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# On the consistency and convergence of particle-based meshfree discretization schemes for the Laplace operator

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ABSTRACT

The Laplace operator appears in the governing equations of continua describes dissipative dynamics, and it also emerges in some second order partial differential equations such as the Poisson equation. In this paper, accuracy and its convergence rates of some meshfree discretization schemes for the Laplace operator are studied as a verification. Moreover, a novel meshfree discretization scheme for the second order differential operator which enables us to use smaller dilation parameter of the compact support of the weight function is proposed, and its application for the meshfree discretization of the Poisson equation demonstrates an improvement of the solution accuracy.



## 1. Introduction

The Laplace operator, or the Laplacian, denoted by symbols $\nabla^2$ or $\Delta$, is a second order differential operator given by the divergence of the gradient of a function in $d$-dimensional Euclidian space. It appears in a lot of second order differential equations that describe physical phenomena, and they can be categorized into three types: parabolic, hyperbolic, and elliptic type. These are important mathematical representations of physics. Furthermore, in the field of fluid dynamics, the Laplace operator occurs in the viscosity (dissipative dynamics) and the pressure Poisson equation; therefore, numerical analyses of differential equations with the Laplace operator, and their discretization procedures, are of interest for computational fluid dynamics.

Various numerical methods have been developed for the solution of ordinary/partial differential equations. For instance, the Finite Element Method(FEM), the Finite Difference Method(FDM), and the Finite Volume Method(FVM), are widely utilized methodologies. Their common feature is that they divide a spatial domain into a set of discrete subdivisions so-called mesh, grid, or cell, which requires pre-defined and fixed connectivity of nodes. Alternatively, variety of meshfree methods, which establish a system of algebraic equations without the use of pre-defined mesh/grid/cell, have been vigorously sought in order to find better discretization procedures without mesh-constraints. Particle methods based on the Lagrangian description are one of the meshfree methods which make the most of meshfree talent, and their most important advantage is that they can easily handle simulations of very large deformations, even with the changes of the topological structure and fragmentation-coalescence of continua.

The Smoothed Particle Hydrodynamics(SPH) method [1,2] and the Moving Particle Semi-implicit(MPS) method [3,4] are extensively used strong-form meshfree and particle methods for numerical analysis of fluid flow with free surfaces. Although they have been shown to be useful in engineering applications, their standard formulae of spatial discretization schemes of the gradient, the divergence, and the Laplace operators lack polynomial completeness (reproducing conditions); therefore, inconsistencies of spatial discretization procedures have been resulted in adverse effects for both computational accuracy and stability. In order to overcome the inconsistency problem of meshfree discretizations, the (weighted) least squares method or equivalents have been utilized in various meshfree and/or particle methods (e.g. [5–14]), and Least Squares Moving Particle Semi-implicit (LSMPS) method [15] is one of the methods based on the least squares technique. Enhancement of accuracy and stability compared with the existing MPS method [3,4] were demonstrated through a applicative validation test problem [15]; however, convergence tests for the second order derivative approximations of the LSMPS method have not been well examined.

In this paper, the consistency of the second order derivative approximations for the strong-form particle methods including the

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LSMPS method are focused on, and the convergence of some meshfree particle discretization schemes for the Laplace operator are studied as a verification. Moreover, a novel meshfree discretization scheme for the second order differential operator which enables us to use smaller dilation parameter of the compact support of the weight function is proposed.

## 2. Meshfree discretization schemes for the Laplace operator

In this section, an overview of meshfree spatial discretization schemes for the Laplace operator (second order derivative approximations of the SPH method, the MPS method, and the LSMPS method) is presented. Furthermore, a novel scheme for the second order differential operator which enables us to utilize smaller dilation parameter of the compact support of the weight function is derived.

### 2.1. The Smoothed Particle Hydrodynamics method approximations

The Smoothed Particle Hydrodynamics (SPH) method was originally developed for the field of astrophysics by Lucy [1], and Gingold and Monaghan [2] in 1977, and it has been applied for numerical analyses of fluid flows and structures (Early contributions have been reviewed in several articles, for instance, [16–20]). In what follows, the SPH method is presented as one of the meshfree discretization methods.

The SPH interpolation is based on the following simple concept,

$$f(\mathbf{x}) = \int_{\mathbb{R}^d} \delta(\mathbf{x}' - \mathbf{x}) f(\mathbf{x}') d\mathbf{x}', \quad \forall \mathbf{x} \in \mathbb{R}^d, \tag{1}$$

where $\delta(\mathbf{x})$ is the Dirac delta distribution, and the key ingredient of the SPH method is to replace the Dirac delta distribution with well-behaved *smoothing* kernel function $w(\mathbf{x}; h)$ ($h$ is a smoothing length) that mimics the useful properties of the Dirac delta distribution. Whereafter, a SPH smoothing interpolation is discretized for a set of scattered nodes $\{\mathbf{x}_j\}_{1 \le j \le N}$, i.e.,

$$\langle f(\mathbf{x}) \rangle = \int_{\mathbb{R}^d} w(\mathbf{x}' - \mathbf{x}; h) f(\mathbf{x}') d\mathbf{x}', \tag{2}$$

$$\approx \sum_j w(\mathbf{x}_j - \mathbf{x}; h) f_j \Delta V_j, \tag{3}$$

where $\Delta V_j$ denotes nodal measures of point $\mathbf{x}_j$, and $f_j = f(\mathbf{x}_j)$. Note that a part $w(\mathbf{x}_j - \mathbf{x}; h)\Delta V_j$ in Eq. (3) can be seen as a shape function in the finite element discretization procedure. The derivatives of a function are obtained by differentiating the discrete interpolated function, for instance, the gradient of a function $f$ is approximated by

$$\langle \nabla f(\mathbf{x}) \rangle \approx \sum_j \left[ \nabla w(\mathbf{x}_j - \mathbf{x}; h) \right] f_j \Delta V_j. \tag{4}$$

