Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 395 (2022) 115012
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Difference between smoothed particle hydrodynamics and moving particle semi-implicit operators

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Received 15 January 2022; received in revised form 10 April 2022; accepted 10 April 2022
Available online 4 May 2022

Abstract

Smoothed particle hydrodynamics (SPH) and moving particle semi-implicit (MPS) methods are representative meshfree particle methods used to compute Lagrangian mechanics. The approximations of differential operators in the SPH and MPS methods have several similarities, but the theoretical discussion of the difference between them is limited. This study mathematically describes the difference via a comprehensive derivation of the first- and second-order derivative operators for each method. The comprehensive derivation indicates that the SPH and MPS operators are consistent with the pressure Poisson equation and moving least-squares approximation, respectively. The variation in consistency can explain the difference in the schemes of the incompressible flow problem. Additionally, the comprehensive derivation of the MPS operators can result in novel second-order and anisotropic operators. This study strengthens the theoretical understanding of the SPH and MPS methods and facilitates the selection of the appropriate method by users. Furthermore, the proposed MPS operators contribute to developing methods with adaptive or multiscale particle distributions.

Keywords: Smoothed particle hydrodynamics; Moving particle semi-implicit; Approximate differential operators; Pressure Poisson equation; Moving least squares

1. Introduction

Smoothed particle hydrodynamics (SPH) [1,2] and moving particle semi-implicit (MPS) [3,4] methods are representative meshfree particle methods for numerically solving Lagrangian mechanics such as incompressible flows, and these methods have been used in various fields including astrophysics, engineering, and biology [1,5,6]. The approximations of the differential operators in the SPH and MPS methods are very similar because they are represented by the weighted averages of the differences between neighboring particles, although their derivations are different. Accordingly, the applications of these methods are very similar. Furthermore, several studies have improved the SPH method by incorporating the ideas of the MPS method [7,8] and vice versa [9].

We pose the following fundamental question:

What is the essential difference between the SPH and MPS methods?

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https://doi.org/10.1016/j.cma.2022.115012

Although some differences in the numerical accuracy have been investigated [10,11], this is an open question from a theoretical perspective. This study answers the question through mathematical analysis of the discrete operators in the SPH and MPS methods.

We review the research on the SPH and MPS operators. Classically, the SPH method derives its operators using the integration approximation (convolution by kernel function) and its discretization on particles [6]. In contrast, the MPS method derives discrete operators using the directional derivatives between particles and their weighted average. However, because both the SPH and MPS operators utilize the weighted average of the differences between neighboring particles, we can transform them into each other by replacing the parameters [12–14] (the transformations are different for the first- and second-order derivative operators). Thus, we cannot identify the essential differences between the SPH and MPS methods from the formulations of the operators. The consistency (truncation error) of the SPH and MPS operators are the same from the viewpoint of the convergence order, and their numerical truncation errors have no noticeable differences [12,13]. However, we can find a difference in the formulation of the pressure Poisson equation in the incompressible flow problem. The incompressible SPH (ISPH) method straightforwardly discretizes the pressure Poisson equation using the SPH operators [8]; in contrast, the MPS method employs the discretization of the source term based on the continuity equation and particle number density [3]. The different formulations represent one of the differences between the SPH and MPS methods, and they may lead to differences in the accuracy and stability of simulations using the methods. However, the difference in the pressure Poisson equation has not been theoretically discussed.

Therefore, this study mathematically investigates the SPH and MPS operators. In particular, we focus on the relationship between the first- and second-order derivative operators in the SPH and MPS methods. To investigate this, we perform comprehensive derivations of these operators for each method. Specifically, we analyze the SPH operators using the pressure Poisson equation appearing in the numerical scheme of the incompressible flow problem [8] (Section 2) and MPS operators using the Taylor expansion and polynomial basis (Section 3). Based on the results, we discuss the difference between the SPH and MPS operators (Section 4). Additionally, we suggest that this difference in the SPH and MPS operators leads to the difference in the formulations of the incompressible flow problem. Finally, we propose novel MPS operators, second-order and anisotropic models, based on the comprehensive derivation of MPS operators (Section 5).

The notations used in this study are as follows:

d	Dimension ($d \geq 2$).
$\mathbb{R}^d$	d-dimensional Euclidean space.
Ω	Bounded domain in $\mathbb{R}^d$.
$y^{(i)}$	ith coordinate of vector $y \in \mathbb{R}^d$.
x_i	ith point (*particle*) in Ω without overlap ($i \neq j \Leftrightarrow x_i \neq x_j$).
N	Number of particles ($N < \infty$).
f	Smooth function on Ω.
A^{T}	Transpose vector or matrix A.
∂_k	Partial derivative with respect to the kth variable.
∇	Gradient operator ($\nabla = (\partial_1, \dots, \partial_d)^{\mathrm{T}}$).
$\nabla\cdot$	Divergence operator.
Δ	Laplacian operator ($\Delta = \partial_1^2 + \cdots + \partial_d^2$).
$\lVert \cdot \rVert$	Euclidean distance.

2. Formulation and derivation of SPH operators

This section introduces the formulation of the differential operators (first-order derivative and Laplacian operators) in the SPH method. Furthermore, we derive the SPH operators based on the pressure Poisson equation used in the ISPH method.

2.1. Formulation of SPH operators

The SPH method approximates the integration of function f based on the Monte Carlo method, as follows:

$$\int_\Omega f(y)\mathrm{d}y \approx \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j). \tag{1}$$

Here, m_j and ρ_j denote the mass and density, respectively, assigned to particle x_j, satisfying

$$\sum_{j=1}^{N} \frac{m_j}{\rho_j} = \text{volume of } \Omega.$$

Further, we introduce the smoothing kernel $w_h^{\mathtt{SPH}} : [0, \infty) \to [0, \infty)$, satisfying the compact support condition

$$w_h^{\mathtt{SPH}}(r) \begin{cases} > 0, & 0 \le r < h, \\ = 0, & r \ge h, \end{cases} \tag{2}$$

unity condition

$$\int_{\mathbb{R}^d} w_h^{\mathtt{SPH}}(\|y\|)\mathrm{d}y = 1, \tag{3}$$

and smoothness condition

$$\dot{w}_h^{\mathtt{SPH}}(0) = \dot{w}_h^{\mathtt{SPH}}(h) = 0. \tag{4}$$

Here, h denotes a positive parameter known as the smoothing length, and $\dot{w}_h^{\mathtt{SPH}}$ is the first-order derivative of $w_h^{\mathtt{SPH}}$. We generally use smoothing kernels such as cubic and quintic B-spline kernels [6]. We define the index set NP_i of the neighboring particles with respect to particle x_i as follows:

$$\mathrm{NP}_i := \{j = 1, \dots, N;\; 0 < \|x_i - x_j\| < h\}.$$

Then, we introduce the SPH operator on particle x_i for the first-order derivative with respect to the kth variable as follows:

$$\langle \partial_k f \rangle_i^{\mathtt{SPH}} := \sum_{j \in \mathrm{NP}_i} \frac{m_j}{\rho_j} \left[f(x_j) - f(x_i) \right] \partial_k w_h^{\mathtt{SPH}}(\|x_i - x_j\|). \tag{5}$$

The corresponding expression for the Laplacian operator is as follows:

$$\langle \Delta f \rangle_i^{\mathtt{SPH}} := 2 \sum_{j \in \mathrm{NP}_i} \frac{m_j}{\rho_j} \frac{f(x_i) - f(x_j)}{\|x_i - x_j\|} \frac{x_i - x_j}{\|x_i - x_j\|} \cdot \nabla w_h^{\mathtt{SPH}}(\|x_i - x_j\|). \tag{6}$$

Here, $\partial_k w_h^{\mathtt{SPH}}$ is expressed as

$$\partial_k w_h^{\mathtt{SPH}}(\|y\|) = \begin{cases} \dfrac{y^{(k)}}{\|y\|} \dot{w}_h^{\mathtt{SPH}}(\|y\|), & y \ne 0, \\ 0, & y = 0, \end{cases}$$

and $\nabla w_h^{\mathtt{SPH}}(\|y\|) = [\partial_1 w_h^{\mathtt{SPH}}(\|y\|), \dots, \partial_d w_h^{\mathtt{SPH}}(\|y\|)]^{\mathrm{T}}$.

