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DEVELOPMENT OF LEAST SQUARES MOVING PARTICLE SEMI-IMPLICIT METHOD

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Abstract. In this paper, with focusing particular attention on a major issue — the lack of consistency conditions on the spatial discretization schemes of the existing MPS method, we develop a new meshfree particle method named *Least Squares Moving Particle Semi-implicit/Simulation* (LSMPS) method. The new schemes have arbitraly higher order consistency conditions, make treatment of boundary conditions exceedingly easy, and can be applied for both Eulerian and Lagrangian framework. Moreover, applications of the new schemes for numerical analysis of incompressible flows with the free surfaces result in enhancement of numerical accuracy and stability.

1 INTRODUCTION

Recently, meshfree particle methods have been receiving a lot of interest in computational mechanics. The MPS (Moving Particle Semi-implicit, or Moving Particle Simulation) method[1] for numerical analysis of incompressible flows with the free surfaces has been shown useful in engineering applications widly. With expanding the techniques of the MPS method, analysis of compressible flows, weakly compressible flows with fully explicit algorithm, and of structural dynamics achieved successful outcomes; however, numerical discretization schemes of the existing MPS method have a major issue — the lack of consistency conditions, which results in contradictory effects for computational accuracy and stability.

With taking particular note of this matter, we develop a new *consistent* meshfree particle method, named *Least Squares Moving Particle Semi-implicit/Simulation* (LSMPS) method. As its name suggests, new spatial discretization schemes are derived based on the weighted Least Squares method, and have arbitrary higher order consistency conditions.

The new schemes can be applied for methods with collocation points (scattered points) in both Eulerian and Lagrangian frameworks, without grid or mesh.

By the way, as a common problem in strong-form meshfree particle methods including the MPS method and the SPH (Smoothed Particle Hydrodynamics) method[2], treatment of boundary conditions, especially in enforcing the Neumann boundary condition is difficult. In order to overcome this difficulty, new schemes (named Generalized LSMPS schemes) based on the *locally Hermite interoperation* technique and weighted least squares method are also developed. In calculation of spatial derivatives, Generalized LSMPS schemes use not only the values of a function but also their derivatives up to a certain degree of order; therefore, with using the values of a function and their first order derivatives, Generalized LSMPS schemes make the treatment of Neumann boundary condition easy. In other words, they can enforce Neumann boundary conditions simply, on the second order partial differential equations like Pressure Poisson equations. Moreover, Generalized LSMPS schemes can be used as the *Meshfree Compact scheme* like the compact schemes used in FDM[3], and provide extra higher-order accuracy.

In this paper, we introduce the new schemes, and test their accuracy and convergence rate in comparison with the Moving Least Squares(MLS) method[4] and the Reproducing Kernel Particle method(RKPM)[5]. Additionally, application of the LSMPS method for numerical analysis of incompressible flows with the free surfaces shows improvement of numerical accuracy and stability compared with the existing MPS method.

2 THE LSMPS METHOD

In this section, spatial discretization schemes of the existing MPS method and the LSMPS method, and time marching algorithm for the LSMPS method are described.

2.1 The existing MPS method

The MPS(Moving Particle Semi-implicit) method[1] is developed by Koshizuka and Oka for numerical analysis of incompressible flow with the free surfaces. Let $\phi(\mathbf{x})$ and $\mathbf{u}(\mathbf{x})$ be sufficiently smooth functions defined on a domain $\Omega \subset (\mathbb{R}^d, \|\cdot\|)$, where d is the number of dimension. Formulations of the spacial discretization schemes on each particle $\mathbf{x}_i$ are the following,

$$\langle \nabla \phi \rangle_{\mathbf{x}_i} = \frac{d}{n^0} \sum_{\Omega_i} \left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e} \right) \frac{\mathbf{x}_j - \mathbf{x}_i}{\|\mathbf{x}_j - \mathbf{x}_i\|} \frac{\phi_j - \phi_i}{\|\mathbf{x}_j - \mathbf{x}_i\|} \right], \tag{1}$$

$$\left\langle \nabla^2 \phi \right\rangle_{\mathbf{x}_i} = \frac{2d}{\lambda^0 n^0} \sum_{\Omega_i} \left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e} \right) (\phi_j - \phi_i) \right], \tag{2}$$

$$\langle \nabla \cdot \mathbf{u} \rangle_{\mathbf{x}_i} = \frac{d}{n^0} \sum_{\Omega_i} \left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e} \right) \frac{\mathbf{x}_j - \mathbf{x}_i}{\|\mathbf{x}_j - \mathbf{x}_i\|} \cdot \frac{\mathbf{u}_j - \mathbf{u}_i}{\|\mathbf{x}_j - \mathbf{x}_i\|} \right], \tag{3}$$

where $w(\|\cdot\|;r_e):\mathbb{R}_+\to\mathbb{R}_+$ is the weight function with support, r_e is the dilation parameter, n^0 and λ^0 are the normalization parameters, and the set of neighboring particles Ω_i is defined as

$$\Omega_i := \left\{ j \;\middle|\; \mathbf{x}_j \in \mathrm{supp}(w_i)\cap\Omega\ ,\ \mathbf{x}_j \neq \mathbf{x}_i \right\},\quad \mathrm{supp}(w_i) := \left\{ \mathbf{x}\in\mathbb{R}^d \;\middle|\; \frac{\|\mathbf{x}-\mathbf{x}_i\|}{r_e} < 1 \right\}. \quad (4)$$

The schemes(eq.(1),(2),(3)) have second order consistency condition (accuracy) if and only if the set $\{\mathbf{x}_i\}_{1\le i\le N}$ constructs a lattice with some symmetry; therefore, they are *inconsistent* schemes generally. In other words, if the particles $\mathbf{x}_i$ are randomly distributed, or, they are on or near the boundaries, the schemes of existing MPS method do not have any consistency condition. Actually, their accuracy become 0-th order or less[6]. To solve this major issue, in the next subsection, LSMPS method is developed.