Following the same procedure yields a SPH approximation for the Laplacian of a function $f$:

$$\left\langle \nabla^2 f(\mathbf{x}) \right\rangle \approx \sum_j \left[ \nabla^2 w(\mathbf{x}_j - \mathbf{x}; h) \right] f_j \Delta V_j. \tag{5}$$

This formulation, however, is not used today since its accuracy and solution stability depend strongly on the nodal distribution [16,21,22] and it lacks polynomial completeness conditions. Alternatively, some approximating discretization schemes for the Laplace operator have been utilized in the SPH method.

#### 2.1.1. Brookshaw type SPH formula

Brookshaw [23] proposed the following SPH formulation for the approximation of the Laplacian of a function:

$$\left\langle \nabla^2 f(\mathbf{x}) \right\rangle_i \approx \sum_{j \in \Lambda_i} \frac{\nabla_i w(\mathbf{x}_j - \mathbf{x}_i; h) \cdot (\mathbf{x}_j - \mathbf{x}_i)}{\|\mathbf{x}_j - \mathbf{x}_i\|^2} \left( f_j - f_i \right) \Delta V_j, \tag{6}$$

$$= \sum_{j \in \Lambda_i} \left[ \frac{1}{r_{ij}} \frac{\partial w(\mathbf{x}_j - \mathbf{x}_i; h)}{\partial r_{ij}} \Delta V_j \right] (f_j - f_i), \tag{7}$$

where $\nabla_i = \nabla|_{\mathbf{x}=\mathbf{x}_i}$, $r_{ij} = \|\mathbf{x}_j - \mathbf{x}_i\|$, and $\Lambda_i$ stands for sets of neighboring nodes $\mathbf{x}_j$ that locate in the compact support of the kernel function of the node $\mathbf{x}_i$. It should be mentioned that this discretization scheme forms a finite difference like formula:

$$\left\langle \nabla^2 f(\mathbf{x}) \right\rangle_i \approx \sum_{j \in \Lambda_i} C_{ij} (f_j - f_i), \tag{8}$$

and various discretization schemes based on finite difference like formulae have been proposed for the SPH method (e.g.[24,25]). Morris[26] applied this brookshaw type SPH formula of the approximating Laplace operator for discretization of the viscosity term in the Navier–Stokes equations, and this scheme [23,26] is one of the most widely used formulae in the SPH method for discretization of the Laplacian; therefore, the accuracy of Brookshaw type SPH Laplace operator (Eq. (6)) will be investigated numerically, later in this study.

#### 2.1.2. Monaghan and Gingold type SPH formula

Monaghan and Gingold [27] proposed the following formula for discretization of the viscosity term of fluid flows:

$$\left\langle \mu \nabla^2 \mathbf{u} \right\rangle_i \approx 2(d+2)\mu \sum_{j \in \Lambda_i} \nabla_i w(\mathbf{x}_j - \mathbf{x}_i; h) \frac{(\mathbf{x}_j - \mathbf{x}_i) \cdot (\mathbf{u}_j - \mathbf{u}_i)}{\|\mathbf{x}_j - \mathbf{x}_i\|^2} \Delta V_j, \tag{9}$$

$$= 2(d+2)\mu \sum_{j \in \Lambda_i} \left[ \frac{\nabla_i w(\mathbf{x}_j - \mathbf{x}_i; h)(\mathbf{x}_j - \mathbf{x}_i)^T}{\|\mathbf{x}_j - \mathbf{x}_i\|^2} \right] (\mathbf{u}_j - \mathbf{u}_i) \Delta V_j, \tag{10}$$

$$= 2(d+2)\mu \sum_{j \in \Lambda_i} \left[ \frac{1}{r_{ij}^3} \frac{\partial w(\mathbf{x}_j - \mathbf{x}_i; h)}{\partial r_{ij}} \Delta V_j (\mathbf{x}_j - \mathbf{x}_i)(\mathbf{x}_j - \mathbf{x}_i)^T \right] (\mathbf{u}_j - \mathbf{u}_i), \tag{11}$$

where $\mu$ denotes the dynamic viscosity, and $\mathbf{u}$ stands for the velocity vector. This formulation for discretization of the viscosity term is also a widely utilized scheme in the SPH method, however, this model do not satisfy the Stokes hypothesis as pointed out by Colagrossi et al. [28]. The consequence of this fact have not been studied deeply and its study of accuracy and inconsistency in the Stokes hypothesis will be postponed for future studies.