2.2. *Comprehensive derivation of SPH operators*

To clarify the relationship between the first-order derivative (5) and Laplacian operators (6) in the SPH method, we consider the following pressure Poisson equation:

$$\Delta p = \frac{\rho}{\tau} \nabla \cdot \widetilde{u} \qquad \text{in } \Omega, \tag{7}$$

which appears in the time discretization based on the projection method for the incompressible Navier–Stokes equations [8]. Here, p, $\widetilde{u}$, ρ, and τ denote the pressure, predicted velocity, density, and time step, respectively. For simplicity, this study does not mention the boundary conditions. Using $v = \rho\, \widetilde{u}/\tau$, we consider the following simple form:

$$\Delta p = \nabla \cdot v \qquad \text{in } \Omega. \tag{8}$$

We show that an approximation of Poisson equation (8) can *naturally* lead to the SPH operators (5) and (6). We assume that p and v are sufficiently smooth. Let $\Omega_h^{\mathtt{in}}$ be the inner domain obtained as

$$\Omega_h^{\mathtt{in}} := \{x \in \Omega;\; B_h(x) \subset \Omega\},$$

where $B_h(x)$ denotes the open domain with center x and radius h, that is,

$$B_h(x) := \{y \in \mathbb{R}^d;\ \|y - x\| < h\}.$$

We first state the following lemma:

Lemma 2.1. *For $x \in \Omega_h^{\mathtt{in}}$ and $k, \ell = 1, \dots, d$,*

$$\int_\Omega \frac{(x-y)^{(k)}(x-y)^{(\ell)}}{\|x-y\|} \dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y = -\delta_{k,\ell}$$

holds, where $\delta_{k,\ell}$ denotes the Kronecker delta.

Proof. From $B_h(x) \subset \Omega$, using the coordinate transformation and compact support condition (2), we obtain

$$\int_\Omega \frac{(x-y)^{(k)}(x-y)^{(\ell)}}{\|x-y\|} \dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y = \int_{\|y\|<h} \frac{y^{(k)}y^{(\ell)}}{\|y\|} \dot{w}_h^{\mathtt{SPH}}(\|y\|)\mathrm{d}y.$$

When $k \neq \ell$, because the integrated function is odd with respect to the origin, we obtain

$$\int_{\|y\|<h} \frac{y^{(k)}y^{(\ell)}}{\|y\|} \dot{w}_h^{\mathtt{SPH}}(\|y\|)\mathrm{d}y = 0.$$

When $k = \ell$, using the symmetry with respect to the origin, polar coordinate transformation, and conditions (3)–(4) of the weight function, we obtain

$$\begin{aligned}
\int_{\|y\|<h} \frac{[y^{(k)}]^2}{\|y\|} \dot{w}_h^{\mathtt{SPH}}(\|y\|)\mathrm{d}y &= \frac{1}{d}\sum_{s=1}^{d} \int_{B_h(0)} \frac{[y^{(s)}]^2}{\|y\|} \dot{w}_h^{\mathtt{SPH}}(\|y\|)\mathrm{d}y \\
&= \frac{1}{d}\int_{B_h(0)} \|y\| \dot{w}_h^{\mathtt{SPH}}(\|y\|)\mathrm{d}y \\
&= \frac{1}{d}\int_{S^{d-1}} J(\theta) \int_0^h r^d \dot{w}_h^{\mathtt{SPH}}(r)\mathrm{d}r\mathrm{d}\theta \\
&= -\int_{S^{d-1}} J(\theta) \int_0^h r^{d-1} w_h^{\mathtt{SPH}}(r)\mathrm{d}r\mathrm{d}\theta \\
&= -\int_{\|y\|<h} w_h^{\mathtt{SPH}}(\|y\|)\mathrm{d}y \\
&= -1.
\end{aligned}$$

Here, S^{d-1} denotes the $(d-1)$-dimensional unit sphere, and $J(\theta)$ is the Jacobian with respect to angle θ. □

Now, we introduce the following operators:

$$\widetilde{\nabla}^{\mathtt{SPH}} \cdot v(x) := \int_\Omega [v(y) - v(x)] \cdot \nabla w_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y,$$

$$\widetilde{\Delta}^{\mathtt{SPH}} p(x) := 2\int_\Omega \frac{p(x)-p(y)}{\|x-y\|}\frac{x-y}{\|x-y\|} \cdot \nabla w_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y.$$

Using Eq. (1), we can consider these operators as approximations of the SPH operators, that is,

$$\widetilde{\nabla}^{\mathtt{SPH}} \cdot v(x_i) \underset{\text{Eq. (1)}}{\approx} \langle \nabla \cdot v\rangle_i^{\mathtt{SPH}} \quad \text{and} \quad \widetilde{\Delta}^{\mathtt{SPH}} p(x_i) \underset{\text{Eq. (1)}}{\approx} \langle \Delta p\rangle_i^{\mathtt{SPH}}.$$

Here, $\langle \nabla \cdot v\rangle_i^{\mathtt{SPH}}$ is the divergence operator in SPH method defined as

$$\langle \nabla \cdot v\rangle_i^{\mathtt{SPH}} := \sum_{k=1}^{d} \langle \partial_k v^{(k)}\rangle_i^{\mathtt{SPH}} = \sum_{j \in \mathrm{NP}_i} \frac{m_j}{\rho_j}\left[v(x_j) - v(x_i)\right] \cdot \nabla w_h^{\mathtt{SPH}}(\|x_i - x_j\|).$$

Using Lemma 2.1, we have the following theorem:

Theorem 2.2. *For $x \in \Omega_h^{\mathtt{in}}$,*

$$\widetilde{\Delta}^{\mathtt{SPH}} p(x) = \widetilde{\nabla}^{\mathtt{SPH}} \cdot v(x) + \mathrm{RES}^{\mathtt{SPH}}(x) \tag{9}$$

holds. Here, $\mathrm{RES}^{\mathtt{SPH}}$ *is the residual obtained by higher-order derivatives of p and v, i.e.,*

$$\begin{aligned}
\mathrm{RES}^{\mathtt{SPH}}(x) &:= \mathrm{RES}_v(x) - \mathrm{RES}_p(x),\\
\mathrm{RES}_p(x) &:= 2\int_\Omega \frac{R_4(p,x,y)}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y,\\
\mathrm{RES}_v(x) &:= \frac{1}{3}\int_\Omega R_3(v,x,y)\cdot\nabla w_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y,
\end{aligned}$$

where R_n denotes the residual of the Taylor expansion defined as

$$R_n(f,x,y) := \int_0^1 (1-t)^{n-1}\frac{[(x-y)^{\mathrm{T}}\nabla]^n f(ty-(1-t)x)}{n!}\mathrm{d}t.$$

