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Error Estimation in Smoothed Particle Hydrodynamics and a New Scheme for Second Derivatives

R. Fatehi[a], M.T. Manzari[a,*]

[a]*Center of Excellence in Energy Conversion, School of Mechanical Engineering, Sharif University of Technology, Tehran, Iran.*

Abstract

Several schemes for discretization of first and second derivatives are available in Smoothed Particle Hydrodynamics (SPH). Here, four schemes for approximation of the first derivative and three schemes for the second derivative are examined using a theoretical analysis based on Taylor series expansion both for regular and irregular particle distributions. Estimation of terms in the truncation errors shows that only the renormalized (the first-order consistent) scheme has acceptable convergence properties to approximate the first derivative. None of the second derivative schemes has the first-order consistency. Therefore, they converge only when the particle spacing decreases much faster than the smoothing length of the kernel function.

In addition, using a modified renormalization tensor, a new SPH scheme is presented for approximating second derivatives that has the property of first-order consistency. To assess the computational performance of the proposed scheme, it is compared with the best available schemes when applied to a 2D heat equation. The numerical results show at least one order of magnitude improvement in accuracy when the new scheme is used. In addition, the new scheme has higher-order convergence rate on regular particle arrangements even for the case of only four particles in the neighborhood of each particle.

Key words: Smoothed Particle Hydrodynamics (SPH), Second derivative, First-order Consistency, Truncation Error, Convergence

1. Introduction

Smoothed Particle Hydrodynamics (SPH) was first introduced by Gingold and Monaghan [1] and Lucy [2] in 1977 and has emerged as a viable numerical scheme in the context of mesh free methods. The method has been successfully applied to numerous scientific applications. Like most other numerical schemes, however, the SPH method experiences continual theoretical and technical developments. In particular, various numerical schemes have been devised to approximate the first and second spatial derivative terms which appear in the governing equations. A typical first derivative term is the pressure gradient which plays an important role in the flow equations. Various numerical schemes have been proposed to deal with such terms including both symmetric [3] and non-symmetric [4] forms. On the other hand, second derivatives are manifested typically in flow problems as viscous terms. At least three different types of schemes have been introduced to discretize such second derivatives [5]. The computational performance of various methods have been investigated and reported in [4, 6, 7, 5]. Despite these valuable efforts, it seems that a sound and fairly general theoretical analysis on this issue is yet to be presented.

To have a numerical method of a desired order of accuracy, it is required that each term in the differential equation be discretized with a certain order of accuracy. In the mesh-free methods like SPH, the spatial derivatives are of particular importance. Another property of numerical methods which is related to accuracy is the rate of convergence. The convergence rate of a numerical method depends on the leading error term in its modified equation. Practically, each term in the governing equation can be discretized using different methods for computation of derivatives which

*Corresponding author

Email addresses: mtmanzari@sharif.edu (M.T. Manzari)

potentially lead to errors of different magnitudes. Therefore, the choice of appropriate approximations for various derivative terms is of crucial importance especially in the SPH method.

In the context of the SPH method, Monaghan and Lattanzio [8] showed that the error of the so-called integral interpolant of SPH is of second order in terms of smoothing length h and also demonstrated that using a higher-order kernel function can improve the accuracy to h^4. This argument is however valid only for the continuous interpolation of field functions. In the discrete summations which are used in the computation of derivatives, there are also other sources of errors. In 1987, Mas-Gallic and Raviart [9] proved that a discrete form for nth derivatives in SPH has an error of order $h^2 + h^{-n}(\Delta/h)^2$ where Δ is the distance between the neighboring particles in one dimension. This means that decreasing the smoothing length h does not lead to convergence unless the particle spacing Δ decreases much faster than h. The dependency of convergence of the SPH method on both particle spacing Δ and smoothing length h was also confirmed in the work of Ben Moussa and Vila [10]. They also showed that to obtain a convergent first derivative approximation in the SPH method, it is required to satisfy both $h \longrightarrow 0$ and $\Delta/h^2 \longrightarrow 0$ conditions.

Another property associated with the numerical schemes is the notion of consistency which is a requirement for convergence. Unlike grid-based methods, in general, evaluation of consistency is not a straightforward matter for mesh-free methods. For these types of methods, Belytschko *et al.* [11] have defined the order of consistency as the maximum order of a polynomial which is represented exactly by an approximation technique. Here, it is shown that the order of accuracy of a scheme is highly affected by its order of consistency.

An extra difficulty arises when one deals with moving particles. In such cases, the spacing between particles can continually change and therefore the assumption of equally spaced particle distribution is no longer valid. As a result, the error estimates based on regular arrangement of particles need to be modified. Colagrossi reported that the convergence rate of a method can be as much as one to three orders of magnitude lower than that for ordered particles [12]. Quinlan *et al.* [13] studied convergence of two SPH schemes for the computation of the first derivative in one dimension. They calculated the derivative of a sinusoidal function using the standard and first-order consistent SPH schemes when particle arrangement is either ordered or disordered. By investigating the numerical errors, they showed that for a uniform distribution, the error of the standard scheme decays as a function of h^2 up to a certain limit which is itself a function of the fraction h/Δ. In the case of the first-order consistent scheme on an ordered particle distribution, however, the method retains its second-order convergence. When the particles are disordered, error of the standard scheme can grow as h is reduced. This highlights the complex behavior of the SPH even for approximation of the first derivative of a fairly simple function.

Concerning the accuracy of second derivative approximations in SPH, there are even fewer works in the literature. Fatehi *et al.* [14] compared three forms of discretization of the second derivative for a heat-like equation in one dimension. Graham and Hughes [7] numerically studied a SPH scheme in 1D and 2D for random placement of particles and concluded that the method converges only in the case of regular particle arrangement and for special values of h/Δ.

In the present paper, a mathematical framework is presented to compare the truncation errors and convergence properties of general SPH schemes for discretization of both first and second spatial derivatives. Four schemes for the first derivative and three schemes for the second derivative are considered. The schemes are briefly presented in the following section. Next, the truncation error associated with each scheme is found using a Taylor series expansion. In section 4, the order of magnitude of different terms in the truncation errors are estimated both for regular and irregular particle arrangements. Finally, a new scheme for approximation of the second derivative is introduced in section 5 and its performance is assessed by solving a 2D heat equation in section 6.

2. SPH Approximation of Derivatives

SPH is a Lagrangian particle-based method in which each computational point is a part of substance and is called particle. The SPH method is built on the notion of interpolation. For an arbitrary field function u the interpolated value $\langle u \rangle$ in terms of the values at neighboring particles u_j is found from

$$\langle u(\mathbf{r}) \rangle = \sum_j \omega_j u_j W(\mathbf{r} - \mathbf{r}_j, h), \tag{1}$$

where ω_j is the weight or the volume of neighboring particle j and W represents the smoothing or kernel function which is a smoothed version of the Dirac delta function and is positive for $\left|\mathbf{r} - \mathbf{r}_j\right| < h$ with a compact support of radius h [1].

Several techniques have been used in SPH to discretize the first and the second spatial derivatives. In this section, a number of frequently used schemes are summarized.

2.1. First derivative

The first derivative of field function u can be approximated using either of the following schemes.

Scheme F1 Standard scheme as first introduced by Monaghan [1]:

$$\langle \nabla u \rangle_i = \sum_j \omega_j u_j \nabla_i W_{ij}, \tag{2}$$

where $W_{ij} = W(\mathbf{r}_i - \mathbf{r}_j, h)$ denotes the kernel function of particle i evaluated at r_j the position of particle j. Also, ∇_i denotes differentiation in space with respect to the coordinates on particle i. In the following, the subscript is dropped for the sake of simplicity.

Scheme F2 Modified version of **Scheme F1**:

$$\langle \nabla u \rangle_i = \sum_j \omega_j \left(u_j - u_i\right) \nabla W_{ij}. \tag{3}$$

The advantage of this form over the standard one is that here, the first derivative of a constant function is exactly zero. This property is known as zeroth-order consistency.

Scheme F3 Symmetric form

$$\langle \nabla u \rangle_i = \sum_j \omega_j \left(u_j + u_i\right) \nabla W_{ij}, \tag{4}$$

is not zeroth-order consistent but it is usually used for discretization of the pressure gradient in the Navier-Stokes and Euler equations. The advantage is that using symmetric forms to discretize forces leads to local momentum conservation.

Scheme F4 Renormalized scheme as introduced by Randles and Libersky [15], Bonet and Lok [16] and Vila [17]:

$$\langle \nabla u \rangle_i = \sum_j \omega_j \left(u_j - u_i\right) \mathbf{B}_i \cdot \nabla W_{ij}, \tag{5}$$

where

$$\mathbf{B}_i = -\left[\sum_j \omega_j \mathbf{r}_{ij} \nabla W_{ij}\right]^{-1}, \tag{6}$$

is the renormalization tensor in which $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is the distance vector of particles i and j. Since ∇W_{ij} is parallel to $\mathbf{r}_{ij}$, the renormalization tensor $\mathbf{B}$ is symmetric. An advantage of this method is that it is first-order consistent. This means by definition that the scheme can exactly calculate the gradient of a linear function. Since this form is not symmetric, conservation is not guaranteed. In 2005, Vila [18] suggested a symmetric version of the renormalized scheme which is conservation preserving but it is not first-order consistent any more.

2.2. Second derivative

There are also different forms to approximate the second derivative $\langle \nabla \cdot \nabla u \rangle_i$ in the context of SPH. In the following, three forms are described.