### 2.2. The Moving Particle Semi-implicit method approximations

The Moving Particle Semi-implicit method [3,4] was developed by Koshizuka and Oka for numerical analyses of incompressible flows with free surfaces. Since the MPS method requires to discretize the pressure Poisson equation and the viscosity term, variety of spatial discretization schemes for the Laplace operator have been proposed.

#### 2.2.1. Koshizuka and Oka type formula

Koshizuka and Oka [3] proposed the following "particle interaction model" to discretize the Laplace operator:

$$\left\langle \nabla^2 f(\mathbf{x}) \right\rangle_i \approx \frac{2d}{\lambda n} \sum_{j \in \Lambda_i} w(\mathbf{x}_j - \mathbf{x}_i; h)(f_j - f_i), \tag{12}$$

where $n$ and $\lambda$ are the normalization coefficients of weighting defined by

$$n = \int_{\mathbb{R}^d} w(\mathbf{x}' - \mathbf{x}; h) d\mathbf{x}', \tag{13}$$

$$\approx \sum_{j \in \Lambda^0} w(\mathbf{x}_j - \mathbf{x}_i; h) \cdot 1, \tag{14}$$

$$\lambda = \left[ \int_{\mathbb{R}^d} w(\mathbf{x}' - \mathbf{x}, h) \mathbf{x}'^2 d\mathbf{x}' \right] \Big/ \left[ \int_{\mathbb{R}^d} w(\mathbf{x}' - \mathbf{x}, h) d\mathbf{x}' \right], \tag{15}$$

$$\approx \left[ \sum_{j \in \Lambda^0} w(\mathbf{x}_j - \mathbf{x}_i; h)(\mathbf{x}_j - \mathbf{x}_i)^2 \cdot 1 \right] \Big/ \left[ \sum_{j \in \Lambda^0} w(\mathbf{x}_j - \mathbf{x}_i; h) \cdot 1 \right], \tag{16}$$

respectively. For the above point collocation integrations, in practical code implementations unity nodal measures (volumes) are employed, and the summations over indices $j \in \Lambda^0$ are taken for nodes distributed on the uniform square lattice in two dimensions and the cubic lattice in three dimensions, respectively.

*2.2.2. Khayyer and Gotoh type formula*

Khayyer and Gotoh [29] proposed "a higher order Laplacian model" for enhancement and stabilization of pressure calculation of the MPS method, and it is derived by taking the divergence of a meshfree gradient approximation:

$$\left\langle \nabla^2 f(\mathbf{x}) \right\rangle_i \approx \nabla \cdot \langle \nabla f(\mathbf{x}) \rangle \tag{17}$$

$$\approx \frac{1}{n} \sum_{j \in \Lambda_i} \left[ (f_j - f_i) \frac{\partial^2 w(\mathbf{x}_j - \mathbf{x}_i; h)}{\partial r_{ij}^2} - \frac{f_j - f_i}{r_{ij}} \frac{\partial w(\mathbf{x}_j - \mathbf{x}_i; h)}{r_{ij}} \right] \tag{18}$$

$$= \sum_{j \in \Lambda_i} \left[ \frac{1}{n} \left\{ \frac{\partial^2 w(\mathbf{x}_j - \mathbf{x}_i; h)}{\partial r_{ij}^2} - \frac{1}{r_{ij}} \frac{\partial w(\mathbf{x}_j - \mathbf{x}_i; h)}{r_{ij}} \right\} \right] (f_j - f_i). \tag{19}$$

It must be noted here that, according to Khayyer and Gotoh [29,30], this scheme for the Laplace operator is a specific formula for two dimensional space, and the other peculiar formulation for three dimensional space is also proposed by Khayyer and Gotoh [30]. Moreover, this scheme does not satisfy the partition of unity condition, namely,

$$\sum_{j \in \Lambda_i} \frac{1}{n} \left\{ \frac{\partial^2 w(\mathbf{x}_j - \mathbf{x}_i; h)}{\partial r_{ij}^2} - \frac{1}{r_{ij}} \frac{\partial w(\mathbf{x}_j - \mathbf{x}_i; h)}{r_{ij}} \right\} \neq 1. \tag{20}$$

Although the name of scheme is "a higher order Laplacian model", the partition of unity, that is the 0th order consistency, is destroyed in general. The accuracy of the two dimensional scheme will be examined numerically, later in this study.

*2.2.3. Least Squares MPS type fomulae*

Least Squares Moving Particle Semi-implicit (LSMPS) method [15] was developed by Tamai and Koshizuka for numerical analyses of incompressible flows with free surfaces. As it name suggests, the weighted least squares method is utilized for the spatial discretization schemes including an implementation of Neumann boundary condition constraints, and the Laplace operator is discretized by the following scheme:

$$\left\langle \nabla^2 f(\mathbf{x}) \right\rangle_i \approx \left\{ \frac{1}{2} \nabla^2 \mathbf{p}(\mathbf{x}) \Big|_{\mathbf{x}=\mathbf{0}} \right\}^T \left[ H_{r_s} [\mathbf{M}_i + \chi \mathbf{N}_i]^{-1} \{ \mathbf{b}_i + \chi \mathbf{c}_i \} \right], \tag{21}$$