Proof. From Lemma 2.1, for $x \in \Omega_h^{\mathtt{in}}$, we obtain

$$\begin{aligned}
0 &= \Delta p(x) - \nabla\cdot v(x)\\
&= \sum_{k,\ell\in\{1,\dots,d\}} [\partial_k\partial_\ell p(x) - \partial_k v(x)^{(\ell)}]\delta_{k,\ell}\\
&= -\sum_{k,\ell\in\{1,\dots,d\}} [\partial_k\partial_\ell p(x) - \partial_k v(x)^{(\ell)}]\int_\Omega \frac{(x-y)^{(k)}(x-y)^{(\ell)}}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y.
\end{aligned} \tag{10}$$

Now, we consider the nth order Taylor expansion of the multivariable function f:

$$f(x) = \sum_{k=0}^n \frac{[(x-y)^{\mathrm{T}}\nabla]^k f(y)}{k!} + R_{n+1}(f,x,y). \tag{11}$$

By using the Taylor expansions (11) of p and v, we obtain

$$\begin{aligned}
&-\sum_{k,\ell\in\{1,\dots,d\}}\partial_k\partial_\ell p(x)\int_\Omega\frac{(x-y)^{(k)}(x-y)^{(\ell)}}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y\\
&= -\int_\Omega\sum_{k,\ell\in\{1,\dots,d\}}\frac{(x-y)^{(k)}(x-y)^{(\ell)}\partial_k\partial_\ell p(x)}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y\\
&= -\int_\Omega\frac{[(x-y)^{\mathrm{T}}\nabla]^2 p(x)}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y.\\
&= 2\int_\Omega\frac{p(x)-p(y)}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y\\
&\quad \underbrace{+2\int_\Omega\frac{(x-y)^{\mathrm{T}}\nabla p(x)}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y}_{=0}\\
&\quad \underbrace{+\frac{1}{3}\int_\Omega\frac{[(x-y)^{\mathrm{T}}\nabla]^3 p(x)}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y}_{=0} + \mathrm{RES}_p(x)\\
&= 2\int_\Omega\frac{p(x)-p(y)}{\|x-y\|}\dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y + \mathrm{RES}_p(x)\\
&= 2\int_\Omega\frac{p(x)-p(y)}{\|x-y\|}\frac{x-y}{\|x-y\|}\cdot\nabla w_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y + \mathrm{RES}_p(x)\\
&= \widetilde{\Delta}^{\mathtt{SPH}} p(x) + \mathrm{RES}_p(x)
\end{aligned}$$

and

$$
\begin{aligned}
&\sum_{k,\ell\in\{1,\ldots,d\}} \partial_k v(x)^{(\ell)} \int_\Omega \frac{(x-y)^{(k)}(x-y)^{(\ell)}}{\|x-y\|} \dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y \\
&= \int_\Omega \sum_{k,\ell\in\{1,\ldots,d\}} \frac{(x-y)^{(k)}\partial_k v(x)^{(\ell)}(x-y)^{(\ell)}}{\|x-y\|} \dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y \\
&= \int_\Omega \frac{[(x-y)^{\mathrm{T}}\nabla]v(x)\cdot(x-y)}{\|x-y\|} \dot{w}_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y \\
&= \int_\Omega [(x-y)^{\mathrm{T}}\nabla]v(x)\cdot\nabla w_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y \\
&= -\int_\Omega [v(y)-v(x)]\cdot\nabla w_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y \\
&\quad \underbrace{-\frac{1}{2}\int_\Omega [(x-y)^{\mathrm{T}}\nabla]^2 v(x)\cdot\nabla w_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y}_{=0} - \mathrm{RES}_v(x) \\
&= -\int_\Omega [v(y)-v(x)]\cdot\nabla w_h^{\mathtt{SPH}}(\|x-y\|)\mathrm{d}y - \mathrm{RES}_v(x) \\
&= -\widetilde{\nabla}^{\mathtt{SPH}}\cdot v(x) - \mathrm{RES}_v(x).
\end{aligned}
$$

Here, underlined terms are zero because the integrated functions are odd. Using the same transformation as that used previously, we obtain thus, from Eq. (10), we obtain Eq. (9). □

From the integration approximation (1) and Theorem 2.2, we can derive the approximation of Poisson Eq. (8) in the SPH method using the following procedures:

$$
\begin{aligned}
\Delta p = \nabla\cdot v \quad \text{in } \Omega \quad &\xrightarrow[\text{Eq. (10) \& Taylor expansion}]{=} \quad \widetilde{\Delta}^{\mathtt{SPH}} p = \widetilde{\nabla}^{\mathtt{SPH}}\cdot v + \mathrm{RES}^{\mathtt{SPH}} \quad \text{in } \Omega_h^{\mathtt{in}} \\
&\xrightarrow[\text{Truncate RES}^{\mathtt{SPH}}]{\approx} \quad \widetilde{\Delta}^{\mathtt{SPH}} p \approx \widetilde{\nabla}^{\mathtt{SPH}}\cdot v \quad \text{in } \Omega_h^{\mathtt{in}} \\
&\xrightarrow[\text{Eq. (1)}]{\approx} \quad \langle \Delta p\rangle_i^{\mathtt{SPH}} \approx \langle\nabla\cdot v\rangle_i^{\mathtt{SPH}} \quad \text{for } i = 1,\ldots,N.
\end{aligned}
\tag{12}
$$

Many studies related to the derivation and consistency for the SPH operators exist [12,15–19], but these works derived the first- and second-order SPH operators individually. In contrast, as shown in Theorem 2.2 and Eq. (12), we approximate both sides of the Poisson equation in the same manner (transformation (10) → Taylor expansion → truncate $\mathrm{RES}^{\mathtt{SPH}}$ → approximation (1)). This implies that the definitions of the SPH operators (5) and (6) are consistent with the pressure Poisson equation.

3. Formulation and derivation of MPS operators

This section introduces the formulation of the differential operators (first-order derivative operator and Laplacian) in the MPS method. Furthermore, we derive the MPS operators based on the Taylor expansion and polynomial approximation associated with the moving least-squares (MLS) method. Additionally, we propose new MPS operators for anisotropic distributions based on the derivation.

3.1. Formulation of MPS operators

The MPS method forms approximations of the differential operators based on the weighted average of the differences between the neighboring particles. For particle x_i, the MPS method introduces the *particle number density* n_i defined as

$$
n_i := \sum_{j\in\mathrm{NP}_i} w_h^{\mathtt{MPS}}(\|x_j - x_i\|).
$$

The MPS method introduces the weight function $w_h^{\mathtt{MPS}}$ with the compact support condition as follows:

$$w_h^{\mathtt{MPS}}(r)\begin{cases} > 0, & 0 < r < h, \\ = 0, & r \geq h. \end{cases}$$

The MPS method does not require the unity (3) and smoothness conditions (4), which are required for the smoothing kernel of the SPH method. We generally use the weight function as an infinite model

$$w_h^{\mathtt{MPS}}(r) = \begin{cases} \dfrac{h}{r} - 1, & 0 < r < h, \\ 0, & \text{otherwise} \end{cases}$$

or a quadratic model

$$w_h^{\mathtt{MPS}}(r) = \begin{cases} (r-h)^2, & 0 < r < h, \\ 0, & \text{otherwise.} \end{cases}$$

Then, we introduce the MPS operator on particle x_i for the first-order derivative with respect to the kth variable as follows:

$$\langle \partial_k f \rangle_i^{\mathtt{MPS}} := \frac{d}{n_i} \sum_{j \in \mathrm{NP}_i} \frac{f(x_j) - f(x_i)}{\|x_j - x_i\|} \frac{x_j^{(k)} - x_i^{(k)}}{\|x_j - x_i\|} w_h^{\mathtt{MPS}}(\|x_j - x_i\|). \tag{13}$$

The corresponding expression for the Laplacian is as follows:

$$\langle \Delta f \rangle_i^{\mathtt{MPS}} := \frac{2d}{n_i \lambda_i} \sum_{j \in \mathrm{NP}_i} \left[f(x_j) - f(x_i) \right] w_h^{\mathtt{MPS}}(\|x_j - x_i\|), \tag{14}$$

where λ_i is defined as

$$\lambda_i := \frac{1}{n_i} \sum_{j \in \mathrm{NP}_i} \|x_j - x_i\|^2 w_h^{\mathtt{MPS}}(\|x_j - x_i\|).$$

Although n_i and λ_i are classically fixed [3] for simplicity, we use non-fixed values as employed in recent models [4].