2.2 The LSMPS method

2.2.1 Stone-Weierstrass theorem of locally compact version

Let $f:\mathbb{R}^d\to\mathbb{R}$ be a sufficiently smooth function (at least $f(\mathbf{x})\in C^0(\bar{\Omega})$) that is defined on a simply connected open set $\Omega\in\mathbb{R}^d$. According to the Stone-Weierstrass theorem of locally compact version, for a fixed point $\bar{\mathbf{x}}\in\bar{\Omega}$, one should always be able to approximate $f(\mathbf{x})$ by a polynomial series locally. Thus, we can define a local function and the open sphere

$$f^l(\mathbf{x},\bar{\mathbf{x}}) := \begin{cases} f(\mathbf{x}) & {}^\forall\mathbf{x}\in\mathbf{B}(\bar{\mathbf{x}}),\\ 0 & \text{otherwise.}\end{cases} \quad (5)$$

$$\mathbf{B}(\bar{\mathbf{x}}) := \left\{\mathbf{x}\in\bar{\Omega} \mid \|\mathbf{x}-\bar{\mathbf{x}}\| < r_e\right\}. \quad (6)$$

If the function $f(\mathbf{x})$ is smooth enough as assumed, there exists a local operator $L_{\bar{\mathbf{x}}}: C^0(\mathbf{B}(\bar{\mathbf{x}}))\mapsto C^p(\mathbf{B}(\bar{\mathbf{x}}))$, s.t.

$$f^l(\mathbf{x},\bar{\mathbf{x}}) \approx L_{\bar{\mathbf{x}}}f(\mathbf{x}) = \mathbf{q}^T(\mathbf{x})\mathbf{a}(\bar{\mathbf{x}}), \quad (7)$$

where $\mathbf{q}(\mathbf{x}) = \{\mathbf{x}^{\boldsymbol{\alpha}} \mid 0\le|\boldsymbol{\alpha}|\le p\}$ is p-th order polynomial basis, and $\mathbf{a}(\bar{\mathbf{x}})$ is coefficient vector. With using Taylor expansion , we can denote the locally approximated function $L_{\bar{\mathbf{x}}}f(\mathbf{x})$ with given values such as $\mathbf{x}_i,\mathbf{x}_j,f(\mathbf{x}_i),f(\mathbf{x}_j)$, and unknowns such as Fréchet derivative $D^{\boldsymbol{\alpha}}_{\mathbf{x}}f(\cdot)$ and error of approximation R^{p+1}_{ij},

$$\sum_{|\boldsymbol{\alpha}|=1}^{p}\left[\frac{1}{\boldsymbol{\alpha}!}\left(\mathbf{x}_j-\mathbf{x}_i\right)^{\boldsymbol{\alpha}} D^{\boldsymbol{\alpha}}_{\bar{\mathbf{x}}}f^h(\mathbf{x}_i)\right] - \{f(\mathbf{x}_j)-f(\mathbf{x}_i)\} = R^{p+1}_{ij}\big(= L_{\bar{\mathbf{x}}}f(\mathbf{x}) - f^l(\mathbf{x})\big), \quad (8)$$

where $\boldsymbol{\alpha} = (\alpha_1,\cdots,\alpha_d)$ is an d-tuple non-negative integers, called multi-index. Throughout this paper, Taylor expansions of locally approximated function(eq.(8)) according to the Stone-Weierstrass theorem and multi-index notation are used without note again.

2.2.2 LSMPS scheme (Standard type)

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a sufficiently smooth function that is defined on a simply connected open set $\Omega \in \mathbb{R}^d$. Standard type spatial discretization schemes for each calculation point(particle) $\mathbf{x}_i$ are defined as the following.

Definition 2.1. (*Standard LSMPS scheme*)

$$\mathbf{D}_{\mathbf{x}} f^h(\mathbf{x}_i) := H_{r_s}\left[\mathbf{M}_i^{-1}\mathbf{b}_i\right] \tag{9}$$

where

$$\mathbf{D}_{\mathbf{x}} := \left\{D_{\mathbf{x}}^{\boldsymbol{\alpha}} \mid 1 \le |\boldsymbol{\alpha}| \le p\right\}, \tag{10}$$

$$H_{r_s} := \mathrm{diag}\left\{\left\{{r_s}^{-|\boldsymbol{\alpha}|}\boldsymbol{\alpha}!\right\}_{1\le|\boldsymbol{\alpha}|\le p}\right\}, \tag{11}$$

$$\mathbf{M}_i := \sum_{\Omega_i}\left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e}\right)\mathbf{p}\left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s}\right)\mathbf{p}^T\left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s}\right)\right], \tag{12}$$

$$\mathbf{b}_i := \sum_{\Omega_i}\left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e}\right)\mathbf{p}\left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s}\right)\left\{f(\mathbf{x}_j) - f(\mathbf{x}_i)\right\}\right], \tag{13}$$

$$\mathbf{p}(\mathbf{x}) := \left\{\mathbf{x}^{\boldsymbol{\alpha}} \mid 1 \le |\boldsymbol{\alpha}| \le p\right\}, \tag{14}$$

r_e : dilation parameter $(0 < r_e)$, r_s : scaling parameter $(0 < r_s < r_e)$.