where

$$H_{r_s} = \mathrm{diag}\left\{ \left\{ r_s^{-|\boldsymbol{\alpha}|} \boldsymbol{\alpha}! \right\}_{1 \le |\boldsymbol{\alpha}| \le p} \right\}, \tag{22}$$

$$\mathbf{M}_i = \sum_{j \in \Lambda_i} w(\mathbf{x}_j - \mathbf{x}_i; h) \mathbf{p}\left( \frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) \mathbf{p}^T \left( \frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right), \tag{23}$$

$$\mathbf{N}_i = w_N(\mathbf{x}_i; h) \mathbf{p}_N(\mathbf{x}_i) \mathbf{p}_N^T(\mathbf{x}_i), \tag{24}$$

$$\mathbf{b}_i = \sum_{j \in \Lambda_i} w(\mathbf{x}_j - \mathbf{x}_i; h) \mathbf{p}\left( \frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) (f_j - f_i), \tag{25}$$

$$\mathbf{c}_i = w_N(\mathbf{x}_i; h) \mathbf{p}_N(\mathbf{x}_i) r_s g_N(\mathbf{x}_i), \tag{26}$$

$$\mathbf{p}(\mathbf{x}) = \{ \mathbf{x}^{\boldsymbol{\alpha}} \mid 1 \le |\boldsymbol{\alpha}| \le p \}, \tag{27}$$

$$\mathbf{p}_N(\mathbf{x}) = \left( \mathbf{n}(\mathbf{x}), \underbrace{0, \cdots, 0}_{\sigma \text{ times}} \right), \tag{28}$$

$$\sigma = \binom{p+d}{d} - (d+1), \tag{29}$$

$$\chi = \begin{cases} 1, & \mathbf{x}_i \in (\text{Neumann boundary}), \\ 0, & \mathbf{x}_i \in (\text{Interior of domain}), \end{cases} \tag{30}$$

$$r_s : \text{the scaling parameter} \quad (0 < r_s \le h), \tag{31}$$

$$p : \text{the order of the basis function } \mathbf{p}(\mathbf{x}), \tag{32}$$

and $\boldsymbol{\alpha} \in \mathbb{N}_0^d$ is the multi-index.

In order to discretize the second order or higher order derivative of a function, higher order basis functions have to be employed. For instance, to obtain the discrete Laplace operator, the order of the basis function $\mathbf{p}(\mathbf{x})$ must be greater than 2. Additionally, employing higher order basis function results in achievement of higher order polynomial completeness and the consistency conditions for discretization of the Laplace operator. In particular, adopting $p$th order basis function for discretization of the Laplace operator results in satisfaction of $(p-1)$th order consistency conditions.

*2.2.4. An alternative 1st order consistent discretization scheme for the Laplace operator*

The LSMPS schemes introduced in the previous Section 2.2.3 can complete higher order consistency conditions of spatial discretization, if the moment matrices $\mathbf{M}_i + \chi \mathbf{N}_i$ are well-conditioned. The smallest order formula for discretization of the Laplace operator is the 1st order consistent scheme, that is, the 2nd order basis function is applied. In concrete terms, for two and three dimensional analyses, the bases are:

$$\mathbf{p}(\mathbf{x}) = \begin{cases} (x, y, x^2, xy, y^2)^T, & d = 2, \\ (x, y, z, x^2, xy, xz, y^2, yz, z^2)^T, & d = 3, \end{cases} \tag{33}$$

and the numbers of vector components are 5 in two dimensional space, and 9 in three dimensional space, respectively. Consequently, in order to satisfy the invertibility of the moment matrix, the number of linearly independent bases $\mathbf{p}((\mathbf{x}_j - \mathbf{x}_i)/r_s)$ must be larger than the number of vector components of basis function $\mathbf{p}(\mathbf{x})$. In other words, in order to make the number of "neighboring particle $j$" to be adequately large, a sufficiently large dilation parameter that determines the compact support of the weight function has to be used; however, this requirement would be stringent for nodes located on or near the domain boundaries. For this reason, a new meshfree discretization scheme for the second order spatial differential operator which enables us to use smaller dilation parameter of the compact support of the weight function is proposed.

Utilizing the Taylor expansion of a sufficiently smooth function $f(\mathbf{x})$ around $\mathbf{x}_i$ yields

$$f(\mathbf{x}_j) = f(\mathbf{x}_i) + \{(\mathbf{x}_j - \mathbf{x}_i)^T\nabla\} f(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_i} + \frac{1}{2}\left\{(\mathbf{x}_j - \mathbf{x}_i)^T\nabla\right\}^2 f(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_i} + \cdots, \tag{34}$$

and abridged notations

$$f_{ij} = f_j - f_i \tag{35}$$

$$= (\mathbf{x}_{ij}^T\nabla) f\Big|_i + \frac{1}{2}(\mathbf{x}_{ij}^T\nabla)^2 f\Big|_i + \frac{1}{6}(\mathbf{x}_{ij}^T\nabla)^3 f\Big|_i + \cdots \tag{36}$$

are used from here on.