Scheme S1 Naturally, one can use each of the schemes defined in section 2.1 to obtain a numerical scheme for the second derivative. These give

$$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \omega_j \langle \nabla u \rangle_j \cdot \nabla W_{ij}, \tag{7}$$

$$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \omega_j \left(\langle \nabla u \rangle_j - \langle \nabla u \rangle_i\right) \cdot \nabla W_{ij}, \tag{8}$$

or

$$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \omega_j \left(\langle \nabla u \rangle_j + \langle \nabla u \rangle_i \right) \cdot \nabla W_{ij}. \tag{9}$$

These forms were used to include physical viscosity in astrophysical problems [19, 20] and to solve 2D heat conduction problems [21] and to study low-Reynolds number incompressible flows [16, 22]. The above forms can be named as double summation forms as they require two summation evaluations. Flebbe *et al.* [19] and Watkins *et al.* [20] used the scheme in Eq. (9) for astrophysical problems and reported some non-physical oscillations in their solution. Fatehi *et al.* [14] showed that using these schemes in a heat-like equation with discontinuous initial condition, essentially leads to oscillatory solutions. The reason can be explained by referring to the extension of the computational stencil which is a well-known issue in grid-based methods [23].

Scheme S2 Another way to construct second derivative is to use the second derivative of the kernel function. Using Eqs. (2), (3), and (4), one obtains

$$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \omega_j u_j \nabla \cdot \nabla W_{ij}, \tag{10}$$

$$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \omega_j \left(u_j - u_i \right) \nabla \cdot \nabla W_{ij}, \tag{11}$$

and

$$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \omega_j \left(u_j + u_i \right) \nabla \cdot \nabla W_{ij}. \tag{12}$$

These forms were used by Takeda *et al.* [24] and Chaniotis *et al.* [25]. Fatehi and coworkers [14] showed that to have monotonicity preserving, when using Eq. (12), the inflection point of the kernel function must be farther than the nearest neighboring particle. Since usual smoothing functions have inflection points between 0 and h, in a complicated flow problem, it is hard to satisfy the above condition. It should be noted that, this discussion is for ordered particles. As reported by Monaghan [3], the form of Eq. (10) is also very sensitive to particle distribution.

Scheme S3 Brookshaw [26] suggested a finite-difference-like form for the first derivation and a SPH summation for the second derivative as

$$\langle \nabla \cdot \nabla u \rangle_i = \sum_j 2\omega_j \frac{u_i - u_j}{r_{ij}} \mathbf{e}_{ij} \cdot \nabla W_{ij}, \tag{13}$$

where $r_{ij} = \left| \mathbf{r}_{ij} \right|$ and $\mathbf{e}_{ij} = \frac{\mathbf{r}_{ij}}{r_{ij}}$ is a unit vector in the inter-particle direction. Basa *et al.* [5] showed that this technique is best among the available SPH schemes for approximation of the second derivatives.

3. Error Analysis

In this section, truncation errors of the above mentioned schemes are assessed. Consider the multi-dimensional Taylor series expansion of the field function u at $\mathbf{r}_j$ about point $\mathbf{r}_i$ as

$$u_j = \sum_{m=0}^{\infty} \left[\frac{1}{m!} \left((\mathbf{r}_j - \mathbf{r}_i) \cdot \nabla \right)^m u \right]_{\mathbf{r}=\mathbf{r}_i}. \tag{14}$$

The first four terms are

$$u_j = u_i - \mathbf{r}_{ij} \cdot \nabla u \Big|_i + \frac{1}{2} \left(\mathbf{r}_{ij} \cdot \nabla \right) \left(\mathbf{r}_{ij} \cdot \nabla \right) u \Big|_i - \frac{1}{6} \left(\mathbf{r}_{ij} \cdot \nabla \right) \left(\mathbf{r}_{ij} \cdot \nabla \right) \left(\mathbf{r}_{ij} \cdot \nabla \right) u \Big|_i + \cdots,$$

where subscript i denotes evaluation of the function and its derivatives at point $\mathbf{r}_i$. Equivalently, it can be rewritten as

$$u_j = u_i - \mathbf{r}_{ij} \cdot \nabla u|_i + \frac{1}{2} \mathbf{r}_{ij} \mathbf{r}_{ij} : \nabla \nabla u|_i - \frac{1}{6} \mathbf{r}_{ij} \mathbf{r}_{ij} \mathbf{r}_{ij} \vdots \nabla \nabla \nabla u|_i + \cdots, \tag{15}$$

where the operator ":" denotes double dot, scalar, or inner product of second-order tensors. Similarly, triple dot product of two third-order tensors $\mathbf{X}$ and $\mathbf{Y}$ can be defined as

$$\begin{aligned}\mathbf{X}\dddot{}\mathbf{Y} &= X_{\alpha\beta\gamma}\mathbf{e}_\alpha\mathbf{e}_\beta\mathbf{e}_\gamma\dddot{}Y_{\delta\lambda\eta}\mathbf{e}_\delta\mathbf{e}_\lambda\mathbf{e}_\eta \\ &\equiv X_{\alpha\beta\gamma}Y_{\alpha\beta\gamma}.\end{aligned} \tag{16}$$

Substituting (15) in the schemes of section 2, one can evaluate the truncation error of each scheme. This is elaborated in the following.

3.1. First derivative

Considering **scheme F1** (Eq. (2)) and using Eq. (15), one obtains

$$\langle\nabla u\rangle_i = \sum_j \omega_j \left(u_i - \mathbf{r}_{ij}\cdot\nabla u|_i + \frac{1}{2}\mathbf{r}_{ij}\mathbf{r}_{ij} : \nabla\nabla u|_i + \cdots\right)\nabla W_{ij}.$$

Since u_i, $\nabla u|_i$, $\cdots$ are constant with respect to j, the above equation can be written as

$$\langle\nabla u\rangle_i = u_i\sum_j \omega_j\nabla W_{ij} - \nabla u|_i\cdot\sum_j \omega_j\mathbf{r}_{ij}\nabla W_{ij} + \frac{1}{2}\,\nabla\nabla u|_i : \sum_j \omega_j\mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij} + \cdots.$$

Therefore, the truncation error Er_i is obtained as

$$\begin{aligned}Er_i &\equiv \langle\nabla u\rangle_i - \nabla u|_i \\ &= u_i\sum_j \omega_j\nabla W_{ij} - \nabla u|_i\cdot\left(\mathbf{I} + \sum_j \omega_j\mathbf{r}_{ij}\nabla W_{ij}\right) + \frac{1}{2}\,\nabla\nabla u|_i : \sum_j \omega_j\mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij} + \cdots.\end{aligned}$$

Rearranging and keeping the first two terms, one obtains

$$Er_i = u_i\sum_j \omega_j\nabla W_{ij} + \nabla u|_i\cdot\left(\mathbf{B}_i^{-1} - \mathbf{I}\right) + \cdots, \tag{17}$$

in which $\mathbf{I}$ is the second-order unitary tensor. Eq. (17) shows that the first term in truncation error of the standard scheme is proportional to u_i. Although the coefficient $\sum_j \omega_j\nabla W_{ij}$ can vanish in the case of ordered particle arrangement, in general, it is non-zero. The order of magnitude of this term is investigated in the next section. The appearance of u_i and even $\nabla u|_i$ cause a great difficulty because when a constant u_0 is added to all points, the error grows proportionally. Also the error increases when one approximates a function with a large first derivative $\nabla u|_i$. It is not acceptable that the truncation error of a derivative approximation includes derivatives of the same order or lower orders.

Similar behavior is observed when using **scheme F3**. In this case, the truncation error becomes

$$Er_i = 2u_i\sum_j \omega_j\nabla W_{ij} + \nabla u|_i\cdot\left(\mathbf{B}_i^{-1} - \mathbf{I}\right) + \cdots, \tag{18}$$

in which the multiplier of the first term has been doubled. In the case of Navier-Stokes equations, when the pressure gradient is discretized in this manner, the whole solution depends on the value of reference pressure P_0 [27]. Thus, to have a reasonable result, P_0 needs to be tuned for each problem. The culprit is the existence of u_i in the truncation error.

In the case of **scheme F2** (Eq. (3)) the truncation error becomes independent of u_i and one obtains

$$Er_i = \nabla u|_i\cdot\left(\mathbf{B}_i^{-1} - \mathbf{I}\right) + \frac{1}{2}\,\nabla\nabla u|_i : \sum_j \omega_j\mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij} + \cdots. \tag{19}$$

The disappearance of u_i is equivalent to achieving zeroth-order consistency. In addition, Eq. (19) shows that the accuracy of this technique is one order of magnitude higher than those of both **F1** and **F3** schemes. However, **scheme F2** still suffers from the existence of $\nabla u|_i$ in the truncation error of $\langle \nabla u \rangle_i$.

In a similar way, it can be shown that the truncation error of the Renormalized scheme (**scheme F4**) is

$$Er_i = \frac{1}{2}\ \nabla\nabla u|_i : \sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\mathbf{B}_i \cdot \nabla W_{ij} - \frac{1}{6}\ \nabla\nabla\nabla u|_i \vdots \sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\mathbf{r}_{ij}\mathbf{B}_i \cdot \nabla W_{ij} + \cdots . \tag{20}$$

Here, the lowest-order term includes the second derivative. This is why the scheme can exactly predict the first derivative of a linear function, an important property which cannot be seen in all other known SPH schemes.