3.2. Comprehensive derivation of MPS operators

We initially showed the comprehensive derivation of the MPS operators in a two-dimensional space ($d = 2$) [20]. This section shows the general case ($d \geq 2$).

We first define the notations. For simplicity, we use $f_{ij} = f(x_j) - f(x_i)$ and $r_{ij} = x_j - x_i$ hereinafter. We define $\theta_{i,k,\ell}$ and θ_i ($i = 1, \ldots, N, k, \ell = 1, \ldots, d$) as follows:

$$\theta_{i,k,\ell} := \sum_{j \in \mathrm{NP}_i} \frac{[r_{ij}^{(k)}]^2 [r_{ij}^{(\ell)}]^2}{\|r_{ij}\|^2} w_h^{\mathtt{MPS}}(\|r_{ij}\|), \tag{15}$$

$$\theta_i := \frac{2}{d(d-1)} \sum_{\ell=k+1}^{d} \sum_{k=1}^{d} \theta_{i,k,\ell}.$$

Here, θ_i denotes the average of $\theta_{i,k,\ell}$ for $k \neq \ell$. Let D and p_{ij} be vectors with length $d(d+3)/2$, belonging to the second-order and lower partial derivatives and to the polynomial bases, respectively. They are defined as follows:

$$D = [\underbrace{\partial_1, \ldots, \partial_d}_{\text{1st order}}, \underbrace{\partial_1^2, \ldots, \partial_d^2}_{\text{2nd order (duplicated)}}, \underbrace{\partial_1 \partial_2, \ldots, \partial_{d-1} \partial_d}_{\text{2nd order (mixed)}}]^{\mathtt{T}},$$

$$p_{ij} = \left[r_{ij}^{(1)}, \ldots, r_{ij}^{(d)}, \frac{[r_{ij}^{(1)}]^2}{2}, \ldots, \frac{[r_{ij}^{(d)}]^2}{2}, r_{ij}^{(1)} r_{ij}^{(2)}, \ldots, r_{ij}^{(d-1)} r_{ij}^{(d)} \right]^{\mathtt{T}}.$$

The second-order Taylor expansion on particle x_i can be expressed as follows:

$$f(x_j) = p_{ij}^{\mathtt{T}} D f(x_i) + R_3(f, x_j, x_i). \tag{16}$$

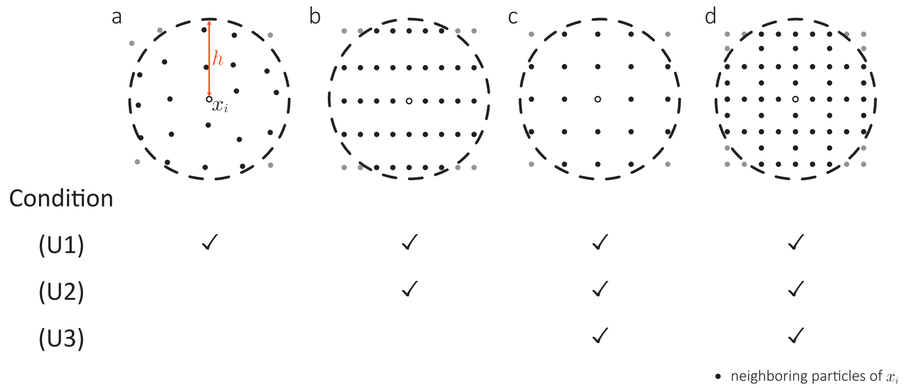

Fig. 1. Examples of neighboring particles that satisfy conditions (U1)–(U3). a, non-structural distribution that satisfies (U1). b, anisotropic structural distribution that satisfies (U1)–(U2). c and d, isotropic structural distributions that satisfy (U1)–(U3).

Using p_{ij}, we define the moment matrix M_i on particle x_i as

$$M_i := \sum_{j\in \mathrm{NP}_i} \frac{p_{ij}p_{ij}^{\mathrm{T}}}{\|r_{ij}\|^2} w_h^{\mathtt{MPS}}(\|r_{ij}\|).$$

We define m_i^α as

$$m_i^\alpha := \sum_{j\in \mathrm{NP}_i} \frac{r_{ij}^\alpha}{\|r_{ij}\|^2} w_h^{\mathtt{MPS}}(\|r_{ij}\|).$$

Here, $\alpha = (\alpha_1, \dots, \alpha_d)$ denotes the d-dimensional multi-index, which is the d-variable of non-negative integers with the following operations:

$$y^\alpha = [y^{(1)}]^{\alpha_1} \times \dots \times [y^{(d)}]^{\alpha_d},$$
$$|\alpha| = \alpha_1 + \cdots + \alpha_d.$$

The term m_i^α can represent the elements of M_i; for instance, when $d = 2$,

$$M_i = \begin{bmatrix} m_i^{(2,0)} & m_i^{(1,1)} & \dfrac{m_i^{(3,0)}}{2} & \dfrac{m_i^{(1,2)}}{2} & m_i^{(2,1)} \\ m_i^{(1,1)} & m_i^{(0,2)} & \dfrac{m_i^{(2,1)}}{2} & \dfrac{m_i^{(0,3)}}{2} & m_i^{(1,2)} \\ \dfrac{m_i^{(3,0)}}{2} & \dfrac{m_i^{(2,1)}}{2} & \dfrac{m_i^{(4,0)}}{4} & \dfrac{m_i^{(2,2)}}{4} & \dfrac{m_i^{(3,1)}}{2} \\ \dfrac{m_i^{(1,2)}}{2} & \dfrac{m_i^{(0,3)}}{2} & \dfrac{m_i^{(2,2)}}{4} & \dfrac{m_i^{(0,4)}}{4} & \dfrac{m_i^{(1,3)}}{2} \\ m_i^{(2,1)} & m_i^{(1,2)} & \dfrac{m_i^{(3,1)}}{2} & \dfrac{m_i^{(1,3)}}{2} & m_i^{(2,2)} \end{bmatrix}.$$

Next, we introduce the conditions for the neighboring particles as follows:

(U1) M_i is invertible.

(U2) $m_i^\alpha = 0$ for all α that contain odd component(s) and $|\alpha| \le 4$.

(U3) The distribution of the neighboring particles is isotropic with respect to all coordinate systems with origin x_i; that is, for all $j \in \mathrm{NP}_i$ and $s, t = 1, \dots, d$, there exists $k \in \mathrm{NP}_i$ such that $r_{ij}^{(s)} = r_{ik}^{(t)}$, $r_{ij}^{(t)} = r_{ik}^{(s)}$, and $r_{ij}^{(\ell)} = r_{ik}^{(\ell)}$ for all ℓ not s or t.

We show examples of the neighboring particles that satisfy conditions (U1)–(U3) in Fig. 1.