Multiplying $w(\mathbf{x}_j - \mathbf{x}_i; h)(\mathbf{x}_j - \mathbf{x}_i) := w_{ij}\mathbf{x}_{ij}$ for the both sides of the Eq. (36) provides

$$w_{ij}\mathbf{x}_{ij} f_{ij} = w_{ij}\mathbf{x}_{ij}\left((\mathbf{x}_{ij}^T\nabla) f\Big|_i\right) + \frac{1}{2} w_{ij}\mathbf{x}_{ij}\left((\mathbf{x}_{ij}^T\nabla)^2 f\Big|_i\right) + \frac{1}{6} w_{ij}\mathbf{x}_{ij}\left((\mathbf{x}_{ij}^T\nabla)^3 f\Big|_i\right) + \cdots, \tag{37}$$

and taking summation over index $j \in \Lambda_i$ with some algebra, one can get

$$\left[\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij}\mathbf{x}_{ij}^T\right]\nabla f\Big|_i = \left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij} f_{ij}\right\} - \frac{1}{2}\left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij}(\mathbf{x}_{ij}^T\nabla)^2 f\Big|_i\right\} - \frac{1}{6}\left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij}(\mathbf{x}_{ij}^T\nabla)^3 f\Big|_i\right\} + \cdots. \tag{38}$$

If a moment matrix

$$\mathbf{M}_{1,i} = \sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij}\mathbf{x}_{ij}^T \tag{39}$$

is not singular, one can obtain the following 1st order consistent gradient approximation:

$$\langle\nabla f\rangle_{1,i} = \mathbf{M}_{1,i}^{-1}\left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij} f_{ij}\right\} \underbrace{- \frac{1}{2}\mathbf{M}_{1,i}^{-1}\left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij}(\mathbf{x}_{ij}^T\nabla)^2 f\Big|_i\right\}}_{\text{Leading truncation error}:\mathcal{O}(h)} \underbrace{- \frac{1}{6}\mathbf{M}_{1,i}^{-1}\left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij}(\mathbf{x}_{ij}^T\nabla)^3 f\Big|_i\right\} + \cdots}_{\text{Truncation error}:\mathcal{O}(h^2)}. \tag{40}$$

This formula of gradient approximation with a specific choice of weight function $w_{ij}$ is widely utilized, for instance, Randles and Libersky [11] (the weight $w_{ij}$ in the Eq. (40) is replaced by $\Delta V_j \partial w_{ij}/\partial r_{ij}$), Suzuki [31] (replaced by $w_{ij}/r_{ij}^2$), and Tamai and Koshizuka [15](the weight is $w_{ij}$, not replaced).

Substituting the Eq. (40) into the Eq. (36) yields

$$f_{ij} = \mathbf{x}_{ij}^T\left[\mathbf{M}_{1,i}\left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij} f_{ij}\right\} - \frac{1}{2}\mathbf{M}_{1,i}^{-1}\left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij}(\mathbf{x}_{ij}^T\nabla)^2 f\Big|_i\right\} - \frac{1}{6}\mathbf{M}_{1,i}^{-1}\left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{x}_{ij}(\mathbf{x}_{ij}^T\nabla)^3 f\Big|_i\right\} + \cdots\right] + \frac{1}{2}(\mathbf{x}_{ij}^T\nabla)^2 f\Big|_i + \frac{1}{6}(\mathbf{x}_{ij}^T\nabla)^3 f\Big|_i + \cdots, \tag{41}$$

then the above equation can be transformed into

$$(\mathbf{x}_{ij}^T\nabla)^2 f\Big|_i - \mathbf{x}_{ij}^T\mathbf{M}_{1,i}^{-1}\left\{\sum_{k\in\Lambda_i} w_{ik}\mathbf{x}_{ik}(\mathbf{x}_{ik}^T\nabla)^2 f\Big|_i\right\} = 2f_{ij} - 2\mathbf{x}_{ij}^T\langle\nabla f\rangle_{1,i} - \frac{1}{3}(\mathbf{x}_{ij}^T\nabla)^3 f\Big|_i + \frac{1}{3}\mathbf{x}_{ij}^T\mathbf{M}_{1,i}^{-1}\left\{\sum_{k\in\Lambda_i} w_{ik}\mathbf{x}_{ik}(\mathbf{x}_{ik}^T\nabla)^3 f\Big|_i\right\} + \cdots \tag{42}$$

$$:= 2f_{ij} - 2\mathbf{x}_{ij}^T\langle\nabla f\rangle_{1,i} + \varepsilon_{ij}, \tag{43}$$

where the dummy indices $j \in \Lambda_i$ for the summations are changed to $k \in \Lambda_i$. The left hand side of the Eq. (42) includes unknowns of the 2nd order derivatives of a function $f$, and can be rewritten as follows:

$$(\mathbf{x}_{ij}^T\nabla)^2 f\Big|_i - \mathbf{x}_{ij}^T\mathbf{M}_{1,i}^{-1}\left\{\sum_{k\in\Lambda_i} w_{ik}\mathbf{x}_{ik}(\mathbf{x}_{ik}^T\nabla)^2 f\Big|_i\right\} = \sum_{|\boldsymbol{\alpha}|=2}\left[\frac{|\boldsymbol{\alpha}|!}{\boldsymbol{\alpha}!}\left[\mathbf{x}_{ij}^{\boldsymbol{\alpha}} - \mathbf{x}_{ij}^T\mathbf{M}_{1,i}^{-1}\left[\sum_{k\in\Lambda_i} w_{ik}\mathbf{x}_{ik}^{\boldsymbol{\alpha}}\mathbf{x}_{ik}\right]\right] D_{\mathbf{x}}^{\boldsymbol{\alpha}} f\Big|_i\right] \tag{44}$$