Derivation: With locally approximated function and its denotation described in subsection 2.2.1., we can obtain

$$\sum_{|\boldsymbol{\alpha}|=1}^{p}\left[\frac{1}{\boldsymbol{\alpha}!}\left(\mathbf{x}_j - \mathbf{x}_i\right)^{\boldsymbol{\alpha}} D_{\mathbf{x}}^{\boldsymbol{\alpha}} f^h(\mathbf{x}_i)\right] - \left\{f(\mathbf{x}_j) - f(\mathbf{x}_i)\right\} = R_{ij}^{p+1}, \tag{15}$$

and by using scaling parameter r_s, eq.(15) can be rewritten as

$$\sum_{|\boldsymbol{\alpha}|=1}^{p}\left[\left\{\frac{\left(\mathbf{x}_j - \mathbf{x}_i\right)^{\boldsymbol{\alpha}}}{r_s^{|\boldsymbol{\alpha}|}}\right\}\left\{\frac{r_s^{|\boldsymbol{\alpha}|}}{\boldsymbol{\alpha}!}D_{\mathbf{x}}^{\boldsymbol{\alpha}} f^h(\mathbf{x}_i)\right\}\right] - \left\{f(\mathbf{x}_j) - f(\mathbf{x}_i)\right\} = R_{ij}^{p+1}, \tag{16}$$

i.e.

$$\mathbf{p}^T\left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s}\right)\left[H_{r_s}^{-1}\mathbf{D}_{\mathbf{x}} f^h(\mathbf{x}_i)\right] - \left\{f(\mathbf{x}_j) - f(\mathbf{x}_i)\right\} = R_{ij}^{p+1}. \tag{17}$$

If we define functional J associated with residual R_{ij}^{p+1} and the weight function w by

$$J(H_{r_s}^{-1}\mathbf{D}_{\mathbf{x}} f^h(\mathbf{x}_i)) := \sum_{\Omega_i}\left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e}\right)\left(R_{ij}^{p+1}\right)^2\right], \tag{18}$$

and by minimizing the quadratic functional J with the weighted least squares method, one can obtain normal equations (Linear system) $\mathbf{M}_i\left[H_{r_s}^{-1}\mathbf{D}_{\bar{\mathbf{x}}}f^h(\mathbf{x}_i)\right]=\mathbf{b}_i$. If and only if $\mathrm{rank}(\mathbf{M}_i)=-1+\frac{1}{d!}\prod_{k=1}^{d}(p+k)$, normal equations have a unique solution s.t.

$$\mathbf{D}_{\mathbf{x}}f^h(\mathbf{x}_i):=H_{r_s}\left[\mathbf{M}_i^{-1}\mathbf{b}_i\right]. \tag{19}$$

$\blacksquare$.

Remark 2.2. It is so important to introduce the scaling parameter r_s. Without scaling for basis $\mathbf{p}$, the moment matrix $\mathbf{M}$ becomes ill-conditioned, which creates an adverse effects both numerical accuracy and stability. To avoid this problem, the Moving Least Squares Reproducing Kernel Particle Method(MLSRKPM)[5] also introduce scaling for basis; however, in the MLSRKPM, dilation parameter $r_e=\varrho$ is used for scaling, on the other hand, in the LSMPS method, scaling parameter r_s is kept to be smaller than dilation parameter r_e. This difference yields smaller condition number of moment matrices which provides more improvement of accuracy and stability.

Theorem 2.3. Let $\mathbf{M}_{r_s}$ be the moment matrix with scaling, and $\mathbf{M}$ be the one without scaling. One can obtain about determinant of the moment matrices,

$$\frac{\det(\mathbf{M}_{r_s})}{\det(\mathbf{M})}\approx {r_s}^{-2d\binom{p+d}{d+1}}, \tag{20}$$

and one can obtain about the condition number of them,

$$\frac{\mathrm{cond}(\mathbf{M}_{r_s})}{\mathrm{cond}(\mathbf{M})}\le {r_s}^{2p}. \tag{21}$$

Remark 2.4. The MLS or the MLSRKPM is suitable for construction of shape functions for weak-form formulations, but is unsuited for calculation of spatial derivatives for strong-form formulations; since the calculation of shape function's derivatives requires high computational costs. On the other hand, the LSMPS schemes can calculate derivatives directly. Moreover, the dimension of moment matrix in the LSMPS is just one smaller than the one in the MLS and the MLSRKPM. These differences bring in advantage of computational costs for strong-form formulations.

Definition 2.5. Let $\mathbf{X}:=\{\mathbf{x}_i\}_{1\le i\le N}$ be the set of particles on the domain $\Omega\subset\mathbb{R}^d$, closed ball $\bar{B}(\mathbf{x},r):=\left\{\mathbf{x}'\in\mathbb{R}^d \mid \|\mathbf{x}-\mathbf{x}'\|\le r\right\}$, fill distance $h_{\mathbf{x},\Omega}:=\sup_{\mathbf{x}\in\Omega}\min_{1\le i\le N}\|\mathbf{x}-\mathbf{x}_i\|$, separation distance $\eta_{\mathbf{x}}:=\frac{1}{2}\min_{j\ne i}\|\mathbf{x}_j-\mathbf{x}_i\|$, and $N_{\min}:=\mathrm{card}\left\{\mathbf{x}^{\boldsymbol{\alpha}}\ \middle|\ 1\le|\boldsymbol{\alpha}|\le p\right\}$. An admissible particle distribution for the standard LSMPS schemes is defined as

$$\Omega\subset\bigcup_{i=1}^{N}\bar{B}(\mathbf{x}_i,h_{\mathbf{x},\Omega}/2), \tag{22}$$

$$N_{\min}\le\mathrm{card}\left\{j\ \middle|\ \mathbf{x}_j\in\bar{B}(\mathbf{x}_i,ch_{\mathbf{x},\Omega})\right\}, c\ge 1, {}^{\forall} i, \tag{23}$$

$${}^{\exists}\delta>0\ \text{ s.t. }\ \eta_{\mathbf{x}}\le h_{\mathbf{x},\Omega}\le\delta\eta_{\mathbf{x}}. \tag{24}$$

