Error estimates of generalized particle methods for the Poisson and heat equations

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Error Estimates of Generalized Particle Methods for the Poisson and Heat Equations

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Introduction

The purpose of this thesis is to establish error estimates of generalized particle methods for the Poisson and heat equations.

A particle method is a class of numerical methods that approximate partial differential equations by using particles distributed in the spatial domain; for example, we can refer to Diffuse Element Method (DEM) [34, 45], Element Free Galerkin Methods (EFGM) [5, 6], Reproducing Kernel Particle Method (RKPM) [14, 39], Local Radial Basis Function Collocation Method (LRBFCM) [23, 49], Smoothed Particle Hydrodynamics (SPH) [26, 38, 40], and Moving Particle Semi-implicit (MPS) [32, 33, 52]. The particle method defines connectivities among the particles by using distance of each other. Therefore particle methods do not require mesh and grid in advance to define the connectivity among the particles, which is much different from other numerical methods such as Finite Difference Method (FDM) [24, 54, 59], Finite Element Method (FEM) [11, 16, 27], Boundary Element Method (BEM) [13, 50], and Finite Volume Method (FVM) [22, 35, 60]. This difference becomes the strong point in case of numerical methods for problems with large deformations and destructions; for example, astrophysics [40], collapses [43], brittle solids [9], flow problems with free surface [33, 42, 44, 53], fluid-structure interaction [15, 20], electronic structure calculations [55].

We can find many mathematical analysis of numerical methods like FDM, FEM, BEM, and FVM; for example, in case of FEM, elliptic problems [16, 30], parabolic problems [4, 21], Navier-Stokes equations [27, 46, 56], natural convection equations [57, 58], and references therein. On the other hands, we encounter a few researches on the numerical analysis of the particle methods; for example, error estimates of a particle method based on the vortex method have been established in case of parabolic and hyperbolic systems in unbounded domains [41, 48], in case of nonlinear conservation lows in unbounded domains [8], and in case of nonlinear conservation lows in bounded domains [7]. However, since the particle distributions and particle volumes in [7, 8, 41, 48] are defined by solutions of differential equations derived from given flow fields. Therefore, the dependence of their particle distributions and particle volumes on flow fields is different from those in practical computations such as SPH and MPS. As another example, there is a truncation error estimate of approximate gradient operators of MPS [29]. However, since the indicator of the particle distributions used in the regularity that is a sufficient condition of the truncation error estimate cannot be generally computed, it is difficult to confirm whether the particle distributions are valid. Moreover, as related results on error estimates of interpolants of particle methods, there exist truncation error estimates of interpolants by Radial Basis Function (RBF) [51, 61] and by Moving Least-Squares (MLS) [36]. However, there are differences in the methods of determining the coefficients of linear combinations. RBF sets the coefficients by solving linear equations derived from the condition of the Lagrange interpolants and MLS sets by solving linear equations derived from the condition to minimize a weighted least-square error. On the other hand, SPH and MPS give the coefficients by particle volumes based on the volume of domain. Therefore the truncation error estimates of RBF and MLS cannot be applied to that of the interpolant of SPH or MPS. Error estimates of SPH or MPS applicable for practical computations have been discussed only from the engineering point of view; for example, numerical tests of truncation errors of interpolants and approximate differential operators of first derivatives in one dimensional space [25, 47] and in three dimensional space [1, 2].

Therefore, as the first step of establishment of mathematical framework of the particle methods, we do investigate the numerical analysis of the particle methods. In this thesis, we introduce a generalized particle method, which can describe a class of particle methods including SPH and MPS, and analyze its truncation errors of interpolants and approximate differential operators. Moreover we apply the generalized particle method to the Poisson and heat equations and analyze its errors of the approximate solutions.

At first, we introduce the generalized particle method for an interpolant and approximate differential operators. The interpolant and the approximate differential operators are constructed by the particle distribution, a set of particle volumes, a weight functions, and an influence radius. In order to obtain error estimates, we introduce three conditions of these parameters. The first is a regularity of the family of the particle distributions, the particle volume set, and the influence radius. This regularity clarifies a uniform distribution of the particle distributions, a determination method of the particle volumes, and a decrement rate of the influence radius corresponding to an increment of number of particles. The second are some hypotheses of the weight function. These hypotheses clarify a usable range of weight functions from the mathematical point of view. The third is an h-connectivity among the particles corresponding to the influence radius h. This h-connectivity is a new concept of connectivity among the particles and provides a necessary length of the influence radius for the particle distributions. Since these conditions can be computed practically, we can verify whether these parameters are valid or not. Under these conditions, we show truncation error estimates of the interpolant and the approximate differential operators with the maximum norm; see [28]. Then the convergence rates with respect to the influence radius depend on the decrement rates of influence radius in the regularity and the choice of the parameters; for example, in case of the approximate operators in SPH, the convergence rates are at most second order.