3.2. Second derivative

As mentioned before, all techniques in the category of **scheme S1** have difficulties because of the notion of extending computational stencil. This is also visible in the truncation errors. For example, assume that the first derivatives in Eqs. (7) to (9) are calculated using Eq. (3) (**scheme F2**). Thus,

$$\langle \nabla u \rangle_i = \nabla u|_i \cdot \mathbf{B}_i^{-1} + \frac{1}{2}\ \nabla\nabla u|_i : \sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij} + \cdots ,$$

and

$$\langle \nabla u \rangle_j = \nabla u|_j \cdot \mathbf{B}_j^{-1} + \frac{1}{2}\ \nabla\nabla u|_j : \sum_k \omega_k \mathbf{r}_{jk}\mathbf{r}_{jk}\nabla W_{jk} + \cdots .$$

where subscript k denotes neighbors of particle j. But from Taylor series expansion, one has

$$\nabla u|_j = \nabla u|_i - \mathbf{r}_{ij} \cdot \nabla\nabla u|_i + \frac{1}{2}\mathbf{r}_{ij}\mathbf{r}_{ij} : \nabla\nabla\nabla u|_i + \cdots ,$$

and

$$\nabla\nabla u|_j = \nabla\nabla u|_i - \mathbf{r}_{ij} \cdot \nabla\nabla\nabla u|_i + \frac{1}{2}\mathbf{r}_{ij}\mathbf{r}_{ij} : \nabla\nabla\nabla\nabla u|_i + \cdots .$$

Therefore,

$$\langle \nabla u \rangle_j = \nabla u|_i \cdot \mathbf{B}_j^{-1} - \mathbf{B}_j^{-1} \cdot \nabla\nabla u|_i \cdot \mathbf{r}_{ij} + \frac{1}{2}\ \nabla\nabla u|_i : \left(\sum_k \omega_k \mathbf{r}_{jk}\mathbf{r}_{jk}\nabla W_{jk} \right) + \cdots ,$$

Substituting this in Eq. (7) leads to

$$\begin{aligned} \langle \nabla \cdot \nabla u \rangle_i = {} & \nabla u|_i \cdot \sum_j \omega_j \mathbf{B}_j^{-1} \cdot \nabla W_{ij} + \sum_j \omega_j \mathbf{B}_j^{-1} \cdot \nabla\nabla u|_i \cdot \mathbf{r}_{ij} \cdot \nabla W_{ij} \\ & + \frac{1}{2}\ \nabla\nabla u|_i : \sum_j \omega_j \left(\sum_k \omega_k \mathbf{r}_{jk}\mathbf{r}_{jk}\nabla W_{jk} \right) \cdot \nabla W_{ij} + \cdots . \end{aligned} \tag{21}$$

Keeping in mind that $\mathbf{B}$ approximates $\mathbf{I}$, one can conclude that the multiplier of $\nabla \cdot \nabla u|_i$ is near unity. So, the truncation error is

$$\begin{aligned} Er_i = {} & \nabla u|_i \cdot \sum_j \omega_j \mathbf{B}_j^{-1} \cdot \nabla W_{ij} + \sum_j \omega_j \mathbf{B}_j^{-1} \cdot \nabla\nabla u|_i \cdot \mathbf{r}_{ij} \cdot \nabla W_{ij} \\ & + \nabla\nabla u|_i : \left[\frac{1}{2} \sum_j \omega_j \left(\sum_k \omega_k \mathbf{r}_{jk}\mathbf{r}_{jk}\nabla W_{jk} \right) \cdot \nabla W_{ij} - \mathbf{I} \right] \\ & + \cdots . \end{aligned} \tag{22}$$

There are two problems. The first problem is the appearance of $\nabla u|_i$ which is similar to the difficulties discussed previously. The other problem is the summation on neighbors k of each neighboring particle j. In a heat-like equation,

this can result in two or more decoupled sets of algebraic equations which leads to non-physical oscillations in the solutions. Note that if **schemes F1** or **F3** were used for the first derivative approximation, the condition was even worse. In those situations, the truncation error would have a leading term involving u_i.

In a similar fashion, the truncation errors associated with equations (8) and (9) are obtained as

$$\begin{aligned} Er_i = &\nabla u|_i \cdot \sum_j \omega_j \left(\mathbf{B}_j^{-1} - \mathbf{B}_i^{-1}\right) \cdot \nabla W_{ij} + \sum_j \omega_j \mathbf{B}_j^{-1} \cdot \nabla\nabla u|_i \cdot \mathbf{r}_{ij} \cdot \nabla W_{ij} \\ &+ \nabla\nabla u|_i : \left[\frac{1}{2}\sum_j \omega_j \left(\sum_k \omega_k \mathbf{r}_{jk}\mathbf{r}_{jk}\nabla W_{jk} - \sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij}\right) \cdot \nabla W_{ij} - \mathbf{I}\right] \\ &+ \cdots, \end{aligned} \tag{23}$$

and

$$\begin{aligned} Er_i = &\nabla u|_i \cdot \sum_j \omega_j \left(\mathbf{B}_j^{-1} + \mathbf{B}_i^{-1}\right) \cdot \nabla W_{ij} + \sum_j \omega_j \mathbf{B}_j^{-1} \cdot \nabla\nabla u|_i \cdot \mathbf{r}_{ij} \cdot \nabla W_{ij} \\ &+ \nabla\nabla u|_i : \left[\frac{1}{2}\sum_j \omega_j \left(\sum_k \omega_k \mathbf{r}_{jk}\mathbf{r}_{jk}\nabla W_{jk} + \sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij}\right) \cdot \nabla W_{ij} - \mathbf{I}\right] \\ &+ \cdots. \end{aligned} \tag{24}$$

Note that although the use of Eq. (8) improves the accuracy of the technique by substituting $\mathbf{B}_j^{-1}$ with $\left(\mathbf{B}_j^{-1} - \mathbf{B}_i^{-1}\right)$ in Eq. (23), it still suffers from the same flaws. So, this scheme is not studied further in the present paper.

Scheme S2 does not have the problem of extended stencil. Instead, Eqs. (10) and (12) suffer from the appearance of u_i in the truncation error of $\langle\nabla \cdot \nabla u\rangle_i$. For example, the truncation error of Eq. (10) is

$$\begin{aligned} Er_i = &u_i \sum_j \omega_j \nabla \cdot \nabla W_{ij} - \nabla u|_i \cdot \sum_j \omega_j \mathbf{r}_{ij} \nabla \cdot \nabla W_{ij} \\ &+ \nabla\nabla u|_i : \left(\frac{1}{2}\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\nabla \cdot \nabla W_{ij} - \mathbf{I}\right) + \cdots. \end{aligned} \tag{25}$$

The main problem here is that the term $\sum_j \omega_j \nabla \cdot \nabla W_{ij}$ does not easily converge to zero. See the discussion in the next section for more details.

Using the scheme given by Eq. (11) one obtains a better condition:

$$Er_i = -\nabla u|_i \cdot \sum_j \omega_j \mathbf{r}_{ij} \nabla \cdot \nabla W_{ij} + \nabla\nabla u|_i : \left(\frac{1}{2}\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\nabla \cdot \nabla W_{ij} - \mathbf{I}\right) + \cdots. \tag{26}$$

Although the leading term in the error is now an order of magnitude lower than that of Eq. (25), the problem of existence of $\nabla u|_i$ is yet remaining.

Scheme S3 also only uses u_i and u_j and thus does not have the problem of non-physical oscillations. For Eq. (13), substituting from Eq. (15) results in

$$\langle\nabla \cdot \nabla u\rangle_i = \sum_j 2\omega_j \left(\mathbf{e}_{ij} \cdot \nabla u|_i - \frac{1}{2}\mathbf{r}_{ij}\mathbf{e}_{ij} : \nabla\nabla u|_i + \frac{1}{6}\mathbf{r}_{ij}\mathbf{r}_{ij}\mathbf{e}_{ij} \vdots \nabla\nabla\nabla u|_i + \cdots\right)\mathbf{e}_{ij} \cdot \nabla W_{ij}.$$

Since $\nabla W_{ij} = \frac{\partial W_{ij}}{\partial \mathbf{r}_{ij}}\mathbf{e}_{ij}$ and $\mathbf{e}_{ij} \cdot \mathbf{e}_{ij} = 1$, the truncation error can be simplified as

$$\begin{aligned} Er_i = &2\ \nabla u|_i \cdot \sum_j \omega_j \nabla W_{ij} + \nabla\nabla u|_i : \left(\mathbf{B}_i^{-1} - \mathbf{I}\right) \\ &+ \frac{1}{3}\ \nabla\nabla\nabla u|_i \vdots \left(\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij}\right) + \cdots. \end{aligned} \tag{27}$$

As can be seen, the error still includes the first derivative term $\nabla u|_i$. In section 5, a new scheme will be presented which resolves this difficulty.

4. Error Estimation

In the previous section, the truncation errors of a number of SPH schemes were obtained in terms of summations of the gradient of the kernel function such as $\sum_j \omega_j \nabla W_{ij}$, $\sum_j \omega_j \mathbf{r}_{ij} \nabla W_{ij}$, *etc*. Here, an order of magnitude analysis for these terms is given.

4.1. Regular arrangement

Assume that the particles are positioned orderly and weights ω_j (here, chosen as the volumes of particles) are constant and equal. By these assumptions, the computation of some terms becomes trivial. For example, it is obvious that on such arrangements, from symmetry, one has

$$\sum_j \omega_j \nabla W_{ij}^{reg} = \mathbf{0}, \tag{28}$$

$$\sum_j \omega_j \mathbf{r}_{ij}^{reg} \mathbf{r}_{ij}^{reg} \nabla W_{ij}^{reg} = \mathbf{0}, \tag{29}$$

and

$$\sum_j \omega_j \mathbf{r}_{ij}^{reg} \nabla \cdot \nabla W_{ij}^{reg} = \mathbf{0}, \tag{30}$$

where superscript "*reg*" denotes summation on a regular arrangement.