Theorem 2.6. Assume $f(\mathbf{x}) \in C^{p+1}(\Omega)$, where $\Omega \subset \mathbb{R}^d$ is a bounded open set, there exists a constant $0 < C_1 < \infty$ and the Standard LSMPS schemes have the following error bounds

$$|D_{\mathbf{x}}^{\boldsymbol{\alpha}} f(\mathbf{x}) - D_{\mathbf{x}}^{\boldsymbol{\alpha}} f^h(\mathbf{x})| \le C_1 r_e^{p+1-|\boldsymbol{\alpha}|} |f(\mathbf{x})|_{C^{p+1}(\Omega)} \tag{25}$$

2.2.3 Generalized LSMPS scheme type-1

Definition 2.7. (*Generalized LSMPS scheme type*-1)

$$\mathbf{D}_{\mathbf{x}} f^h(\mathbf{x}_i) := H_{r_s} \left[\mathbf{M}_i^{-1} \mathbf{b}_i \right] \tag{26}$$

where

$$\mathbf{D}_{\mathbf{x}} := \left\{ D_{\mathbf{x}}^{\boldsymbol{\alpha}} \mid 1 \le |\boldsymbol{\alpha}| \le p \right\}, \tag{27}$$

$$H_{r_s} := \mathrm{diag} \left\{ \left\{ {r_s}^{-|\boldsymbol{\alpha}|} \boldsymbol{\alpha}! \right\}_{1 \le |\boldsymbol{\alpha}| \le p} \right\}, \tag{28}$$

$$\mathbf{M}_i' := \sum_{|\boldsymbol{\beta}|=0}^{q} \sum_{\Omega_i} \left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e} \right) \frac{r_s^{|\boldsymbol{\beta}|}}{\boldsymbol{\beta}!} D_{\mathbf{x}}^{\boldsymbol{\beta}} \mathbf{p} \left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) \frac{r_s^{|\boldsymbol{\beta}|}}{\boldsymbol{\beta}!} D_{\mathbf{x}}^{\boldsymbol{\beta}} \mathbf{p}^T \left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) \right], \tag{29}$$

$$\mathbf{b}_i' := \sum_{|\boldsymbol{\beta}|=0}^{q} \sum_{\Omega_i} \left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e} \right) \frac{r_s^{|\boldsymbol{\beta}|}}{\boldsymbol{\beta}!} D_{\mathbf{x}}^{\boldsymbol{\beta}} \mathbf{p} \left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) \left[D_{\mathbf{x}}^{\boldsymbol{\beta}} f(\mathbf{x}_j) - D_{\mathbf{x}}^{\boldsymbol{\beta}} f(\mathbf{x}_i) \right] \right], \tag{30}$$

$$\mathbf{p}(\mathbf{x}) := \left\{ \mathbf{x}^{\boldsymbol{\alpha}} \mid 1 \le |\boldsymbol{\alpha}| \le p \right\}, \tag{31}$$

r_e : dilation parameter $(0 < r_e)$, r_s : scaling parameter $(0 < r_s < r_e)$.

Derivation: With locally approximated function $L_{\bar{\mathbf{x}}} f(\mathbf{x})$ described in subsection 2.2.1., and with its derivatives $D_{\mathbf{x}}^{\boldsymbol{\beta}} L_{\bar{\mathbf{x}}} f(\mathbf{x}), 0 \le |\boldsymbol{\beta}| \le q \le p$, we can obtain

$$\sum_{|\boldsymbol{\alpha}|=1}^{p-|\boldsymbol{\beta}|} \left[\frac{1}{\boldsymbol{\alpha}!} (\mathbf{x}_j - \mathbf{x}_i)^{\boldsymbol{\alpha}} D_{\mathbf{x}}^{\boldsymbol{\alpha}} D_{\mathbf{x}}^{\boldsymbol{\beta}} f^h(\mathbf{x}_i) \right] - \left\{ D_{\mathbf{x}}^{\boldsymbol{\beta}} f(\mathbf{x}_j) - D_{\mathbf{x}}^{\boldsymbol{\beta}} f(\mathbf{x}_i) \right\} = R_{ij,\boldsymbol{\beta}}^{p+1}. \tag{32}$$

By taking sum of multi-index $\boldsymbol{\beta} : 0 \le |\boldsymbol{\beta}| \le q$ for eq.(32),

$$\sum_{|\boldsymbol{\beta}|=0}^{q} \left[\frac{r_s^{|\boldsymbol{\beta}|}}{\boldsymbol{\beta}!} D_{\mathbf{x}}^{\boldsymbol{\beta}} \mathbf{p}^T \left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) \left[H_{r_s}^{-1} \mathbf{D}_{\mathbf{x}} f^h(\mathbf{x}_i) \right] \right] - \sum_{|\boldsymbol{\beta}|=0}^{q} \left[D_{\mathbf{x}}^{\boldsymbol{\beta}} f(\mathbf{x}_j) - D_{\mathbf{x}}^{\boldsymbol{\beta}} f(\mathbf{x}_i) \right] = \sum_{|\boldsymbol{\beta}|=0}^{q} R_{ij,\boldsymbol{\beta}}^{p+1}. \tag{33}$$