Next, we establish error estimates of the Poisson equation discretized by the generalized particle method. Under the h-connectivity condition and the hypotheses of the weight functions, we prove the unique solvability and the discrete maximum principle of the discrete Poisson equation. As the truncation error estimates and the discrete maximum principle lead to the stability of the discrete Poisson equation, we obtain the error estimate with a discrete L^∞ norm. The convergence rates with respect to the influence radius are at most second order.

Moreover, we establish error estimates of the heat equation discretized by the generalized particle method in space and the θ-method in time. We show the unique solvability of the discrete heat equation. Furthermore, we prove the discrete maximum principle and the stability of the discrete heat equation with a condition of time step in case of $\theta \in [0, 1)$ and without in case of $\theta = 1$. Therefore we obtain the error estimates with the discrete L^∞ norm in space and time, and the convergence rates with respect to the time step are first order ($\theta \neq 1/2$) and second order ($\theta = 1/2$), and with respect to the influence radius are at most second order. Moreover, by considering an discrete L^2 norm in space, we show a stability of the discrete heat equation with a condition of time step in case of $\theta \in [0, 1/2)$ and without in case of $\theta \in [1/2, 1]$. Then we establish error estimates with the discrete L^2 norm in space and the discrete L^∞ norm in time, where these convergence rates agree with that of the error estimates with the discrete L^∞ norm.

Finally, we show some numerical results corresponding to the theoretical ones. We consider parameters satisfying the sufficient conditions of the error estimates. Then we compute numerically truncation errors of the interpolant and the approximate differential operators and relative errors of the approximate solutions of the generalized particle methods for the Poisson and heat equations. We confirm convergence of the errors under the sufficient conditions of each theorem and almost agreements between numerical convergence rates and theoretical ones.

An outline of this thesis is as follows. In Chapter 1, we formulate a generalized particle method, prepare some conditions of parameters, and prove truncation error estimates of an interpolant and approximate differential operators of the generalized particle method. In Chapter 2, we derive a generalized particle method for the Poisson equation and prove its error estimates. In Chapter 3, we introduce a generalized particle method for the heat equation and prove its error estimates. In Chapter 4, we present some numerical results corresponding to our results. In Appendix A, we introduce conventional particle methods, which are SPH and MPS, and show these error estimates by clarifying the relationship between the generalized particle method and these conventional particle methods.

Contents

Chapter 1

Generalized particle method

The purpose of this chapter is to formulate a generalized particle method and prepare some conditions and theorems used in the subsequent numerical analysis. Section 1.1 prepares notation and function spaces used later on. Section 1.2 introduces approximate operators of the generalized particle method: an interpolant, an approximate gradient operator, and an approximate Laplace operator. Section 1.3 gives some conditions of parameters of the generalized particle method used in the subsequent numerical analysis. Section 1.4 shows truncation error estimates for the approximate operators. The truncation error estimates of the interpolant was presented in Imoto and Tagami [28].

1.1 Preliminaries

We prepare notation and function spaces used later on. Let $\mathbb{R}^+$ and $\mathbb{R}_0^+$ be the set of positive real numbers and the set of nonnegative real numbers, respectively. Let $\mathbb{N}_0$ be the set of nonnegative integers.

Let S be an open set in $\mathbb{R}^d$ ($d \in \mathbb{N}$). Let $C(\overline{S})$ be the space of real continuous functions defined in $\overline{S}$. The norm of $C(\overline{S})$ is define dy

$$\|v\|_{C(\overline{S})} := \max_{x \in \overline{S}} |v(x)| .$$

For $k \in \mathbb{N}$, let $C^k(\overline{S})$ be the space of functions in $C(\overline{S})$ with derivatives up to the kth order and $|.|_{C^k(\overline{S})}$ and $\|.\|_{C^k(\overline{S})}$ denote their semi-norm and norm defined by

$$|v|_{C^k(\overline{S})} := \max_{|\alpha|=k} \|D^\alpha v\|_{C(\overline{S})} ,$$
$$\|v\|_{C^k(\overline{S})} := \max_{j=0,1,\ldots,k} |v|_{C^j(\overline{S})} ,$$

respectively. Here $|.|_{C^0(\overline{S})}$ coincides with $\|.\|_{C(\overline{S})}$.

1.2 Formulations

Let Ω be a bounded domain in $\mathbb{R}^d$ ($d \in \mathbb{N}$) with piecewise Lipschitz continuous boundary. For Ω and $H \in \mathbb{R}^+$, a domain Ω_H is defined by

$$\Omega_H := \left\{ x \in \mathbb{R}^d; \exists y \in \Omega \text{ s.t. } |x-y| < H \right\}.$$

For H and $N \in \mathbb{N}$, let $X_{N,H}$ be a set of points $x_i \in \Omega_H$ ($i = 1, 2, \ldots, N$) satisfying $x_i \neq x_j$ ($i \neq j$). Hereafter we call x_i and $X_{N,H}$ a particle and a particle distribution, respectively. Figure 1.1 shows an example of the particle distribution $X_{N,H}$.

