order consistent (SOC) schemes (bottom) for the first derivative of 1D function $u(x) = 1 + \cos(\pi x)$ on regular (left) and irregular particle spacing (right) with values of $h/\Delta x$ 2.5 (solid line) 3.5 (dash line) 4.5 (dash dot line).

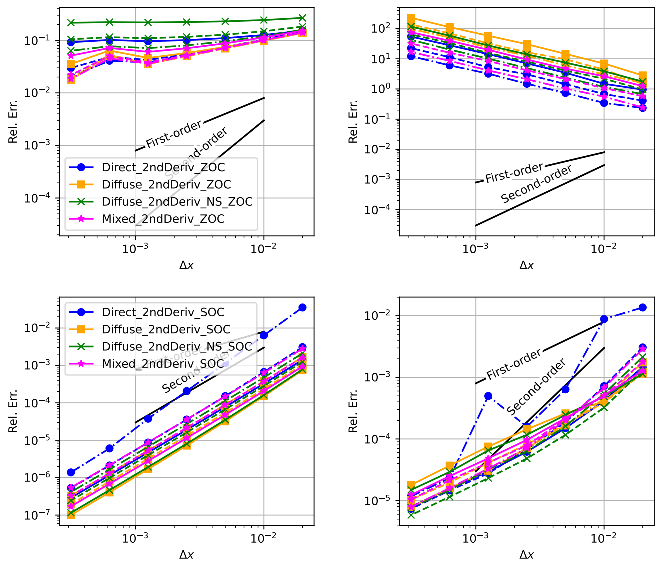

Fig. 2. Convergence of different zeroth-order consistent (ZOC) schemes (top) and second-order consistent (SOC) schemes (bottom) for the second derivative of 1D function $u(x) = 1 + \cos(\pi x)$ on regular (left) and irregular particle spacing (right) with values of $h/\Delta x$ 2.5 (solid line) 3.5 (dash line) 4.5 (dash dot line).

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