$$:= \mathbf{q}_{ij}^T\mathbf{D}_2 f\Big|_i, \tag{45}$$

where

$$\mathbf{q}_{ij} := \left\{\frac{|\boldsymbol{\alpha}|!}{\boldsymbol{\alpha}!}\left[\mathbf{x}_{ij}^{\boldsymbol{\alpha}} - \mathbf{x}_{ij}^T\mathbf{M}_{1,i}^{-1}\left[\sum_{k\in\Lambda_i} w_{ik}\mathbf{x}_{ik}^{\boldsymbol{\alpha}}\mathbf{x}_{ik}\right]\right] \;\Big|\; |\boldsymbol{\alpha}| = 2\right\}, \tag{46}$$

$$\mathbf{D}_2 f\Big|_i := \{D_{\mathbf{x}}^{\boldsymbol{\alpha}} f(\mathbf{x})|_{\mathbf{x}_i} \;|\; |\boldsymbol{\alpha}| = 2\}. \tag{47}$$

Multiplying $w_{ij}\mathbf{q}_{ij}$ for the both hand sides of the Eq. (43) provides

$$w_{ij}(\mathbf{q}_{ij}\mathbf{q}_{ij}^T)\mathbf{D}_2 f\Big|_i = w_{ij}\mathbf{q}_{ij}(2f_{ij} - 2\mathbf{x}_{ij}^T\langle\nabla f\rangle_{1,i}) + w_{ij}\mathbf{q}_{ij}\varepsilon_{ij}, \tag{48}$$

and taking summation over index $j \in \Lambda_i$ yields

$$\left[\sum_{j\in\Lambda_i} w_{ij}\mathbf{q}_{ij}\mathbf{q}_{ij}^T\right]\mathbf{D}_2 f\Big|_i = \left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{q}_{ij}(2f_{ij} - 2\mathbf{x}_{ij}^T\langle\nabla f\rangle_{1,i})\right\} + \left\{\sum_{j\in\Lambda_i} w_{ij}\mathbf{q}_{ij}\varepsilon_{ij}\right\}. \tag{49}$$

If a matrix

$$\mathbf{M}_{2,i} := \sum_{j\in\Lambda_i} w_{ij}\mathbf{q}_{ij}\mathbf{q}_{ij}^T \tag{50}$$

is not singular, one can obtain the following formula of a discretization scheme for the 2nd order spatial derivatives:

$$\langle \mathbf{D}_2 f(\mathbf{x}) \rangle_i = \mathbf{M}_{2,i}^{-1} \left\{ \sum_{j \in \Lambda_i} w_{ij} \mathbf{q}_{ij} (2 f_{ij} - 2 \mathbf{x}_{ij}^T \langle \nabla f \rangle_{1,i}) \right\} + \underbrace{\mathbf{M}_{2,i}^{-1} \left\{ \sum_{j \in \Lambda_i} w_{ij} \mathbf{q}_{ij} \varepsilon_{ij} \right\}}_{\text{Truncation errors}}. \quad (51)$$

The above derivation procedure is analogous to an existing study for the SPH method [32]; however, since the definitions of the moment matrix $\mathbf{M}_{2,\, i}$ and the renormalization tensor $\widehat{\mathbf{B}}_i$ in [32] are different, the system equations to be solved are different.

It should be pointed out that the proposed formulation can be derived by utilizing the weighted least squares method, i.e., the minimization procedure of a discrete functional

$$J = \sum_{j \in \Lambda_i} w_{ij} \varepsilon_{ij}^2, \quad (52)$$

is equivalent. Furthermore, the numbers of vector components of the bases $\mathbf{q}_{ij}$ are 3 for two dimensions and 6 for three dimensions; therefore, a necessary condition to satisfy the invertibility of the moment matrix which impose a limitation of the regularity of nodal distribution is relaxed. In other words, smaller dilation parameter can be employed for the new approach. Finally, without going into detail of a rigorous mathematical proof, the proposed scheme is 1st order consistent; therefore, there exists a positive constant independent from the dilation parameter $h$ s.t.

$$|D_x^{\boldsymbol{\alpha}} f(\mathbf{x}) - \langle D_x^{\boldsymbol{\alpha}} f(\mathbf{x}) \rangle_i| \le C h^1 |f(\mathbf{x})|_{C^3(\Omega)}, \quad |\boldsymbol{\alpha}| = 2. \quad (53)$$