Then, we obtain the following theorem for the derivation of the MPS operators.

Theorem 3.1. *If the neighboring particles of particle x_i satisfy condition (U1), then*

$$\widetilde{D} f(x_i) = Df(x_i) + \mathrm{RES}^{\mathrm{MPS}} \tag{17}$$

holds, where

$$\widetilde{D} f(x_i) := M_i^{-1} \sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|^2} p_{ij} w_h^{\mathrm{MPS}}(\|r_{ij}\|),$$
$$\mathrm{RES}^{\mathrm{MPS}} := M_i^{-1} \sum_{j \in \mathrm{NP}_i} p_{ij} \frac{R_3(f, x_j, x_i)}{\|r_{ij}\|^2} w_h^{\mathrm{MPS}}(\|r_{ij}\|).$$

Moreover, if the neighboring particles of particle x_i satisfy conditions (U1)–(U3), then MPS operators (13) and *(14) are consistent with $\widetilde{D} f(x_i)$; that is,*

$$\langle \partial_k f \rangle_i^{\mathrm{MPS}} = \widetilde{\partial}_k f(x_i), \quad k = 1, \dots, d, \tag{18}$$
$$\langle \Delta f \rangle_i^{\mathrm{MPS}} = \widetilde{\Delta} f(x_i), \tag{19}$$

where $\widetilde{D} = [\widetilde{\partial}_1, \dots, \widetilde{\partial}_d, \widetilde{\partial}_1^2, \dots, \widetilde{\partial}_d^2, \widetilde{\partial}_1 \widetilde{\partial}_2, \dots, \widetilde{\partial}_{d-1} \widetilde{\partial}_d]^{\mathrm{T}}$ and $\widetilde{\Delta} = \widetilde{\partial}_1^2 + \cdots + \widetilde{\partial}_d^2$.

Proof. By multiplying both sides of the second-order Taylor expansion (16) with $p_{ij} w_h^{\mathrm{MPS}}(\|r_{ij}\|)/\|r_{ij}\|^2$ and summing for $j \in \mathrm{NP}_i$, we obtain

$$\sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|^2} p_{ij} w_h^{\mathrm{MPS}}(\|r_{ij}\|) = M_i Df(x_i) + \sum_{j \in \mathrm{NP}_i} p_{ij} \frac{R_3(f, x_j, x_i)}{\|r_{ij}\|^2} w_h^{\mathrm{MPS}}(\|r_{ij}\|).$$

From the invertible condition (U1), by multiplying both sides of the above equation with M_i^{-1}, we obtain Eq. (17).

Next, we show Eqs. (18) and (19). From condition (U2), we can represent the moment matrix M_i as follows:

$$M_i = \begin{bmatrix} n_{i,1} & & & & & & \\ & \ddots & & & & & \\ & & n_{i,d} & & & & \\ & & & \frac{1}{4}\Theta_i & & & \\ & & & & \theta_{i,1,2} & & \\ & & & & & \ddots & \\ & & & & & & \theta_{i,d-1,d} \end{bmatrix}, \tag{20}$$

where

$$n_{i,k} := \sum_{j \in \mathrm{NP}_i} \frac{[r_{ij}^{(k)}]^2}{\|r_{ij}\|^2} w_h^{\mathrm{MPS}}(\|r_{ij}\|), \quad k = 1, \dots, d \tag{21}$$

and Θ_i is a $d \times d$ matrix obtained as $\Theta_i = (\theta_{i,k,\ell})$ $(k, \ell = 1, \dots, d)$ ($\theta_{i,k,\ell}$ is defined in Eq. (15)). The empty elements in Eq. (20) are zero. In addition, from condition (U3), we obtain

$$\begin{aligned} n_{i,k} &= \frac{1}{d} \sum_{\ell=1}^{d} \sum_{j \in \mathrm{NP}_i} \frac{[r_{ij}^{(\ell)}]^2}{\|r_{ij}\|^2} w_h^{\mathrm{MPS}}(\|r_{ij}\|) \\ &= \frac{1}{d} \sum_{j \in \mathrm{NP}_i} w_h^{\mathrm{MPS}}(\|r_{ij}\|) \\ &= \frac{n_i}{d} \end{aligned}$$

for $k = 1, \ldots, d$ and $\theta_{i,k,\ell} = \theta_i$ for $k \neq \ell$. Hence, we can represent the moment matrix M_i as the following block matrix:

$$M_i = \begin{bmatrix} \dfrac{n_i}{d} I_d & & \\ & \dfrac{1}{4}\Theta_i & \\ & & \theta_i I_{d(d-1)/2} \end{bmatrix},$$

where I_k denotes the $k \times k$ identity matrix. Then, we can calculate the inverse M_i^{-1} as follows:

$$M_i^{-1} = \begin{bmatrix} \dfrac{d}{n_i} I_d & & \\ & 4\Theta_i^{-1} & \\ & & \dfrac{1}{\theta_i} I_{d(d-1)/2} \end{bmatrix}.$$

We explicitly calculate Θ_i^{-1}. From

$$\begin{aligned}
\theta_{i,k,k} &= \frac{1}{d} \sum_{\ell=1}^{d} \sum_{j \in \mathrm{NP}_i} \frac{[r_{ij}^{(\ell)}]^4}{\|r_{ij}\|^2} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \frac{1}{d} \sum_{j \in \mathrm{NP}_i} \frac{1}{\|r_{ij}\|^2} \left\{ \sum_{\ell=1}^{d} [r_{ij}^{(\ell)}]^2 \right\}^2 w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&\quad - \frac{2}{d} \sum_{\ell=1}^{d} \sum_{s=\ell+1}^{d} \sum_{j \in \mathrm{NP}_i} \frac{[r_{ij}^{(\ell)}]^2 [r_{ij}^{(s)}]^2}{\|r_{ij}\|^2} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \frac{1}{d} \sum_{j \in \mathrm{NP}_i} \|r_{ij}\|^2 w_h^{\mathtt{MPS}}(\|r_{ij}\|) - \frac{2}{d} \sum_{\ell=1}^{d} \sum_{s=\ell+1}^{d} \theta_{i,\ell,s} \\
&= \frac{n_i \lambda_i - d(d-1)\theta_i}{d},
\end{aligned}$$

Θ_i becomes the $d \times d$ symmetric matrix, obtained as follows:

$$[\Theta_i]_{k\ell} = \begin{cases} \dfrac{n_i \lambda_i - d(d-1)\theta_i}{d}, & k = \ell, \\ \theta_i, & k \neq \ell. \end{cases}$$

Using Cramer's rule, we can calculate Θ_i^{-1} as follows:

$$[\Theta_i^{-1}]_{k\ell} = \begin{cases} \dfrac{d(n_i \lambda_i - d\theta_i)}{n_i \lambda_i (n_i \lambda_i - d^2 \theta_i)}, & k = \ell, \\ -\dfrac{d^2 \theta_i}{n_i \lambda_i (n_i \lambda_i - d^2 \theta_i)}, & k \neq \ell. \end{cases}$$