On the other hand, other summations can be treated as numerical approximations of Riemann integrals. For example,

$$\begin{aligned} \mathbf{B}_i^{-1,reg} &= -\sum_j \omega_j \mathbf{r}_{ij}^{reg} \nabla W_{ij}^{reg} \\ &= \left\langle -\int_{\Omega_i} (\mathbf{r} - \mathbf{r}_i) \nabla W (\mathbf{r} - \mathbf{r}_i, h) \, d\Omega \right\rangle, \end{aligned} \tag{31}$$

where Ω_i is the support of the kernel function and $d\Omega$ is the differential element of space. Using integration by parts and the divergence theorem, one obtains

$$\int_{\Omega_i} (\mathbf{r} - \mathbf{r}_i) \nabla W (\mathbf{r} - \mathbf{r}_i, h) \, d\Omega = \int_{\partial\Omega_i} (\mathbf{r} - \mathbf{r}_i) W (\mathbf{r} - \mathbf{r}_i, h) \, d\mathbf{s} - \mathbf{I} \int_{\Omega_i} W (\mathbf{r} - \mathbf{r}_i, h) \, d\Omega,$$

where $\partial\Omega_i$ is the boundary of Ω_i and $d\mathbf{s}$ is a differential element on it. By definition, W is zero on $\partial\Omega_i$ and $\int_{\Omega_i} W (\mathbf{r} - \mathbf{r}_i, h) \, d\Omega$ is unity. Thus, $\mathbf{B}_i^{-1,reg}$ approximates unitary tensor $\mathbf{I}$. But, Eq. (31) is a midpoint quadrature formula and the error of $\sum_j \omega_j f(\mathbf{r}_j)$ over a regular particle distribution with equal spacing Δ is $C\Omega_i \Delta^2 \nabla^2 f(\mathbf{z})$ where $\mathbf{z}$ is a point in the domain Ω_i. Therefore,

$$\mathbf{B}_i^{-1,reg} \approx \mathbf{I} \left(1 + C\Omega_i \Delta^2 \nabla^2 W(\mathbf{z} - \mathbf{r}_i, h) \right).$$

Note that $\Omega_i \propto h^D$ where D is the number of dimensions. In addition, $\nabla^2 W$ can be approximated as $\frac{W_0}{h^2}$ where W_0 is the multiplier of the kernel function which is proportional to h^{-D}.

A more accurate estimation carried out by Quinlan *et al.* [13] using second Euler-MacLaurin formula shows that for a sufficiently continuous function g in one dimension and ordered particles, one has

$$\sum_j \omega_j g_j W'_{ij} - g'_i \approx g'_i \times O\left(\left(\frac{\Delta}{h} \right)^{\beta+2} \right) + g'''_i \times \left[O\left(h^2\right) + O\left(h^2 \left(\frac{\Delta}{h} \right)^{\beta+2} \right) \right] + \cdots, \tag{32}$$

where prime denotes a derivation in spatial dimension and β is the boundary smoothness of the kernel function W which is defined as the largest integer so that the βth derivative and all lower derivatives of kernel are zero at the edges of the compact support [13]. It is at least 2 for common kernel functions used in SPH. Eq. (32) is obtained supposing

Table 1: The orders of magnitude of the leading terms of truncation errors of some SPH schemes for the first and second derivatives on a regular particle distribution.

Scheme No.	Eq. No.	Scheme	Leading term in truncation error
F1	(2)	$\langle\nabla u\rangle_i = \sum_j \omega_j u_j \nabla_i W_{ij}$	$\lvert\nabla u\rvert_i \times O\left(\left(\frac{\Delta}{h}\right)^{\beta+1}\right)$
F4	(5)	$\langle\nabla u\rangle_i = \sum_j \omega_j \left(u_j - u_i\right)\mathbf{B}_i \cdot \nabla W_{ij}$	$\left\lvert\nabla^3 u\right\rvert_i \times O\left(h^2\right)$
S2	(10)	$\langle\nabla \cdot \nabla u\rangle_i = \sum_j \omega_j u_j \nabla \cdot \nabla W_{ij}$	$u_i \times O\left(\frac{1}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right)$
S2	(11)	$\langle\nabla \cdot \nabla u\rangle_i = \sum_j \omega_j \left(u_j - u_i\right)\nabla \cdot \nabla W_{ij}$	$\left\lvert\nabla^2 u\right\rvert_i \times O\left(\left(\frac{\Delta}{h}\right)^{\beta-1}\right)$
S3	(13)	$\langle\nabla \cdot \nabla u\rangle_i = \sum_j 2\omega_j \frac{u_i - u_j}{r_{ij}}\mathbf{e}_{ij} \cdot \nabla W_{ij}$	$\left\lvert\nabla^2 u\right\rvert_i \times O\left(\left(\frac{\Delta}{h}\right)^{\beta+1}\right)$

even number β. If β is odd, $\beta + 2$ is replaced by $\beta + 1$. In the following, β is assumed odd which is consistent with the kernel function used.

When the above conclusion is extended to multi-dimensions, then

$$\mathbf{I} - \mathbf{B}_i^{-1,reg} \approx O\left(\left(\frac{\Delta}{h}\right)^{\beta+1}\right), \tag{33}$$

and

$$\sum_j \omega_j \mathbf{r}_{ij}^{reg} \mathbf{r}_{ij}^{reg} \mathbf{r}_{ij}^{reg} \nabla W_{ij}^{reg} \approx O\left(h^2\right) + O\left(h^2\left(\frac{\Delta}{h}\right)^{\beta+1}\right). \tag{34}$$

At a constant ratio of $\frac{h}{\Delta}$, the summation in Eq. (34) converges to zero as $\Delta \longrightarrow 0$. This is a worthwhile property. The opposite is the previous term in Eq. (33) which converges only by letting $\frac{h}{\Delta} \longrightarrow \infty$.

In a similar way, one can rewrite Eq. (32) for odd β and second derivative of kernel function W''. Then, the truncation error of the numerical quadrature $\sum_j \omega_j g_j W_{ij}''$ is

$$\begin{aligned}\sum_j \omega_j g_j W_{ij}'' - g_i'' \approx & g_i \times O\left(\frac{1}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right) + g'' \times O\left(\left(\frac{\Delta}{h}\right)^{\beta-1}\right) \\ & + g_i'''' \times O\left(h^2\right) + \cdots,\end{aligned} \tag{35}$$

Using the same assumptions and for common kernel functions for which the divergence theorem

$$\int_{\Omega_i} \nabla \cdot \nabla W\left(\mathbf{r} - \mathbf{r}_i, h\right) d\Omega = \int_{\partial\Omega_i} \nabla W\left(\mathbf{r} - \mathbf{r}_i, h\right) \cdot d\mathbf{s} = 0,$$

is valid, one has

$$\sum_j \omega_j \nabla \cdot \nabla W_{ij}^{reg} \approx O\left(\frac{1}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right), \tag{36}$$

and

$$\sum_j \omega_j \mathbf{r}_{ij}^{reg} \mathbf{r}_{ij}^{reg} \nabla \cdot \nabla W_{ij}^{reg} \approx O\left(\left(\frac{\Delta}{h}\right)^{\beta-1}\right). \tag{37}$$

Substituting the above values in the truncation errors obtained in the previous section (Eqs. (17) to (27)), one can obtain an estimation of errors of these schemes on a regular distribution of particles. These are listed in Table 1 for some of the schemes discussed here. It should be noted that the orders of the leading terms of truncation errors of **schemes F2** and **F3** are the same as that of **scheme F1** and also the orders for **scheme S1** are the same as that of **scheme S2** (Eq. (11)) and **scheme S3** in the case of regular arrangement.

4.2. Irregular arrangement

The above discussion was given for a regular equally spaced particle. For a general particle distribution, this is not true especially for a multi-dimensional flow problem in which particles are moving in a complex manner. Hence, it is necessary to study the errors of the method when the particles are distributed irregularly. When the particle arrangement is not regular, the value of any typical summation S can be decomposed into two parts; S^{reg} which was investigated before and $\tilde{S}$ which is the contribution due to the deviation from the regular arrangement.

Assume that each particle j is displaced by $\mathbf{d}_{ij}$ from its regular position $\mathbf{r}_{ij}^{reg}$. One can write

$$\begin{aligned} W\left(\mathbf{r}_{ij}\right) =& W\left(\mathbf{r}_{ij}^{reg}+\mathbf{d}_{ij}\right) \\ =& W\left(\mathbf{r}_{ij}^{reg}\right)+\mathbf{d}_{ij}\cdot\nabla W\left(\mathbf{r}_{ij}^{reg}\right)+\cdots, \end{aligned}$$

or in short notation

$$W_{ij} = W_{ij}^{reg}+\mathbf{d}_{ij}\cdot\nabla W_{ij}^{reg}+\cdots,$$

and similarly

$$\nabla W_{ij} = \nabla W_{ij}^{reg}+\mathbf{d}_{ij}\cdot\nabla\nabla W_{ij}^{reg}+\cdots,$$

and

$$\nabla\nabla W_{ij} = \nabla\nabla W_{ij}^{reg}+\mathbf{d}_{ij}\cdot\nabla\nabla\nabla W_{ij}^{reg}+\cdots.$$

As a result, one can write for instance

$$\sum_j \omega_j\nabla W_{ij} \approx \sum_j \omega_j\nabla W_{ij}^{reg}+\sum_j \omega_j\mathbf{d}_{ij}\cdot\nabla\nabla W_{ij}^{reg}.$$

From Eq. (28), the first term on the right-hand side is zero. For the second term, one can define $\tilde{d}_i$ as a measure of deviations of the neighboring particles of i. It is obvious that $0 \le \tilde{d}_i < \Delta$. Then using Eq. (36) one finds

$$\begin{aligned} \sum_j \omega_j\nabla W_{ij} \approx& \tilde{d}_i\sum_j \omega_j\nabla\cdot\nabla W_{ij}^{reg} \\ \approx& O\left(\frac{\tilde{d}_i}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right). \end{aligned} \tag{38}$$

Although this is a rough estimation which is different from [13], this approximation is sufficient for the present investigation.