## 3. Numerical experiments of the accuracy and its convergence rate

### 3.1. Problem settings and results

In order to compare accuracy and the convergence rates of discretization schemes for the Laplace operator, the Laplacian of the following non-linear function:

$$\begin{aligned} f(x, y) = {} & \frac{3}{4} \exp\left\{ -\frac{(9x-2)^2}{4} - \frac{(9y-2)^2}{4} \right\} \\ & + \frac{3}{4} \exp\left\{ \frac{(9x+1)^2}{49} - \frac{(9y+1)^2}{10} \right\} \\ & + \frac{1}{2} \exp\left\{ \frac{(9x-7)^2}{4} - \frac{(9y-3)^2}{4} \right\} \\ & - \frac{1}{5} \exp\left\{ -(9x-4)^2 - (9y-7)^2 \right\}, \end{aligned} \quad (54)$$

defined on a domain

$$\Omega = \left\{ (x, y) \in \mathbb{R}^2 \mid [0, 1] \times [0, 1] \right\}, \quad (55)$$

is calculated. Arrangements of a set of nodes $\{\mathbf{x}_i\}_{1 \le i \le N}$ is given quasi-randamly by the following generation process: (i) distribute nodal points $\left\{\mathbf{x}_i'\right\}_{1 \le i \le N}$ on the two dimensional uniform square lattice with width $\Delta x = \Delta y (:= L_0)$, (ii) give relative perturbation $\{\delta \mathbf{x}_i\}_{1 \le i \le N}$ by two dimensional normal distribution with parameters $\mu = 0$, $\sigma = 0.1$, where $\mu$, $\sigma$ denote the expectation of the distribution and the standard deviation, respectively. Consequently, positions of irregularly distributed points are obtained from

$$\{\mathbf{x}_i\}_{1 \le i \le N} = \left\{ \mathbf{x}_i' + \delta \mathbf{x}_i \right\}_{1 \le i \le N}. \quad (56)$$

As a measure of accuracy, discrete relative supreme error norm

$$e_\infty = \frac{\max_{\mathbf{x}_i \in \Omega} \left| \nabla^2 f(\mathbf{x}_i) - \left\langle \nabla^2 f(\mathbf{x}) \right\rangle_i \right|}{\max_{\mathbf{x} \in \Omega} |\nabla^2 f(\mathbf{x})|} \quad (57)$$

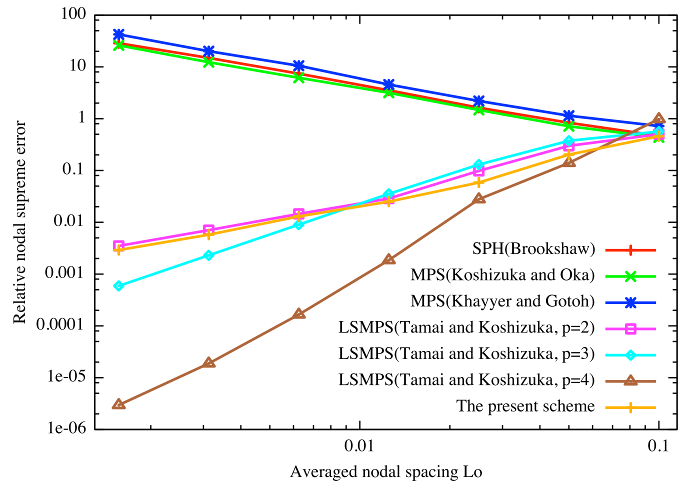


**Fig. 1.** Relative nodal supreme errors of meshfree spatial discretization schemes for the Laplace operator ($p$ is the order of the basis function for the weight least squares approximation).

is utilized. One of the Wendland kernels [33] defined by

$$w(r; h) = \begin{cases} \left(1 - \dfrac{r}{h}\right)^4 \left(1 + 4\dfrac{r}{h}\right), & 0 < \dfrac{r}{h} \le 1, \\ 0, & 1 < \dfrac{r}{h}, \end{cases} \quad (58)$$

is applied as the weight function, and its dilation parameters $h$ applied for each schemes are listed in the Table. 1. The results are shown in the Fig. 1.

### 3.2. Discussions

Fig. 1 shows that some spatial discretization schemes for the Laplace operator are not convergent but divergent. The relative nodal supreme errors of the Brookshaw type SPH (Eq. (6)), the Koshizuka-Oka type MPS (Eq. 12), and the Khayyer-Gotoh type MPS (Eq. 17) growth when smaller averaged nodal spacing $L_0 = \Delta x = \Delta y$ is applied, and the rates of convergence are about *minus-one*. This result of a numerical experiment suggests that these formulations are inconsistent and should be corrected to achieve a certain order of consistency condition. On the other hand, the weighted least squares method based schemes are appropriately convergent. If a sufficiently fine nodal resolution is given, higher order formulae distinguish themselves and provide more accurate approximations; however, with focusing attention on the cases with a coarse resolution of the spatial subdivisions, a new scheme presented in this study has an advantage: the accuracy of the proposed scheme is superior the existing LSMPS scheme with 2nd or 3rd order bases. Moreover, since a new discretization for the Laplace operator enables us to apply smaller dilation parameters, the bandwidth of the discretized Laplace operator, which is a sparse matrix, must be narrower; therefore, computational efficiency of solving the system equation would be also enhanced.