Therefore, we obtain

$$\begin{aligned}
\widetilde{\partial}_k f(x_i) &= [\widetilde{D} f(x_i)]^{(k)} \\
&= \frac{d}{n_i} \sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{r_{ij}^{(k)}}{\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \langle \partial_k f \rangle_i^{\mathtt{MPS}}
\end{aligned}$$

for $k = 1, \ldots, d$ and

$$
\begin{aligned}
\widetilde{\Delta} f(x_i) &= \sum_{k=1}^{d} (\widetilde{D} f(x_i))^{(d+k)} \\
&= 4 \sum_{k=1}^{d} \sum_{\ell=1}^{d} [\Theta_i^{-1}]_{k\ell} \sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{[r_{ij}^{(\ell)}]^2}{2\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \sum_{k=1}^{d} \left\{ \frac{4d(n_i\lambda_i - d\theta_i)}{n_i\lambda_i(n_i\lambda_i - d^2\theta_i)} \sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{[r_{ij}^{(k)}]^2}{2\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \right. \\
&\quad \left. - \frac{4d^2\theta_i}{n_i\lambda_i(n_i\lambda_i - d^2\theta_i)} \sum_{\ell \neq k} \sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{[r_{ij}^{(\ell)}]^2}{2\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \right\} \\
&= \frac{2d(n_i\lambda_i - d\theta_i)}{n_i\lambda_i(n_i\lambda_i - d^2\theta_i)} \sum_{j \in \mathrm{NP}_i} f_{ij} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&\quad - \frac{2d^2(d-1)\theta_i}{n_i\lambda_i(n_i\lambda_i - d^2\theta_i)} \sum_{j \in \mathrm{NP}_i} f_{ij} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \frac{2d}{n_i\lambda_i(n_i\lambda_i - d^2\theta_i)} [(n_i\lambda_i - d\theta_i) - d(d-1)\theta_i] \sum_{j \in \mathrm{NP}_i} f_{ij} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \frac{2d}{n_i\lambda_i} \sum_{j \in \mathrm{NP}_i} f_{ij} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \langle \Delta f \rangle_i^{\mathtt{MPS}}. \quad \square
\end{aligned}
$$

In addition, we describe the relationship with the MLS method [21,22] as follows.

Remark 3.2. The MLS approximation with basis p_{ij} is consistent with $\widetilde{D} f(x_i)$; that is, for the weighted least-square error

$$
\sum_{j \in \mathrm{NP}_i} (c^{\mathrm{T}} p_{ij} - f_{ij})^2 w_h^{\mathtt{MPS}}(\|r_{ij}\|), \tag{22}
$$

the solution $c^{\mathtt{MLS}}$ minimizing Eq. (22) with respect to c, satisfies

$$
\widetilde{D} f(x_i) = c^{\mathtt{MLS}}.
$$

From Theorem 3.1 and Remark 3.2, we can comprehensively derive the MPS operators using the following procedures:

$$
\begin{aligned}
&\text{Taylor expansion} \quad \xrightarrow[\text{Theorem 3.1 (17)}]{=} \quad \widetilde{D} f(x_i) = D f(x_i) + \mathrm{RES}^{\mathtt{MPS}} \\
&\qquad\qquad\qquad\quad \xrightarrow[\text{Truncate } \mathrm{RES}^{\mathtt{MPS}}]{\approx} \quad \widetilde{D} f(x_i) \approx D f(x_i) \text{ (MLS approximation)} \\
&\qquad\qquad\qquad\quad \xrightarrow[\text{Theorem 3.1 (18)–(19)}]{=} \quad \begin{cases} \langle \partial_k f \rangle_i^{\mathtt{MPS}} = (\widetilde{D} f(x_i))^{(k)}, \ k = 1, \ldots, d, \\ \langle \Delta f \rangle_i^{\mathtt{MPS}} = \displaystyle\sum_{k=1}^{d} (\widetilde{D} f(x_i))^{(d+k)}. \end{cases}
\end{aligned} \tag{23}
$$

Unlike the SPH operators, the MPS operators are derived based on the MLS approximation under uniform particle distribution conditions. Based on the different comprehensive derivations, we will discuss the difference between the SPH and MPS operators in the next section. Additionally, by developing a comprehensive derivation of the existing MPS operators, we propose new MPS operators in Section 5.

4. Discussion of the difference between SPH and MPS operators

We first explain the *similarity* between the SPH and MPS operators. The first-order derivative operators can be transformed into each other as follows:

$$\begin{aligned}
\langle \partial_k f \rangle_i^{\mathtt{SPH}} &= \sum_{j \in \mathrm{NP}_i} \frac{m_j}{\rho_j} f_{ij} \partial_k w_h^{\mathtt{SPH}}(\|r_{ji}\|) \\
&= -\sum_{j \in \mathrm{NP}_i} \frac{m_j}{\rho_j} f_{ij} \frac{r_{ij}^{(k)}}{\|r_{ij}\|} \dot{w}_h^{\mathtt{SPH}}(\|r_{ij}\|) \\
&\left(\text{replace } -\frac{m_j}{\rho_i} \dot{w}_h^{\mathtt{SPH}}(\|r_{ij}\|) \text{ and } \frac{d}{n_i \|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|)\right) \\
&\leftrightarrow \frac{d}{n_i} \sum_{j \in \mathrm{NP}_i} f_{ij} \frac{r_{ij}^{(k)}}{\|r_{ij}\|^2} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \langle \partial_k f \rangle_i^{\mathtt{MPS}}.
\end{aligned} \tag{24}$$

Further, we can transform the Laplacian operators in the following way:

$$\begin{aligned}
\langle \Delta f \rangle_i^{\mathtt{SPH}} &= 2 \sum_{j \in \mathrm{NP}_i} \frac{m_j}{\rho_j} \frac{f_{ji}}{\|r_{ji}\|} \frac{r_{ji}}{\|r_{ji}\|} \cdot \nabla w_h^{\mathtt{SPH}}(\|r_{ji}\|) \\
&= -2 \sum_{j \in \mathrm{NP}_i} \frac{m_j}{\rho_j} f_{ij} \dot{w}_h^{\mathtt{SPH}}(\|r_{ij}\|) \\
&\left(\text{replace } -\frac{m_j}{\rho_i} \dot{w}_h^{\mathtt{SPH}}(\|r_{ij}\|) \text{ and } \frac{d}{\lambda_i n_i} w_h^{\mathtt{MPS}}(\|r_{ij}\|)\right) \\
&\leftrightarrow \frac{2d}{\lambda_i n_i} \sum_{j \in \mathrm{NP}_i} f_{ij} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \\
&= \langle \Delta f \rangle_i^{\mathtt{MPS}}.
\end{aligned} \tag{25}$$

The transformation in the case of integral forms has been shown by Souto-Iglesias et al. [13]. From these transformations, we can understand that the SPH and MPS operator are similar formulations.

However, the replaced parameters that convert the SPH and MPS operators are different for the first-order derivative and Laplacian operators. This implies that the relationships between the first- and second-order derivative operators differ in the SPH and MPS methods.

Next, we discuss the *difference* between the SPH and MPS operators. We have shown the comprehensive derivations of the SPH and MPS operators. The SPH operators were consistent with the pressure Poisson equation (Section 2), whereas the MPS operators were consistent with the second-order Taylor expansion (Section 3). As mentioned in the previous paragraph, the first- and second-order derivative operators in the SPH and MPS methods are not converted by replacing the same parameters. Thus, the comprehensive derivations of each do not apply to the other. Consequently, we can conclude that there is an *essential difference* between the SPH and MPS operators (see Fig. 2).

This difference can explain the contrast in the schemes for the incompressible Navier–Stokes equations. The ISPH method straightforwardly discretizes the pressure Poisson equations using the SPH operators. In contrast, the MPS method models the source term (the right-hand side of Eq. (7)) using the particle number density. This may be because the MPS operators have lesser consistency with the pressure Poisson equations than the SPH operators. The similar discussion can be seen in the previous study [14].