If we define functional J' associated with residual $R_{ij,\boldsymbol{\beta}}^{p+1}$ and the weight function w

$$J'(H_{r_s}^{-1} \mathbf{D}_{\mathbf{x}} f^h(\mathbf{x}_i)) := \sum_{|\boldsymbol{\beta}|=0}^{q} \sum_{j \in \Omega_i} \left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e} \right) \left(R_{ij,\boldsymbol{\beta}}^{p+1} \right)^2 \right], \tag{34}$$

and by minimizing the quadratic functional J' with the weighted least squares method, one can obtain the normal equations (Linear system) $\mathbf{M}'_i \left[H_{r_s}^{-1} \mathbf{D}_{\bar{\mathbf{x}}} f^h(\mathbf{x}_i) \right] = \mathbf{b}_i$. If and only if $\mathrm{rank}(\mathbf{M}'_i) = -1 + \frac{1}{d!} \prod_{k=1}^{d} (p+k)$, the normal equations have a unique solution s.t.

$$\mathbf{D}_{\mathbf{x}} f^h(\mathbf{x}_i) := H_{r_s} \left[\mathbf{M}_i'^{-1} \mathbf{b}_i \right]. \tag{35}$$

$\blacksquare$.

Theorem 2.8. Assume $f(\mathbf{x}) \in C^{p+1}(\Omega)$, where $\Omega \subset \mathbb{R}^d$ is a bounded open set, there exists a constant $0 < C_2 < \infty$ and the Generalized LSMPS schemes type-1 have the following error bounds

$$|D_{\mathbf{x}}^{\boldsymbol{\alpha}} f(\mathbf{x}) - D_{\mathbf{x}}^{\boldsymbol{\alpha}} f^h(\mathbf{x})| \leq C_2 r_e^{p+1-|\boldsymbol{\alpha}|} |f(\mathbf{x})|_{C^{p+1}(\Omega)}. \tag{36}$$

Remark 2.9. Linear independence of the basis $D_{\mathbf{x}}^{\boldsymbol{\beta}} \mathbf{p}(\mathbf{x}), 0 \leq |\boldsymbol{\beta}| \leq q$ relieves the requirement of the large number of particles to invert the moment matrix, i.e. the smaller dilation parameter can be used for Generalized LSMPS schemes type-1 than the one of the Standard schemes.

2.2.4 Generalized LSMPS scheme type-2

Definition 2.10. (*Generalized LSMPS scheme type-2*)

$$\mathbf{D}_{\mathbf{x}} f^h(\mathbf{x}_i) := H'_{r_s} \left[\mathbf{M}_i^{-1} \mathbf{b}''_i \right] \tag{37}$$

where

$$\mathbf{D}_{\mathbf{x}} := \left\{ D_{\mathbf{x}}^{\boldsymbol{\alpha}} \mid 1 \leq |\boldsymbol{\alpha}| \leq p \right\}, \tag{38}$$

$$H'_{r_s} := \mathrm{diag} \left\{ \left\{ \sum_{\substack{\boldsymbol{\beta}:\ 0 \leq |\boldsymbol{\beta}| \leq q \\ \boldsymbol{\beta} \leq \boldsymbol{\alpha},\ \boldsymbol{\beta} \neq \boldsymbol{\alpha}}} C(\boldsymbol{\beta}, p, q) {r_s}^{-|\boldsymbol{\alpha}|} (\boldsymbol{\alpha} - \boldsymbol{\beta})! \right\}_{1 \leq |\boldsymbol{\alpha}| \leq p} \right\}, \tag{39}$$

$$\mathbf{M}_i := \sum_{j \in \Omega_i} \left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e} \right) \mathbf{p}\left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) \mathbf{p}^T \left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) \right], \tag{40}$$

$$\mathbf{b}''_i := \sum_{|\boldsymbol{\beta}|=0}^{q} \sum_{\Omega_i} \left[w\left(\frac{\|\mathbf{x}_j - \mathbf{x}_i\|}{r_e} \right) \mathbf{p}\left(\frac{\mathbf{x}_j - \mathbf{x}_i}{r_s} \right) \right.$$
$$\left. \times C(\boldsymbol{\beta}, p, q) (\mathbf{x}_j - \mathbf{x}_i)^{\boldsymbol{\beta}} \left[D_{\mathbf{x}}^{\boldsymbol{\beta}} f(\mathbf{x}_j) - D_{\mathbf{x}}^{\boldsymbol{\beta}} f(\mathbf{x}_i) \right] \right], \tag{41}$$

$$\mathbf{p}(\mathbf{x}) := \left\{ \mathbf{x}^{\boldsymbol{\alpha}} \mid 1 \leq |\boldsymbol{\alpha}| \leq p \right\}, \tag{42}$$

r_e : dilation parameter $(0 < r_e)$, r_s : scaling parameter $(0 < r_s < r_e)$.

$$C(\boldsymbol{\beta},p,q)=\begin{cases}(-1)^{|\boldsymbol{\beta}|}\dfrac{|\boldsymbol{\beta}|!}{\boldsymbol{\beta}!}\dfrac{p!}{(p+q)!} & (|\boldsymbol{\beta}|=q)\\ (-1)^{|\boldsymbol{\beta}|}\dfrac{|\boldsymbol{\beta}|!}{\boldsymbol{\beta}!}\dfrac{q(p+q-|\boldsymbol{\beta}|)!}{(p+q!)} & (0<|\boldsymbol{\beta}|<q)\\ 1 & (|\boldsymbol{\beta}|=0)\end{cases} \tag{43}$$