For the renormalization tensor $\mathbf{B}$, the analysis is slightly more complex. One has

$$\begin{aligned} \mathbf{B}_i^{-1} =& -\sum_j \omega_j\mathbf{r}_{ij}\nabla W_{ij} \\ =& -\sum_j \omega_j\mathbf{r}_{ij}^{reg}\nabla W_{ij}^{reg}-\sum_j \omega_j\mathbf{d}_{ij}\nabla W_{ij}^{reg} \\ & -\sum_j \omega_j\mathbf{r}_{ij}^{reg}\mathbf{d}_{ij}\cdot\nabla\nabla W_{ij}^{reg}-\sum_j \omega_j\mathbf{d}_{ij}\mathbf{d}_{ij}\cdot\nabla\nabla W_{ij}^{reg}. \end{aligned}$$

The first term on the right-hand side was assessed in Eq. (33). The third and fourth terms are of orders higher than the second term, so they are omitted. As a result, one finds

$$\mathbf{I}-\mathbf{B}_i^{-1} \approx O\left(\left(\frac{\Delta}{h}\right)^{\beta+1}\right)+O\left(\frac{\tilde{d}_i}{h}\left(\frac{\Delta}{h}\right)^{\beta+1}\right). \tag{39}$$

By a similar analysis, the order of other terms are also obtained. The results are shown in Table 2.

Now, by substituting the orders of magnitude of Table 2 into the truncation errors of the previous section, the estimation of error for various SPH schemes is completed. (Table 3) Three schemes for the first derivative are shown.

Table 2: The order of magnitude of summations appeared in truncation errors of SPH schemes.

Summation	Order of magnitude
$\sum_j \omega_j \nabla W_{ij}$	$O\left(\frac{\tilde{d}_i}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right)$
$\mathbf{B}_i^{-1} = -\sum_j \omega_j \mathbf{r}_{ij} \nabla W_{ij}$	$O(1)$
$\mathbf{I} - \mathbf{B}_i^{-1}$	$O\left(\left(\frac{\Delta}{h}\right)^{\beta+1}\right) + O\left(\frac{\tilde{d}_i}{h}\left(\frac{\Delta}{h}\right)^{\beta+1}\right)$
$\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij} \nabla W_{ij}$	$O\left(\tilde{d}_i\left(\frac{\Delta}{h}\right)^{\beta+1}\right)$
$\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\mathbf{r}_{ij} \nabla W_{ij}$	$O\left(h^2\right) + O\left(\tilde{d}_i \Delta \left(\frac{\Delta}{h}\right)^{\beta+1}\right)$
$\sum_j \omega_j \nabla\nabla W_{ij}$	$O\left(\frac{1}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right) + O\left(\frac{\tilde{d}_i}{h^3}\left(\frac{\Delta}{h}\right)^{\beta-1}\right)$
$\sum_j \omega_j \mathbf{r}_{ij} \nabla\nabla W_{ij}$	$O\left(\frac{\tilde{d}_i}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right)$

Table 3: The orders of magnitude of the leading terms of truncation errors of some SPH schemes for the first and the second derivative on an arbitrary particle distribution.

Scheme No.	Eq. No.	Scheme	Leading term in truncation error
F1	(2)	$\langle \nabla u \rangle_i = \sum_j \omega_j u_j \nabla_i W_{ij}$	$u_i \times O\left(\frac{\tilde{d}_i}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right)$
F2	(3)	$\langle \nabla u \rangle_i = \sum_j \omega_j \left(u_j - u_i\right) \nabla W_{ij}$	$\lvert\nabla u\rvert_i \times \left(O\left(\left(\frac{\Delta}{h}\right)^{\beta+1}\right) + O\left(\frac{\tilde{d}_i}{h}\left(\frac{\Delta}{h}\right)^{\beta+1}\right)\right)$
F4	(5)	$\langle \nabla u \rangle_i = \sum_j \omega_j \left(u_j - u_i\right) \mathbf{B}_i \cdot \nabla W_{ij}$	$\left\lvert\nabla^2 u\right\rvert_i \times O\left(\tilde{d}_i\left(\frac{\Delta}{h}\right)^{\beta+1}\right)$
S2	(10)	$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \omega_j u_j \nabla \cdot \nabla W_{ij}$	$u_i \times \left(O\left(\frac{1}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right) + O\left(\frac{\tilde{d}_i}{h^3}\left(\frac{\Delta}{h}\right)^{\beta-1}\right)\right)$
S2	(11)	$\langle \nabla \cdot \nabla u \rangle_i = \sum_j \omega_j \left(u_j - u_i\right) \nabla \cdot \nabla W_{ij}$	$\lvert\nabla u\rvert_i \times O\left(\frac{\tilde{d}_i}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right)$
S3	(13)	$\langle \nabla \cdot \nabla u \rangle_i = \sum_j 2\omega_j \frac{u_i - u_j}{r_{ij}} \mathbf{e}_{ij} \cdot \nabla W_{ij}$	$\lvert\nabla u\rvert_i \times O\left(\frac{\tilde{d}_i}{h^2}\left(\frac{\Delta}{h}\right)^{\beta-1}\right)$

The omitted **scheme F3** has the same condition as **scheme F1**. Table 3 demonstrates that the only acceptable SPH technique to discretize the first derivatives is **scheme 4** because of two properties; First, its leading term in truncation error includes a second derivative *i.e.* first-order consistency. The other is that the truncation error diminishes as the particle spacing Δ decreases. Although the scheme converges linearly, it is a valuable property because for a fixed $\frac{h}{\Delta}$ ratio, the other schemes converge only when the particles are ordered. As mentioned before, it is a known fact that for convergence, other SPH methods need both $\Delta \longrightarrow 0$ and $\frac{h}{\Delta} \longrightarrow \infty$ [18]. Table 3 clearly shows this fact. For example, **scheme F1** needs Δ to decrease faster than $h^{1+1/\beta}$. This is tolerable in theory. But in practice, increasing $\frac{h}{\Delta}$ means growing number of neighbors and consequently higher computational costs especially in two or three dimensions. Indeed, a desirable technique is one which needs smaller neighboring particles or $\frac{h}{\Delta}$.

It is notable that the above two properties are not independent. For a first derivative scheme, if the truncation error has a term including u_i, its multiplier must have dimension $[L]^{-1}$ where L is a characteristic length and may be h or Δ. Accordingly, if it contains $\nabla u|_i$, its multiplier must be non-dimensional. These coefficients may not converge to zero as $\Delta \longrightarrow 0$. This is the sign of trouble and means that the truncation error diminishes only by making $\frac{h}{\Delta} \longrightarrow \infty$.

The above discussions are also true for second derivative schemes. Table 3 compares three SPH techniques for second derivatives. The others listed in section 2.2 are of similar order of accuracy. The first one (Eq. (25)) has more difficulties. The truncation error does not vanish except when Δ decreases faster than $h^{(\beta+1)/(\beta-1)}$. The two others are the best available techniques in SPH. Order of error for these two schemes in Table 3 are the same. So, they have the same problem as **scheme F1**. That is appearance of $\nabla u|_i$ in the truncation error and the order of its multiplier. The authors are not aware of any second derivative scheme in the SPH literature which has a better condition or in other words be first-order consistent. In the following section, a new technique is presented which resolves these problems for the second derivative.

5. A New Scheme For Second Derivative

A suitable method for discretization of second derivatives must have third derivative $\nabla\nabla\nabla u|_i$ as the leading term of its truncation error. Consider **scheme S3** in section 2.2. The truncation error in Eq. (27) has two extra terms. To improve the accuracy of this scheme, these terms should be trimmed. The first term can be removed by subtracting the term $2\sum_j \omega_j \mathbf{e}_{ij} \cdot \langle\nabla u\rangle_i \, \mathbf{e}_{ij}\nabla W_{ij}$. Then,

$$\sum_j 2\omega_j \left(\frac{u_i - u_j}{r_{ij}} - \mathbf{e}_{ij} \cdot \langle\nabla u\rangle_i\right) \mathbf{e}_{ij}\nabla W_{ij} = 2\left(\nabla u|_i - \langle\nabla u\rangle_i\right) \cdot \sum_j \omega_j \mathbf{e}_{ij}\mathbf{e}_{ij}\nabla W_{ij} - \nabla\nabla u|_i : \sum_j \omega_j \mathbf{r}_{ij}\mathbf{e}_{ij}\mathbf{e}_{ij}\nabla W_{ij} + \cdots .$$

The only proper choice for the numerical approximation $\langle\nabla u\rangle_i$ is **scheme F4**. Thus, substituting $\nabla u|_i - \langle\nabla u\rangle_i$ from Eq. (20) gives

$$\sum_j 2\omega_j \left(\frac{u_i - u_j}{r_{ij}} - \mathbf{e}_{ij} \cdot \langle\nabla u\rangle_i\right) \mathbf{e}_{ij}\nabla W_{ij} = - \nabla\nabla u|_i : \left[\sum_j \omega_j \mathbf{r}_{ij}\mathbf{e}_{ij}\mathbf{e}_{ij}\nabla W_{ij} + \left(\sum_j \omega_j \mathbf{e}_{ij}\mathbf{e}_{ij}\nabla W_{ij}\right) \cdot \mathbf{B}_i \cdot \left(\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij}\right)\right] + \cdots .$$

In this way, the term including $\nabla u|_i$ vanishes. So, the accuracy of this scheme is an order of magnitude higher than **scheme S3**. The order of error in this modified technique is now $O\left(\left(\frac{\Delta}{h}\right)^{\beta+1}\right) + O\left(\frac{\tilde{d}_i}{h}\left(\frac{\Delta}{h}\right)^{\beta+1}\right)$. To go ahead further, a new renormalization tensor $\hat{\mathbf{B}}_i$ is defined such that

$$\hat{\mathbf{B}}_i : \left[\sum_j \omega_j \mathbf{r}_{ij}\mathbf{e}_{ij}\mathbf{e}_{ij}\nabla W_{ij} + \left(\sum_j \omega_j \mathbf{e}_{ij}\mathbf{e}_{ij}\nabla W_{ij}\right) \cdot \mathbf{B}_i \cdot \left(\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij}\right)\right] = -\mathbf{I}, \tag{40}$$

This tensor differs from the usual renormalization tensor $\mathbf{B}_i$ by incorporating a high-order term which may vanish in the case of regular arrangement. Since $\hat{\mathbf{B}}_i$ is symmetric, calculation of this tensor in 2D leads to solving a linear system of simultaneous equations with three unknowns.