It has been reported that the SPH method is more stable than the MPS method in incompressible flow simulations [10]. Moreover, we mathematically proved the stability for only the ISPH method [23,24]. Furthermore, the improved second-order derivative operators of the SPH methods have been proposed while maintaining the relationship between the first- and second-order derivative operators [25]. Hence, the relationship between the first- and second-order derivative operators in the SPH method is critical for stability and accuracy, and it may yield better discretization of the incompressible Navier–Stokes equations.

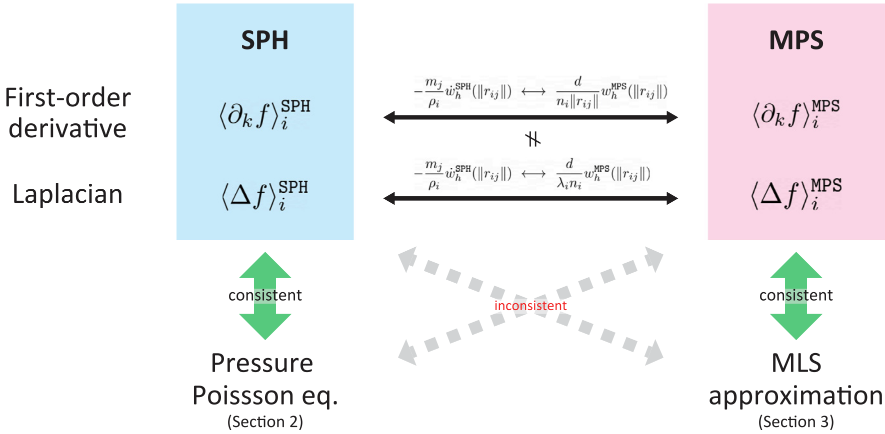

Fig. 2. Relationship and consistency between SPH and MPS operators.

5. Additional results for MPS operators

Considering the components of $\widetilde{D} f(x_i)$ in Theorem 3.1, we can derive the following second-order derivative operators:

Second-order partial derivative operators

- Regular derivative operator:

$$\langle \partial_k^2 f \rangle_i^{\mathtt{MPS}} := \frac{2d}{n_i\lambda_i - d^2\theta_i} \sum_{j\in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{[r_{ij}^{(k)}]^2}{\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|) - \frac{2d^2\theta_i}{n_i\lambda_i(n_i\lambda_i - d^2\theta_i)} \sum_{j\in \mathrm{NP}_i} f_{ij} w_h^{\mathtt{MPS}}(\|r_{ij}\|). \tag{26}$$

- Mixed derivative operator:

$$\langle \partial_k \partial_\ell f \rangle_i^{\mathtt{MPS}} := \frac{1}{\theta_i} \sum_{j\in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{r_{ij}^{(k)} r_{ij}^{(\ell)}}{\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|), \quad (k \neq \ell). \tag{27}$$

Notably, $\langle \partial_k^2 f \rangle_i^{\mathtt{MPS}}$ and $\langle \partial_k \partial_\ell f \rangle_i^{\mathtt{MPS}}$ consist of $(d+1)$th, $\dots$, $2d$th and $2d$th, $\dots$, $d(d+3)/2$th components of $\widetilde{D} f(x_i)$, respectively, under conditions (U1)–(U3). Therefore, we can comprehensively derive second-order partial derivative operators (26)–(27) and conventional operators (13)–(14) using the same procedure as Eq. (23).

The regular operator (26) is complex, unlike the mixed operator (27), which is simple. The regular derivative operator (26) contains the approximation term for the kth direction (first term) and a correction term independent of a specific direction (second term). This fact is consistent with that of the second-order derivative operators in the SPH method [25]. However, we note that these second-order MPS operators can never be derived from the SPH operators by transformation using existing knowledge, such as the replacements in Eqs. (24) and (25). The mixed derivative operator for a two-dimensional space was initially proposed and verified based on numerical results for an incompressible flow problem in our previous study [20].

Next, considering anisotropy (without condition (U3)), we introduce new MPS operators for anisotropic particle distributions. We recall $n_{i,k}$ defined in Eq. (21) and the $d \times d$ matrix Θ_i defined as $\Theta_i = (\theta_{i,k,\ell})$ $(k, \ell = 1, \dots, d)$, where $\theta_{i,k,\ell}$ is defined in Eq. (15). Then, we define the MPS operators for anisotropic particle distributions.

Anisotropic operators

- First-order derivative operator:

$$\langle \partial_k f \rangle_i^{\mathtt{Aniso}} := \frac{1}{n_{i,k}} \sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{r_{ij}^{(k)}}{\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|). \tag{28}$$

- Second-order derivative operator:

$$\langle \partial_k^2 f \rangle_i^{\mathtt{Aniso}} := \left[2\Theta_i^{-1} \sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{q_{ij}}{\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|) \right]^{(k)}, \tag{29}$$

where $q_{ij} := \{[r_{ij}^{(1)}]^2, \ldots, [r_{ij}^{(d)}]^2\}^{\mathtt{T}}$.

- Second-order mixed derivative operator:

$$\langle \partial_k \partial_\ell f \rangle_i^{\mathtt{Aniso}} := \frac{1}{\theta_{i,k,\ell}} \sum_{j \in \mathrm{NP}_i} \frac{f_{ij}}{\|r_{ij}\|} \frac{r_{ij}^{(k)} r_{ij}^{(\ell)}}{\|r_{ij}\|} w_h^{\mathtt{MPS}}(\|r_{ij}\|), \quad k \neq \ell. \tag{30}$$

- Laplacian operator:

$$\langle \Delta f \rangle_i^{\mathtt{Aniso}} := \sum_{k=1}^{d} \langle \partial_k^2 f \rangle_i^{\mathtt{Aniso}}. \tag{31}$$

The anisotropic operators can be derived by computing the inverse of the moment matrix represented by Eq. (20). The anisotropic operators (Eqs. (28) to (31)) are equal to the conventional and proposed operators (Eqs. (13), (14), (26), and (27)) under isotropic conditions (U1)–(U3).

Finally, we present the numerical results for the proposed MPS operators. First, we investigate the second-order partial derivative operators (26) and (27). We set the domain $\Omega = [0, 1] \times [0, 1]$. We consider the uniform and non-uniform particle distributions. We set the uniform distribution as the grid distribution with a spacing distance $\Delta x = 2^{-3}, 2^{-4}, 2^{-5}, 2^{-6}$ (Fig. 3a left) and generate the non-uniform particle distributions by adding a random perturbation that follows the uniform distribution $\mathcal{U}_{[-0.2\Delta x, 0.2\Delta x]}$ with a uniform distribution (Fig. 3b left). We compute the truncation error for the differential operator D based on the relative error

$$E_{\mathrm{D}} = \frac{1}{{}^{\#}\Lambda^{\mathtt{in}}} \sum_{i \in \Lambda^{\mathtt{in}}} \frac{\|\mathrm{D} f(x_i) - \langle \mathrm{D} f \rangle_i\|}{\max_{x \in \Omega} \|\mathrm{D} f(x)\|},$$

where $\Lambda^{\mathtt{in}} := \{j;\ x_j \in \Omega_h^{\mathtt{in}}\}$, ${}^{\#}\Lambda^{\mathtt{in}}$ denotes the number of particles in $\Omega_h^{\mathtt{in}}$, and $\langle \mathrm{D} f \rangle_i$ is the discrete operator of $\mathrm{D} f(x_i)$. We set f as $f(x) = \sin(x^{(1)} + 2x^{(2)})$ and $f(x) = \exp(x^{(1)} + 2x^{(2)})$. The proposed operators converge in the second order in the uniform case, but diverge in the non-uniform case, similar to the existing Laplace operator (Fig. 3). Since both the proposed and existing second-order MPS operators consist of the components of $\widetilde{D} f(x_i)$, their approximation processes are the same, as shown in Eq. (23). Therefore, this similarity can guarantee that the proposed operators are well defined. Although the truncation errors of proposed operators are not accurate for non-uniform distributions, they may be applicable for practical situations, similar to how the conventional MPS method is useful.