Derivation: With $(p+q)$-th order locally approximated function $L_{\bar{\mathbf{x}}}f(\mathbf{x})$ and its denotation described in subsection 2.2.1., we can obtain

$$\sum_{|\boldsymbol{\alpha}|=1}^{p}\left[\frac{1}{\boldsymbol{\alpha}!}(\mathbf{x}_j-\mathbf{x}_i)^{\boldsymbol{\alpha}}D_{\mathbf{x}}^{\boldsymbol{\alpha}}f^h(\mathbf{x}_i)\right]+\sum_{|\boldsymbol{\alpha}|=p+1}^{p+q}\left[\frac{1}{\boldsymbol{\alpha}!}(\mathbf{x}_j-\mathbf{x}_i)^{\boldsymbol{\alpha}}D_{\mathbf{x}}^{\boldsymbol{\alpha}}f^h(\mathbf{x}_i)\right] \\ -\{f(\mathbf{x}_j)-f(\mathbf{x}_i)\}=R_{ij,\boldsymbol{\beta}=\mathbf{0}}^{p+q+1}, \tag{44}$$

and its derivatives $D_{\mathbf{x}}^{\boldsymbol{\beta}}L_{\bar{\mathbf{x}}}f(\mathbf{x})$ $(0\le|\boldsymbol{\beta}|\le q<p)$,

$$\sum_{|\boldsymbol{\alpha}|=1}^{p-|\boldsymbol{\beta}|}\left[\frac{1}{\boldsymbol{\alpha}!}(\mathbf{x}_j-\mathbf{x}_i)^{\boldsymbol{\alpha}}D_{\mathbf{x}}^{\boldsymbol{\alpha}}D_{\mathbf{x}}^{\boldsymbol{\beta}}f^h(\mathbf{x}_i)\right]-\{D_{\mathbf{x}}^{\boldsymbol{\beta}}f(\mathbf{x}_j)-D_{\mathbf{x}}^{\boldsymbol{\beta}}f(\mathbf{x}_i)\}=R_{ij,\boldsymbol{\beta}}^{p+1}. \tag{45}$$

The second sum terms (sum of $\boldsymbol{\alpha}: p+1\le|\boldsymbol{\alpha}|\le p+q$) in eq.(44) can be eliminated by $C(\boldsymbol{\beta},p,q)(\mathbf{x}_j-\mathbf{x}_i)^{\boldsymbol{\beta}}\times$ eq.(45), i.e. taking sum of eq.(44) and eq.(45) with multi-index $\boldsymbol{\beta}: 0\le|\boldsymbol{\beta}|\le q$ yields

$$\sum_{|\boldsymbol{\beta}|=0}^{q}\left[\mathbf{p}^T\left(\frac{\mathbf{x}_j-\mathbf{x}_i}{r_s}\right)\left[H_{r_s}^{\prime -1}\mathbf{D}_{\mathbf{x}}f^h(\mathbf{x}_i)\right]\right] \\ -\sum_{|\boldsymbol{\beta}|=0}^{q}\left[C(\boldsymbol{\beta},p,q)(\mathbf{x}_j-\mathbf{x}_i)^{\boldsymbol{\beta}}\left\{D_{\mathbf{x}}^{\boldsymbol{\beta}}f(\mathbf{x}_j)-D_{\mathbf{x}}^{\boldsymbol{\beta}}f(\mathbf{x}_i)\right\}\right]=\sum_{|\boldsymbol{\beta}|=0}^{q}R_{ij,\boldsymbol{\beta}}^{p+q+1}. \tag{46}$$

By using the weighted least squares method, similar to the Standard schemes and Generalized LSMPS schemes type-1, we can obtain the normal equations and their solutions

$$\mathbf{D}_{\mathbf{x}}f^h(\mathbf{x}_i):=H'_{r_s}\left[\mathbf{M}_i^{-1}\mathbf{b}''_i\right]. \tag{47}$$

$\blacksquare$.

Theorem 2.11. Assume $f(\mathbf{x})\in C^{p+q+1}(\Omega)$, where $\Omega\subset\mathbb{R}^d$ is a bounded open set, there exists a constant $0<C_3<\infty$ and the Generalized LSMPS schemes type-2 have the following error bounds

$$|D_{\mathbf{x}}^{\boldsymbol{\alpha}}f(\mathbf{x})-D_{\mathbf{x}}^{\boldsymbol{\alpha}}f^h(\mathbf{x})|\le C_3 r_e^{p+q+1-|\boldsymbol{\alpha}|}|f(\mathbf{x})|_{C^{p+q+1}(\Omega)}. \tag{48}$$

Remark 2.12. The rational coefficient $C(\boldsymbol{\beta}, p, q)$ contributes achievement of the extra higher order consistency conditions for the Generalized LSMPS schemes type-2. Moreover, with regarding the schemes as implicit formulations, they can be used as *Meshless Compact Schemes.*

2.2.5 Time marching

In the LSMPS method for numerical analysis of incompressible flows, the following pressure-correction schemes[7] with s-th order backorder difference formula, based on the projection method are applied.

$$\frac{1}{\Delta t}\left(\beta_s\tilde{\mathbf{u}}^{k+1} - \sum_{j=0}^{s-1}\beta_j\mathbf{u}^{k-j}\right) = \nu\nabla^2\tilde{\mathbf{u}}^{k+1} - \nabla p^\star + f^k, \quad \tilde{\mathbf{u}}^{k+1}|_{\Gamma_N} = 0, \tag{49}$$

$$\frac{\beta_s}{\Delta t}\left(\mathbf{u}^{k+1} - \tilde{\mathbf{u}}^{k+1}\right) + \nabla\phi^{k+1} = 0, \quad \nabla\cdot\mathbf{u}^{k+1} = 0, \quad \mathbf{u}^{k+1}\cdot\mathbf{n}|_{\Gamma_N} = 0. \tag{50}$$

where ϕ^{k+1} is the modified pressure defined by

$$\phi^{k+1} = p^{k+1} - p^\star + \nu\nabla\cdot\tilde{\mathbf{u}}^{k+1}, \tag{51}$$

and $p^\star$ is the r-th order extrapolated pressure defined by

$$p^\star = \sum_{j=0}^{r-1}\gamma_j p^{k-j}, \tag{52}$$

in particular,

$$p^\star = \begin{cases} 0 & (r=0), \\ p^k & (r=1), \\ 2p^k - p^{k-1} & (r=2). \end{cases} \tag{53}$$

Also, we tested $(s,r) = (1,0), (1,1), (2,0), (2,1)$ and confirmed their stability.