Therefore, the new **scheme S4** takes the following form

$$\langle \nabla \cdot \nabla u \rangle_i \equiv \hat{\mathbf{B}}_i : \sum_j 2\omega_j \mathbf{e}_{ij} \nabla W_{ij} \left(\frac{u_i - u_j}{r_{ij}} - \mathbf{e}_{ij} \cdot \sum_j \omega_j \left(u_j - u_i \right) \mathbf{B}_i \cdot \nabla W_{ij} \right). \tag{41}$$

Using the estimations given in Table 2, the order of the leading term in its truncation error becomes

$$Er_i \approx \left| \nabla^3 u \right|_i \times O\left(\tilde{d}_i \left(\frac{\Delta}{h} \right)^{\beta+1} \right). \tag{42}$$

Equation (41) presents a new scheme for approximation of the second derivatives and can be used for example for discretization of the thermal conduction terms in the energy equation and viscous terms in the Navier-Stokes equations. Since the deviation distance $\tilde{d}_i$ is smaller than the regular distance Δ, **scheme S4** is first-order accurate and converges regardless of the ratio $\frac{h}{\Delta}$. This means that the new scheme predicts the second derivative of either constant, linear, or quadratic functions exactly.

6. Numerical Example

To examine the accuracy of the proposed scheme and to compare its performance with other schemes, a 2D heat conduction problem $\frac{\partial T}{\partial t} = \alpha \nabla^2 T$ is considered on a unit square of thermal diffusivity α initially at uniform temperature $T(x, y, 0) = 0$ whose boundaries are at

$$\begin{aligned} T(0, y, t) &= 0, \\ T(1, y, t) &= 0, \\ T(x, 0, t) &= 0, \\ T(x, 1, t) &= \sin(\pi x). \end{aligned}$$

The analytical solution for this problem is given by

$$T(x, y, t) = \left(\sum_{m=1}^{\infty} \frac{2m}{\pi(m^2 + 1)} (-1)^m e^{-\beta t} \sin(m\pi y) + \frac{\sinh(\pi y)}{\sinh(\pi)} \right) \sin(\pi x), \tag{43}$$

where $\beta = \alpha\pi^2(1+m^2)$ and the value of thermal diffusivity was chosen as unity. This problem was solved using **scheme S3** (Eq. (13)) and the proposed **scheme S4** (Eq. (41)) for discretization of the Laplacian operator in heat equation. The simulation was conducted on both regular and irregular particle arrangements to compare the compatibilities of the methods.

The numerical results T_i^{num} were compared with the exact solution $T(x_i, y_i, t)$ at time $t = 0.1$ and three types of errors were reported: L_2-norm, L_∞-norm, and Conservation Error (EC) which is defined as the error in total energy of the domain

$$L_2 = \sqrt{\frac{1}{N} \sum_i^N \left(T(x_i, y_i, t) - T_i^{num} \right)^2}, \tag{44}$$

$$L_\infty = \max_{1 \le i \le N} \left(\left| T(x_i, y_i, t) - T_i^{num} \right| \right), \tag{45}$$

$$EC = \left| \int \left(T(x, y, t) - T^{num} \right) dxdy \right| = \frac{1}{N} \left| \sum_i^N \left(T(x_i, y_i, t) - T_i^{num} \right) \right|, \tag{46}$$

where N is the total number of particles.

In all simulations, a first-order time discretization was used and Courant number based on the minimum distance between particles is set as 0.2 which means that the time-step size $\Delta t = 0.2\frac{\Delta^2}{\alpha}$ is constant for a given resolution in the case of regular particle arrangements. Also, the quintic Wendland function

$$W(r,h) = W_0 \times \begin{cases} (1-\frac{r}{h})^4(4\frac{r}{h}+1) & 0 \le \frac{r}{h} < 1 \\ 0 & 1 \le \frac{r}{h} \end{cases} \tag{47}$$

was used as kernel where $W_0 = 7/(\pi h^2)$ for 2D problems. The boundary smoothness β of this function is 3.

6.1. Regular arrangement

First, a regular arrangement of particles was considered. Particles were placed on vertices of a square grid in the computational domain $[0,1]\times[0,1]$. Five resolutions were used with a total of 10×10, 20×20, 40×40, 80×80, and 160×160 particles to study the convergence of the methods. The simulations were conducted using Wendland kernel function with various smoothing radii h ranging from 3.5Δ to as low as 1.5Δ. The numerical results obtained using **scheme S3** (Eq. (13)) and **scheme S4** (Eq. (41)) are compared in Fig. 1. In this figure, the values of errors are shown in a log-log scale for **scheme S3** (left) and **scheme S4** (right) as functions of particle spacing Δ.

The error values in the left column of Fig. 1 show that the behavior of the **scheme S3** depends extremely on the ratio $\frac{h}{\Delta}$. For long smoothing radii ($h = 3.5\Delta$ and $h = 3.0\Delta$) the method behaves like a first-order method and the error decreases with particle spacing with a constant slope. But decreasing the smoothing length decreases this slope and for $h \le 2\Delta$ the diagram is virtually constant.

Although Table 1 shows the order of magnitude of the first term in truncation errors on a regular distribution of particles, it is not sufficient for the explanation of the behavior of the error in the left column of Fig. 1. So, it will be instructive to consider again the truncation error of **scheme S3** with more terms:

$$\begin{aligned} Er_i =& 2\ \nabla u|_i \cdot \sum_j \omega_j \nabla W_{ij} + \nabla\nabla u|_i : \left(\mathbf{B}_i^{-1} - \mathbf{I}\right) \\ &+ \frac{1}{3}\ \nabla\nabla\nabla u|_i \vdots \left(\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij}\right) \\ &- \frac{1}{12}\ \nabla\nabla\nabla\nabla u|_i :: \left(\sum_j \omega_j \mathbf{r}_{ij}\mathbf{r}_{ij}\mathbf{r}_{ij}\mathbf{r}_{ij}\nabla W_{ij}\right) + \cdots, \end{aligned} \tag{48}$$

where the operator "::" denotes "four dots product" which applies contraction four times and is defined similar to Eq. (16). On a regular arrangement, the first and third terms on the right-hand side of Eq. (48) are zero and from the estimations in section 4, by substituting β with 3 for the employed kernel function, one has

$$Er_i \approx \left|\nabla^2 u\right|_i \times O\left(\left(\frac{\Delta}{h}\right)^4\right) + \left|\nabla^4 u\right|_i \times \left[O\left(\Delta^2\left(\frac{h}{\Delta}\right)^2\right) + O\left(\Delta^2\left(\frac{\Delta}{h}\right)^2\right)\right]. \tag{49}$$

This equation can explain the reason for the particular performance of **scheme S3**. When smoothing radius is large enough, the first term is much smaller than the second term and the method is convergent. Decreasing the ratio $\frac{h}{\Delta}$ makes the two terms comparable which can be seen in Fig. 1 (left) for $h = 2.5\Delta$. In this case, when particle spacing is large enough, the second term on the right-hand side of Eq. (49) is dominant and the method performs linearly. Then, when Δ and hence h is reduced, the second term decreases more rapidly and the first term becomes significant. For smaller smoothing lengths, the first term is dominant at the whole range of Δ and horizontal lines are obtained.

Figure 1 (left) also shows that the best result of **scheme S3** is obtained with $h = 2.0\Delta$. Increasing the smoothing length leads to a greater stencil with more computations involving farther neighbors but not to a better accuracy. This fact is also observable in Eq. (49) where the dominant term (the coefficient of the fourth derivative) involves $\left(\frac{h}{\Delta}\right)^2$. On the other hand, shorter smoothing radii for this scheme leads to higher errors as there will be less than required neighboring particles to approximate the second derivative.

There is also another error which originates from the boundary conditions because of the lack of enough particles in the kernel support of the particles near the boundary. This error also increases with the smoothing length.