Next, we verify the proposed anisotropic operators (28) and (31) by comparing the isotropic operators (13) and (14) on the anisotropic particle distribution. We omit the verification of the mixed derivative operator (30) because it is equal to the isotropic operator (27) in the case of a two-dimensional space. We used the same methods as previously described for domain Ω, function f, and relative error E_{D}. We created an anisotropic particle distribution by generating particles with a half-spacing distance for the first axis (Fig. 4a). We can observe better accuracy and convergence of the anisotropic operators than the conventional operators (Fig. 4b and c)

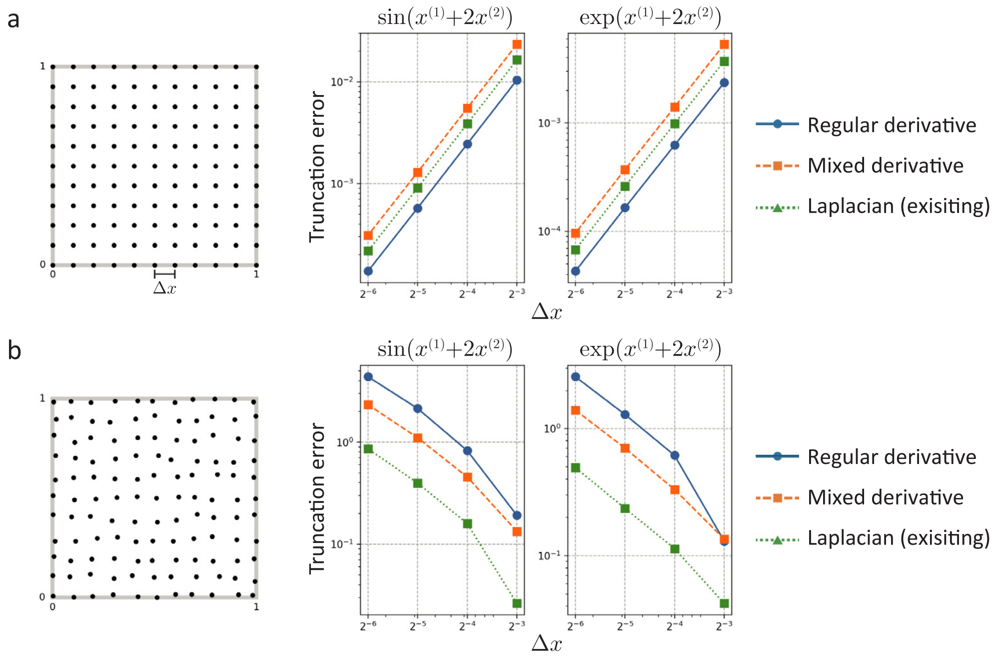

Fig. 3. Particle distributions and truncation errors for the second-order derivative operators: regular derivative (26), mixed derivative (27), and existing Laplacian operators (14). a, Uniform distribution case; b, non-uniform distribution case. The particle distributions are shown for case $\Delta x = 0.1$.

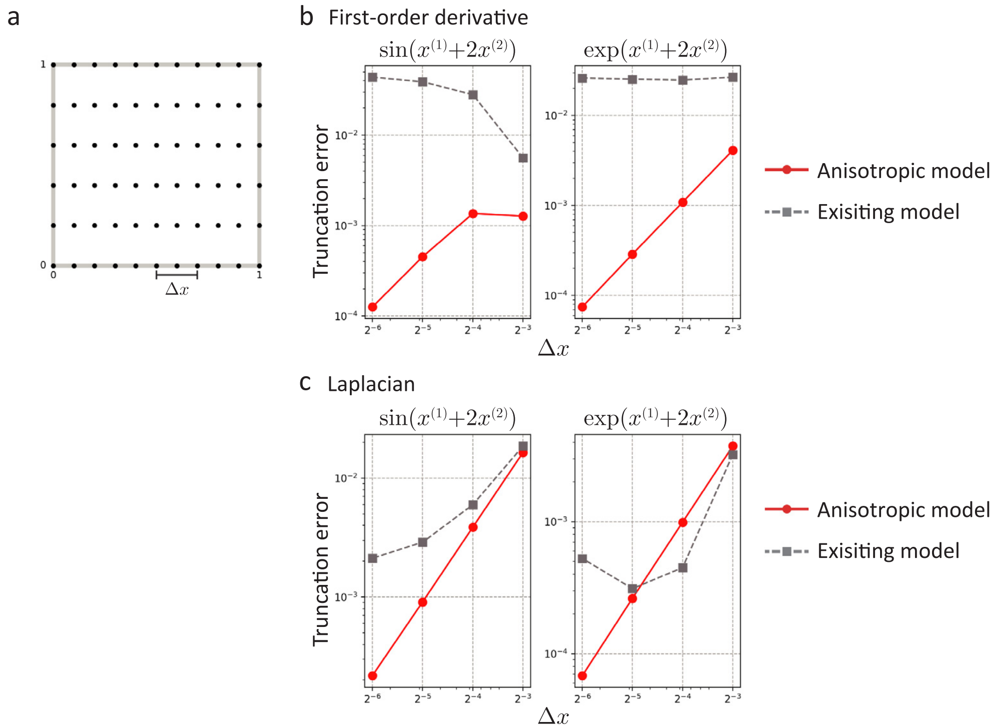

Fig. 4. Particle distribution and truncation errors for the anisotropic operators (28) and (31) and existing operators (13) and (14). a, Anisotropic particle distribution with $\Delta x = 0.1$; b, truncation errors for first-order derivative operators (28) and (13); c, truncation errors for Laplacian operators (31) and (14).

6. Conclusion

We have investigated the difference between SPH and MPS operators via a comprehensive derivation of each method's first- and second-order operators. First, we have derived the SPH operators using the pressure Poisson equation and integration approximation. Next, we have derived the MPS operators using the Taylor expansion and polynomial basis. Further, we have clarified that the MPS derivation is equal to an MLS approximation with an appropriate basis. From the different derivations, we have concluded that the difference between the SPH and MPS operators is the targets (the pressure Poisson equation or MLS approximation) that their first- and second-order operators are consistent with (Fig. 2). Furthermore, we have confirmed that the consistency of the SPH method has advanced the numerical and theoretical stability analyses of incompressible flow problems. In addition, we have proposed novel second-order derivative and anisotropic operators from the comprehensive derivation of the conventional MPS operators. Finally, we have verified these operators through numerical truncation error analysis and have confirmed that they had equal or greater accuracy than the conventional MPS operators.

We expect that this study will help in the development of a theoretical analysis of the SPH and MPS methods or help in the selection of the appropriate method by users. Furthermore, the new MPS operators can contribute to the development of methods with adaptive or multiscale particle distributions. However, this study cannot guarantee the stability or accuracy of practical computations using the SPH and MPS methods. In the future, we will enhance the theoretical study of the SPH and MPS methods by focusing on aspects such as convergence and stability, to inspire confidence in their numerical results.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Yusuke Imoto reports financial support was provided by JSPS KAKENHI and JST PREST.

Acknowledgments

This work was supported by JSPS, Japan KAKENHI [grant number 17K17585] and JST, Japan PREST [grant number JPMJPR2021].

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