Remark 2.13. This time marching scheme is *consistent* and called *rotational form*[7]. The key point is enforcing the *non-homogeneous Neumann Boundary Conditions* for the pressure, i.e. the Poisson equations of the modified pressure ϕ^{k+1} with homogeneous Neumann B.C enforce the pressure p^{k+1} to satisfy the non-homogeneous Neumann B.C s.t.

$$\nabla p^{k+1}\cdot\mathbf{n}|_{\Gamma_N} = \left(f^k - \nu\nabla\times\nabla\times\mathbf{u}^{k+1}\right)\cdot\mathbf{n}|_{\Gamma_N}. \tag{54}$$

Remark 2.14. Although we use the backorder difference method in this paper, the choice of a particular time discretization is not so important. Of course, Adams-Bashforth method, Adams-Moulton method, Runge-Kutta method, etc. are perfectly acceptable.

3 NUMERICAL TESTS

In this section, the advantage of introducing the scaling parameter r_s, and accuracy (convergence rate) of new schemes are presented.

3.1 Calculation conditions

Let $f(x, y)$ be the Franke's test function

$$f(x,y) = \frac{3}{4}\exp\left\{-\frac{(9x-2)^2}{4} - \frac{(9y-2)^2}{4}\right\} + \frac{3}{4}\exp\left\{-\frac{(9x+1)^2}{49} - \frac{(9y+1)^2}{10}\right\} + \frac{1}{2}\exp\left\{-\frac{(9x-7)^2}{4} - \frac{(9y-3)^2}{4}\right\} - \frac{1}{5}\exp\left\{-(9x-4)^2 - (9y-7)^2\right\} \quad (55)$$

defined on a domain $\Omega := \{(x, y) \in \mathbb{R}^2 \mid [0, 1] \times [0, 1]\}$. Particles are distributed quasi-randomly by the following processes; (i) distribute particles $\{\mathbf{x}'_i\}_{1\le i\le N}$ on the square lattice with the width h, and (ii) give relative perturbation $\delta\mathbf{x}_i$ (by normal distribution, $\mu = 0, \sigma = 0.15$) to their positions, i.e. quasi-randomly arranged particles are $\mathbf{x}_i = \mathbf{x}'_i + \delta\mathbf{x}_i$. Maximum condition number $\kappa_\infty = \max_{\mathbf{x}_i\in\Omega}\{\mathrm{cond}(\mathbf{M}_i)\}$ is calculated for presenting the advantages of scaling for basis $\mathbf{p}$ with r_s, in comparison with the MLS(without scaling) and the MLSRKPM(with scaling by $r_e = \varrho$). Also, discrete relative supreme error norm $e^{\boldsymbol{\alpha}}_\infty := \max_{\mathbf{x}_i\in\Omega} |D^{\boldsymbol{\alpha}}_{\mathbf{x}} f^h(\mathbf{x}_i) - D^{\boldsymbol{\alpha}}_{\mathbf{x}} f(\mathbf{x}_i)| / \max_{\mathbf{x}_i\in\Omega} |D^{\boldsymbol{\alpha}}_{\mathbf{x}} f(\mathbf{x}_i)|$ is calculated for testing accuracy and convergence rate, in comparison with the standard LSMPS schemes, the Generalized LSMPS schemes, the standard MLS, and the Generalized MLS. 4-th order spline function is chosen as the weight function. The dilation parameters are $r_e = 3.5h$ ($p = 2$), $4.1h$ ($p = 3$), $4.5h$ ($p = 4$), and the scaling parameters are one-third of them.