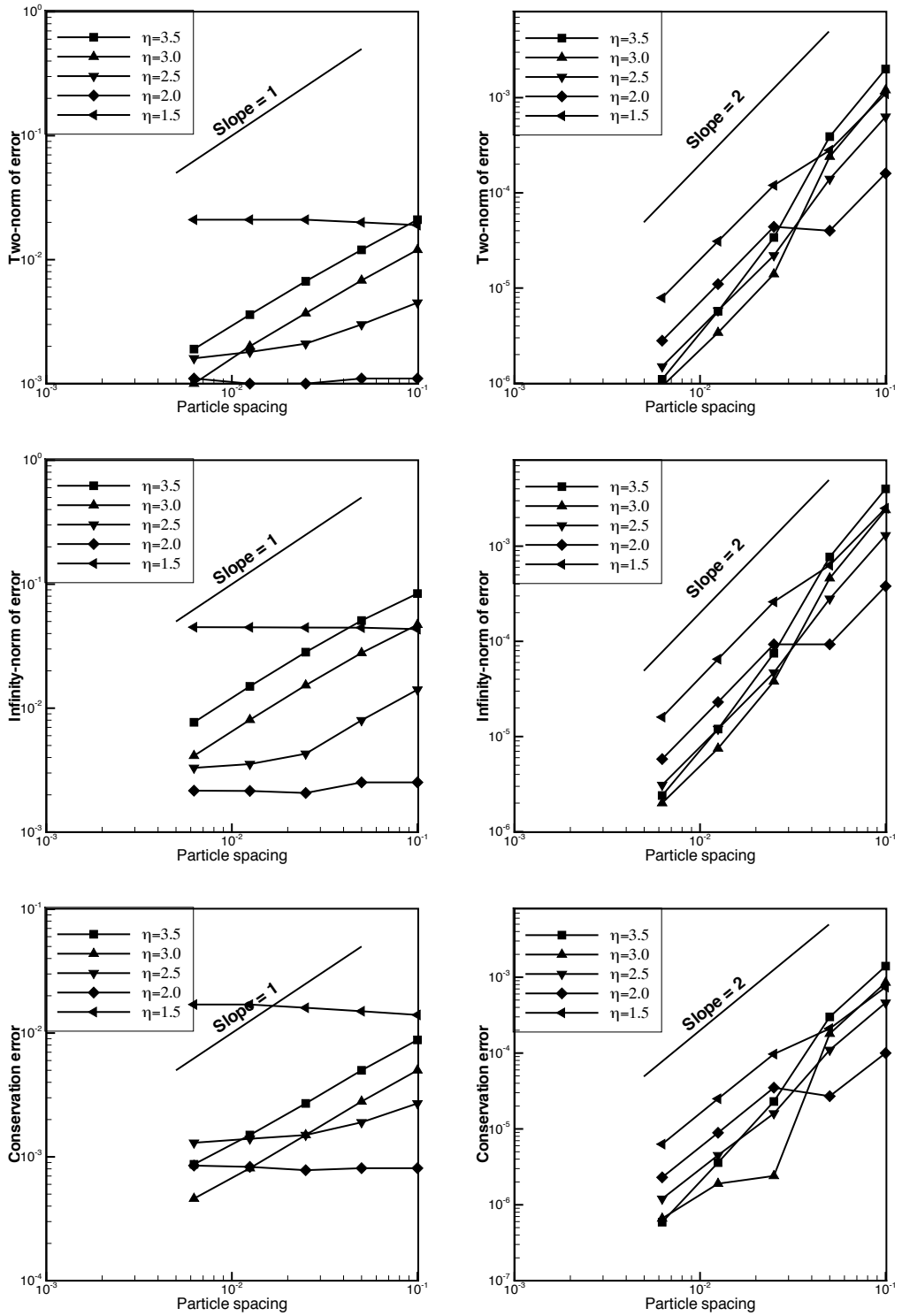

Figure 1: L_2-norm (top), L_∞-norm (middle), and conservation (bottom) errors of SPH results using **scheme S3** (left) and **scheme S4** (right) versus particle spacing Δ for various smoothing radii on regular arrangements ($\eta = \frac{h}{\Delta}$).

The behavior of the proposed **scheme S4** is totally different as seen in the right column of Fig. 1. The order of magnitude of errors are 2 to 3 orders lower than those of the previous method. In addition, the method performs near second order for all smoothing radii on a regular distribution of particles. This means that the scheme is an order of magnitude more accurate than **scheme S3**. The most impressive advantage of **scheme S4** which can be seen in Fig. 1 (Right) is that it converges well even for a short smoothing radius $h = 1.5\Delta$. More precisely, this means that computation is done with only 8 neighboring particles. This is important because reducing the number of neighboring particles means less computational cost and CPU time.

The reason is that **scheme S4** does not have the first term in Eq. (49). So, the truncation error on a regular distribution is second order:

$$Er_i \approx \left|\nabla^4 u\right|_i \times \left[O\left(\Delta^2\left(\frac{h}{\Delta}\right)^2\right) + O\left(\Delta^2\left(\frac{\Delta}{h}\right)^2\right)\right]. \tag{50}$$

Since both **schemes S3** and **S4** are not symmetric and thus are not conservative neither locally nor globally, one could not expect the error in energy conservation (EC) to be zero. However, Fig. 1 (bottom), this error follows the same pattern as the other error norms for both techniques. The values of the conservation error for the proposed **scheme S4** are low enough to be acceptable in solving conventional problems using SPH.

6.2. Irregular arrangement

In this section, the performance of the numerical methods is examined on irregular arrangements of particles. To establish this type of particle distribution, here, a random deviation is applied to the previously used regular arrangements in such a manner that each particle moves somewhat randomly. That is

$$x_i = x_i^{reg} + \epsilon\kappa_{i,x}\Delta,$$

and

$$y_i = y_i^{reg} + \epsilon\kappa_{i,y}\Delta,$$

where $\kappa_{i,x}$ and $\kappa_{i,y}$ are random values between -0.25 and 0.25 which are generated by the computer for each particle in the domain except for boundary particles. Also, ϵ is the randomness factor representing the deviation factor $\tilde{d}$ and is selected here as two values 0.2 and 0.4. It means that the particles can approach each other or retreat to a maximum distance of 0.28Δ. So, in the case of $h = 1.5\Delta$, the number of neighboring particles may become insufficient. Therefore, for $\epsilon = 0.4$, this case is omitted.

The calculated norms of errors using **scheme S3** and **scheme S4** for the heat diffusion problem on irregular arrangement of particles are shown in Fig. 2 for $\epsilon = 0.2$ and Fig. 3 for $\epsilon = 0.4$ as functions of particle spacing Δ for various smoothing lengths.

The left diagrams show the performance of **scheme S3**. A comparison with the values for the case of uniform spacing (Fig. 1) shows growth in the errors. This is because of inclusion of those terms in the truncation errors which vanished on a regular arrangement due to symmetry. For example, the term $\sum_j \omega_j \nabla W_{ij}$ in Eq. (48) is now non-zero. Except for the case $h = 1.5\Delta$ which has very high error values, all others have a convergence rate about unity. The most accurate case ($h = 2.5\Delta$) has errors higher than the worst case of **scheme S4**.

In contrast, the numerical errors of the proposed **scheme S4** (right diagrams) in Figs. 2 and 3 are several orders of magnitude lower than those of the previous scheme. Here, the errors still approximately obey the second-order convergence as predicted especially for the higher smoothing radius ratios $\eta = 3$ and $\eta = 3.5$. This behavior can be explained by using two leading terms in the truncation error given by Eqs.(42) and (50). For the quintic Wendland kernel function with boundary smoothness $\beta = 3$ one has

$$Er_i \approx \left|\nabla^3 u\right|_i \times O\left(\tilde{d}_i\left(\frac{\Delta}{h}\right)^4\right) + \left|\nabla^4 u\right|_i \times O\left(\Delta^2\left(\frac{h}{\Delta}\right)^2\right). \tag{51}$$

This means that by increasing the ratio $\frac{h}{\Delta}$, the first term in the error which involves the effect of the randomness of particle positions decreases rapidly (by a power of 4). So, the second term becomes dominant and the scheme behaves like a second-order method.

Compared with [13], the values selected here for randomness factor ϵ are relatively large. For such values, despite the fact that errors somewhat increases with ϵ, the change of behavior of errors due to ϵ in Figs. 2 and 3 is not significant.