## 4. Application of the new scheme for the Poisson equation

### 4.1. Problem settings and results

A Poisson problem with a given solution $f(x, y)$ defined by the Eq. (54):

$$-\nabla^2 f(x, y) = (\mathrm{R.H.S}), \quad (59)$$

is solved with Dirichlet boundary condition. For comparison, the LSMPS scheme with 2nd order basis (Eq. (21), $p = 2$) and the

**Table 1**
Dilation parameters $h$ adopted for each discretization schemes for the Laplace operator ($L_0 = \Delta x = \Delta y$ denotes the averaged nodal spacing).

| Type of scheme | Dilation paramter h |
|---|---|
| SPH (Brookshaw [23], Eq. (6)) | $2.7L_0$ |
| MPS (Koshizuka and Oka [3], Eq. (12)) | $2.7L_0$ |
| MPS (Khayyer and Gotoh [29], Eq. (17)) | $2.7L_0$ |
| LSMPS (Tamai and Koshizuka[15], with 2nd order basis, Eq. (21)) | $3.5L_0$ |
| LSMPS (Tamai and Koshizuka [15], with 3rd order basis, Eq. (21)) | $4.1L_0$ |
| LSMPS (Tamai and Koshizuka [15], with 4th order basis, Eq. (21)) | $4.5L_0$ |
| The present scheme, Eq. (51) | $2.7L_0$ |

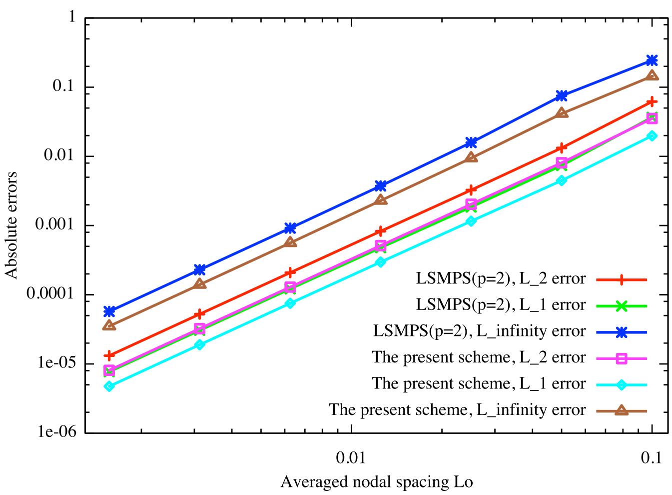


**Fig. 2.** Absolute $L_2$, $L_1$, and $L_\infty$ errors of the numerical solutions of the Poisson equation.

present scheme (Eq. (51)) are applied to discretize the Laplace operator appears in the Poisson equation. A spike shaped weight function defined by

$$w(r;h) = \begin{cases} \left(1 - \dfrac{r}{h}\right)^2, & 0 < \dfrac{r}{h} \leq 1, \\ 0, & 1 < \dfrac{r}{h}, \end{cases} \tag{60}$$

is employed. Note that this weight function is a recommended one for the LSMPS method [15] , and utilized in other studies(e.g.: in the SPH method this weight is employed for the pressure gradient term [34,35], and in the MPS method [36] for all spatial discretization). The dilation parameters $h$ that determine the compact support of the weight function are the same as listed in the Table. 1, and discrete absolute errors defined by

$$E_{L^2} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(f(\mathbf{x}_i)_{\text{exact}} - f(\mathbf{x}_i)_{\text{nuerical}}\right)^2}, \tag{61}$$

$$E_{L^1} = \frac{1}{N}\sum_{i=1}^{N}\left|f(\mathbf{x}_i)_{\text{exact}} - f(\mathbf{x}_i)_{\text{nuerical}}\right|, \tag{62}$$

$$E_{L^\infty} = \max_{1\leq i\leq N}\left|f(\mathbf{x}_i)_{\text{exact}} - f(\mathbf{x}_i)_{\text{nuerical}}\right|, \tag{63}$$

are compared. The results are displayed in Fig. 2.

### 4.2. Discussions

Fig. 2 demonstrates that, both numerical solutions of the Poisson equation with Dirichlet boundary condition obtained by employing the existing LSMPS scheme [15] with 2nd order basis and the novel proposed scheme in this paper, are 2nd order convergent in $L^2$, $L^1$, and $L^\infty$-norms. If Neumann boundary condition is given for a part of the domain boundary, the convergence rate of $L^\infty$-norm would be one; however, implementation of Neumann boundary condition will not be discussed in this paper. The rates of convergence of the LSMPS scheme ($p = 2$) and the present scheme are the same order; however, utilizing the new scheme results in more accurate numerical solutions. The reason for this improvement is the simple fact that the new implementation of discrete Laplace operator enables us to utilize smaller dilation parameters of the weight function. Less numbers of neighboring particles provided by the usage of smaller dilation parameter make the discretized Laplace operator matrix to be more sparse one. Moreover, when the computational domain is small and boundaries are close to each other, reduction of total computational time for solving the Poisson equation owing to the change of the discretization scheme for the Laplace operator is approximately in proportion to the averaged number of neighboring particles. In consequence, faster computation of solving sparse linear systems derived from the second order partial differential equations would be substantialized.

## 5. Conclusion

In this paper, the consistency of the second order derivative approximations for the strong-form meshfree particle methods including the LSMPS method are focused on, and the convergence of some meshfree particle discretization schemes for the Laplace operator are studied as a verification.

Moreover, a novel meshfree discretization scheme for the second order differential operator which enables us to use smaller dilation parameter of the compact support of the weight function is developed, and its application for the meshfree discretization of the Poisson equation demonstrates an improvement of the solution accuracy.

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