3.2 Calculation results

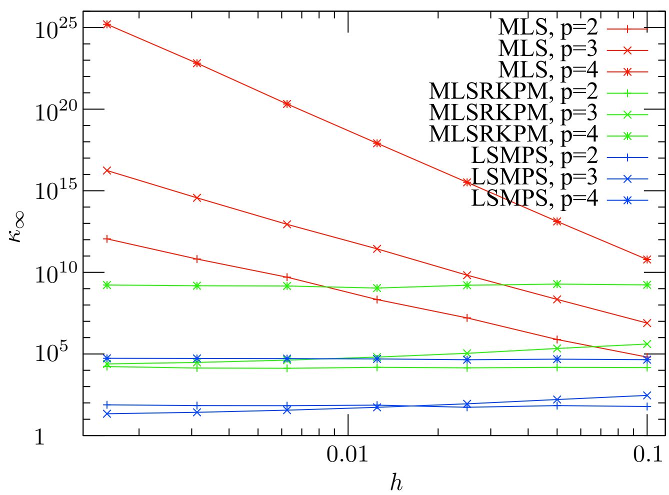

Figure 1: Maximum condition number of the moment matrix

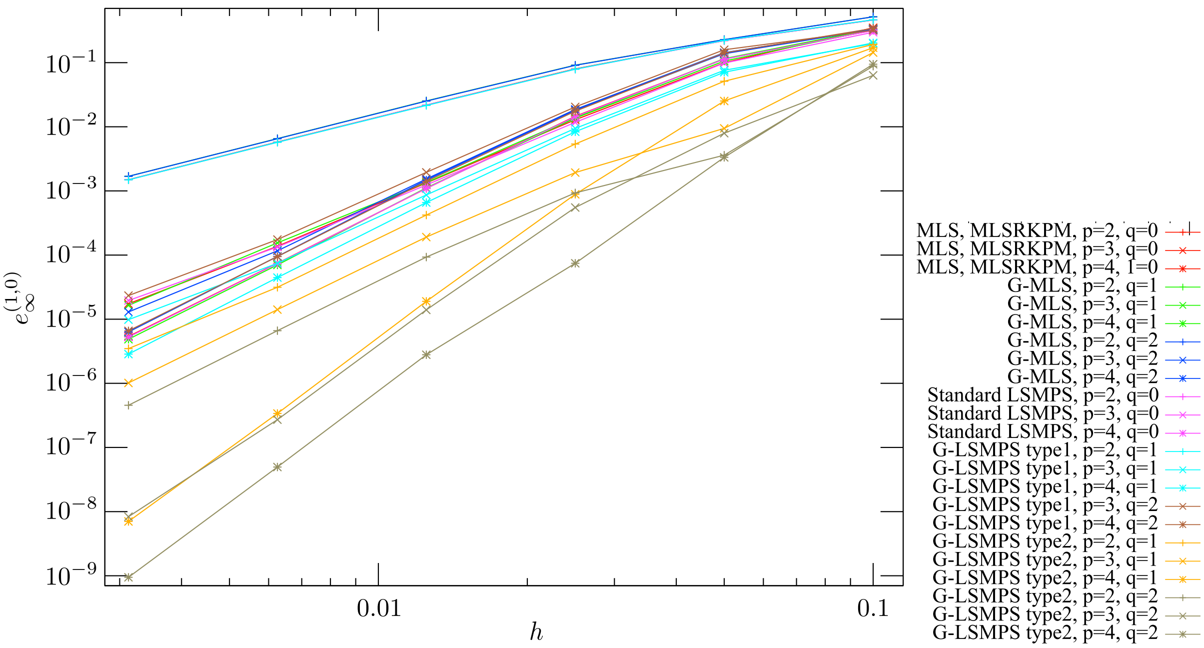

Figure 2: Convergence rates of $e_\infty^{(1,0)}$ (the first derivative $D_x f(x, y)$) with each scheme

3.3 Consideration

According to the Fig.1, the LSMPS schemes have lower condition number of the moment matrices than other methods', which provides more improvement of numerical stability for solving the linear system. Of course, scaling parameter $r_s (< r_e = \varrho)$ can be applied for the MLS and the MLSRKPM. Then, according to the Fig.2, accuracy of the Standard LSMPS schemes achieve the same level of the MLS or the MLSRKPM, although less computational costs are required, and the GMLS and the Generalized LSMPS schemes type-1 achieve the same or a little better accuracy than the standard MLS and the standard LSMPS schemes. Finally, worthy of special mention is the excellent accuracy and higher order convergence rates of the Generalized LSMPS schemes type-2, that they can obtain the extra higher order truncation limits. The Generalized LSMPS schemes type-2 are the most accurate schemes for the strong-form meshfree methods.

4 NUMERICAL EXAMPLES OF INCOMPRESSIBLE FLOWS

We applied the standard LSMPS schemes ($(p, q, r, s) = (2, 0, 1, 2)$) for numerical analysis of incompressible flow with the free surfaces, and calculation results of two patch tests advocated by Colagrossi[8] are shown in Fig.3. The details of the patch tests' system are described in [8]. In these calculations, NO stabilization techniques (such as artificial-viscosity in the SPH method) are introduced. Applications of them result in enhancement of numerical accuracy and stability, and they can treat not only positive pressure field problem but also negative pressure field one, which the existing MPS method cannot calculate stably.

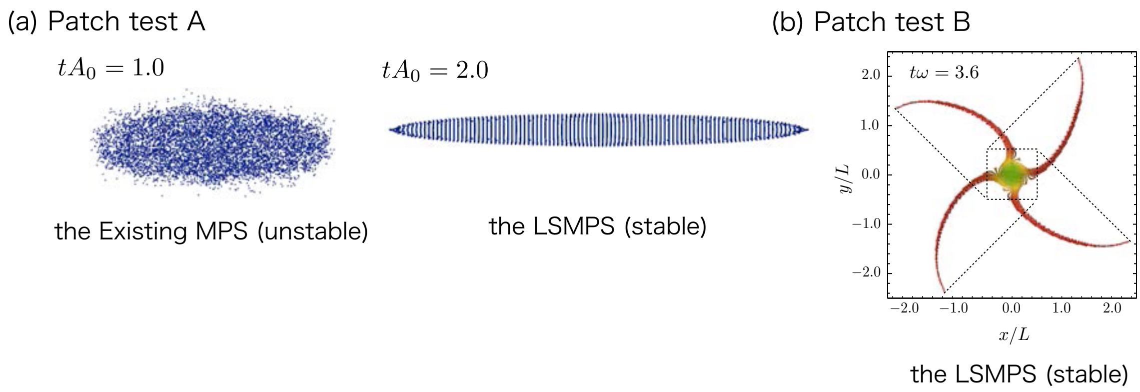

Figure 3: Calculation results of patch tests (patch test B cannot be calculated by the existing MPS)

5 CONCLUSIONS

We develop a new *consistent* particle method, named *Least Squares Moving Particle Semi-implicit/Simulation* (LSMPS) method. New schemes including the Standard type, the Generalized type-1, and the Generalized type-2 are introduced, and their accuracy are compared with the MLS and so on. Especially, the Generalized LSMPS schemes type-2 as meshfree compact schemes are superior in accuracy and the convergence rates. With using the LSMPS method, solutions of P.D.E with higher order accuracy can be obtained.

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