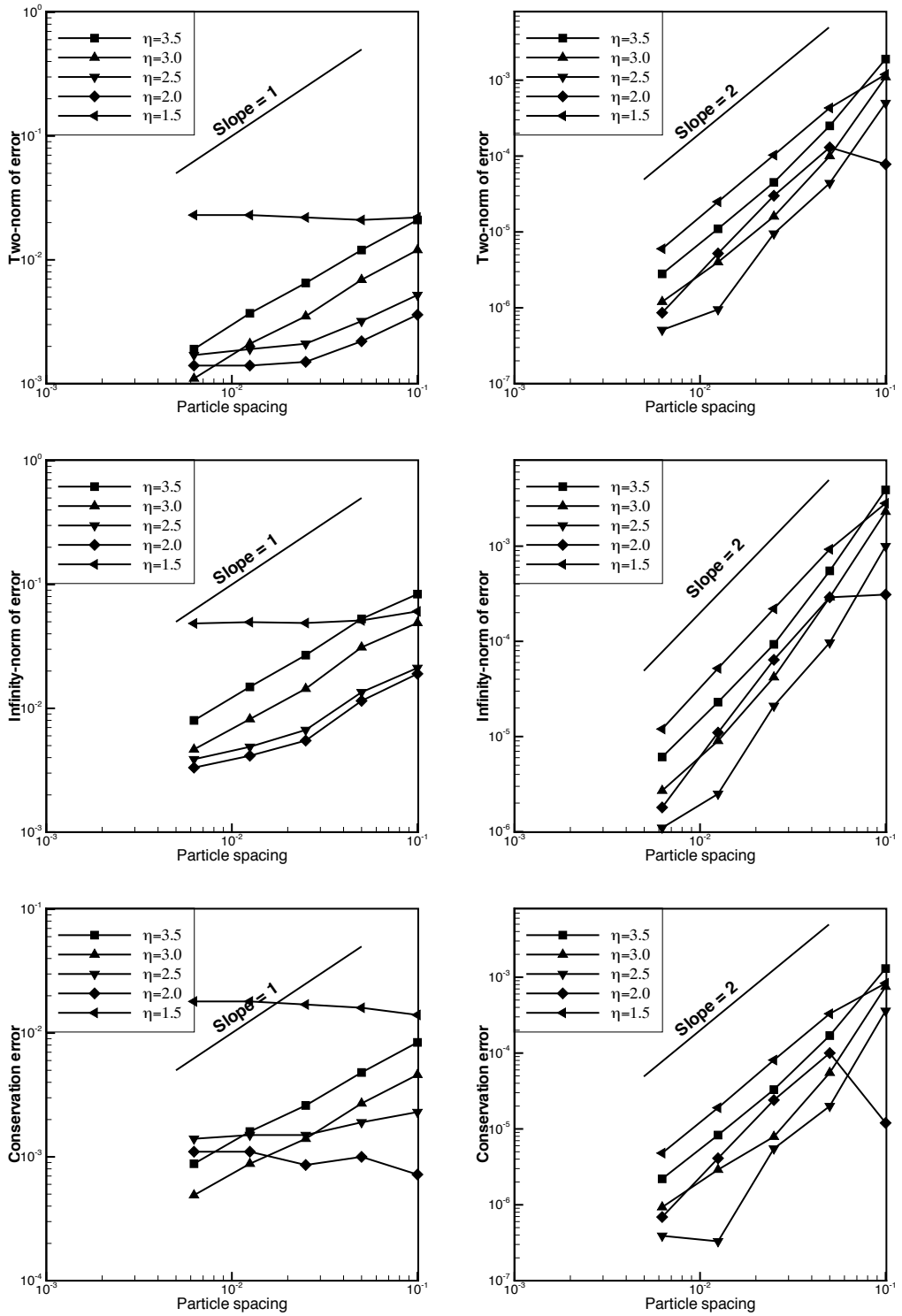

Figure 2: L_2-norm (top), L_∞-norm (middle), and conservation (bottom) errors of SPH results using **scheme S3** (left) and **scheme S4** (right) versus particle spacing Δ for various smoothing radius ratios $\eta = \frac{h}{\Delta}$ on irregular arrangements with randomness $\epsilon = 0.2$.

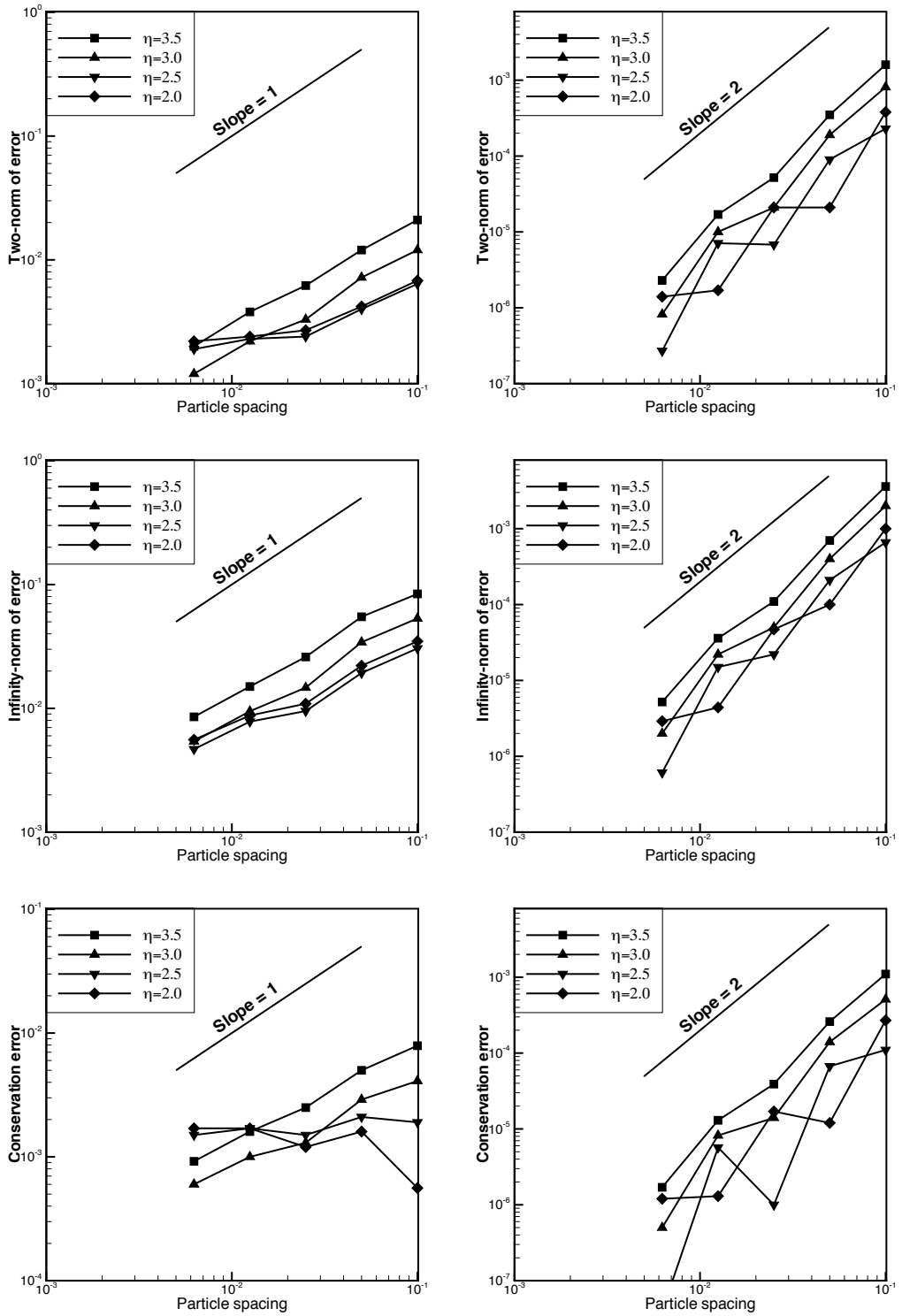

Figure 3: L_2-norm (top), L_∞-norm (middle), and conservation (bottom) errors of SPH results using **scheme S3** (left) and **scheme S4** (right) versus particle spacing Δ for various smoothing radius ratios $\eta = \frac{h}{\Delta}$ on irregular arrangements with randomness $\epsilon = 0.4$.

6.3. Computational cost

It is obvious that the proposed **scheme S4** has more computational cost than **scheme S3** on the same conditions due to three extra numerical stages. One extra calculation is approximation of the first derivative by **scheme F4**. Although this value may be already available in some cases. For example, in solving viscous flow equations, gradient of velocities may be calculated before approximating their Laplacian. The second extra computation is calculation of tensor $\hat{\mathbf{B}}$ which involves solving a linear set of equations with 3 unknowns in 2D and 6 unknowns in 3D. In heat conduction problems, since the SPH particles are fixed, this calculation is only performed once for each set of data. For fluid flow problems, however, the tensor must be updated at each time-step. Finally, the second derivative is approximated by **scheme S4** which has slightly more computations including multiplication of two second-order tensors. This is the third extra work in **scheme S4**.

Nevertheless, the proposed scheme is still very promising because of its accuracy. For instance, solving the heat conduction problem on 160×160 uniformly distributed particles with smoothing radii $h = 3.5\Delta$ takes 233 seconds using **scheme S3** while it takes 856 seconds to be solved using **scheme S4** on a 3 Ghz Intel Core 2 E8400 CPU. However, if one solves the same problem with $h = 1.5\Delta$ using **scheme S4**, the CPU time is reduced to 239 seconds. It is important to note that the error of this computation will be at least two orders of magnitude lower than that of **scheme S3** with $h = 3.5\Delta$.

7. Conclusions

In this paper, a theoretical framework was presented to assess the accuracy of different SPH schemes for discretization of the first and second derivatives in multi-dimensions. Using this framework, it was shown that some of the frequently used SPH schemes for approximation of the first derivative $\langle \nabla u \rangle_i$ involve values u_i and/or the derivative $\nabla u|_i$ in their truncation error which cause some difficulties in simulations. For example, the accuracy of a pressure gradient may be affected by the sign of pressure at each particle or even value of the reference pressure. Also, it was observed that all available SPH schemes for approximation of second derivative suffer from similar problems and in the best case are zero-order consistent.

In addition, using the theory of numerical integration, the order of magnitude of the coefficients in the truncation errors were estimated. This is done for both regular and irregular particle spacing. In this way, the order of each term and the effect of the smoothing radius ratio $\frac{h}{\Delta}$ were clarified, so that one can predict the convergence properties of every SPH scheme analytically.

Finally, a new SPH scheme was presented for the second derivative which is consistent enough to exactly predict the second derivative of a quadratic function. Examining the new technique for 2D unsteady heat equation on regular and irregular particle arrangements showed that it has at least one order of magnitude less errors in comparison with the best available scheme. In addition, on uniform particle distribution, second-order convergence was observed even for smoothing radii as small as 1.5Δ which means a considerable decrease in computational cost without growth in errors. In addition, for irregular distribution of particles it was shown that this scheme behaves near second-order accurate for smoothing radii larger than 2Δ. Although the proposed scheme is not symmetric and so does not conserve momentum or energy exactly, the conservation error was as low as those for other error norms and can be successfully used in practical studies.

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