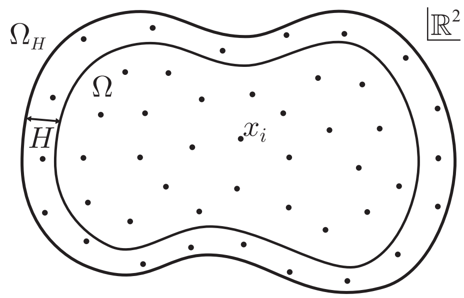

Figure 1.1: An example of the particle distribution $X_{N,H}$.

For H and $N \in \mathbb{N}$, let $V_{N,H}$ be a set of positive numbers $V_i \in \mathbb{R}^+$ ($i = 1, 2, \ldots, N$) satisfying

$$\sum_{i=1}^{N} V_i = \text{meas}(\Omega_H). \tag{1.1}$$

Here, meas(S) denotes the volume of $S \subset \mathbb{R}^d$. Hereafter we call V_i and $V_{N,H}$ a particle volume and a particle volume set, respectively.

An admissible set of weight functions W is defined by

$$W := \left\{ w \in C^1(\mathbb{R});\ \text{supp}(w) = [0,1],\ \int_{\mathbb{R}^d} w(|x|)dx = 1 \right\}.$$

For $w \in W$ and h ($0 < h < H$), set w_h by

$$w_h(r) := \frac{1}{h^d} w\left(\frac{r}{h}\right), \quad r \in \mathbb{R}_0^+.$$

Hereafter we call w and h a weight function and an influence radius, respectively. For $i = 1, 2, \ldots, N$, a function $\phi_i \in C(\overline{\Omega}_H)$ is given by $\phi_i(x) := w_h(|x - x_i|)$ ($x \in \overline{\Omega}_H$). Let W_h be the linear span of ϕ_i.

For $S \subset \mathbb{R}^d$, let Λ_S and Λ_S^* be

$$\Lambda_S := \{i; x_i \in X_{N,H} \cap S,\ i = 1, 2, \ldots, N\},$$
$$\Lambda_S^* := \{i; x_i \in X_{N,H} \setminus S,\ i = 1, 2, \ldots, N\},$$

respectively. For $X_{N,H}$, $V_{N,H}$, w, and h, the interpolant $\Pi_h : C(\overline{\Omega}_H) \to W_h$, the approximate gradient operator $\nabla_h : C(\overline{\Omega}_H) \to W_h^d$, and the approximate Laplace operator $\Delta_h : C(\overline{\Omega}_H) \to W_h$ are defined by

$$\Pi_h v(x) := \sum_{i=1}^{N} V_i v(x_i) w_h(|x - x_i|), \tag{1.2}$$

$$\nabla_h v(x) := d \sum_{i \in \Lambda_x^*} V_i \frac{v(x) - v(x_i)}{|x - x_i|} \frac{x - x_i}{|x - x_i|} w_h(|x - x_i|), \tag{1.3}$$

$$\Delta_h v(x) := -2d \sum_{i \in \Lambda_x^*} V_i \frac{v(x) - v(x_i)}{|x - x_i|^2} w_h(|x - x_i|), \tag{1.4}$$

respectively. We call numerical methods discretizing these approximate operators in space generalized particle methods because the approximate operators can describe ones of conventional particle methods such as SPH or MPS (see Appendix A).

1.3 Conditions of parameters

This section prepares some conditions of parameters of the generalized particle method: the particle distribution $X_{N,H}$, the particle volume set $V_{N,H}$, the influence radius h, and the weight function w. Subsection 1.3.1 defines a regularity of the family $\{X_{N,H}, V_{N,H}, h\}$. Subsection 1.3.2 introduces some conditions of the weight function w. The regularity and the conditions of the weight function appear everywhere in the subsequent numerical analysis. Subsection 1.3.3 defines a connectivity of the particle distribution $X_{N,H}$, which required in Chapter 2.

1.3.1 Regularity

For $X_{N,H}$, let σ_i be the Voronoi cell defined by

$$\sigma_i := \{x \in \Omega_H;\ \forall x_j (\neq x_i) \in X_{N,H}, |x_i - x| < |x_j - x|\}.$$

The decomposition of Ω_H by $\sigma = \{\sigma_i\}_{i=1}^N$ is called the Voronoi decomposition and its example is shown in Figure 1.2. For $X_{N,H}$, the covering radius r_c is defined by

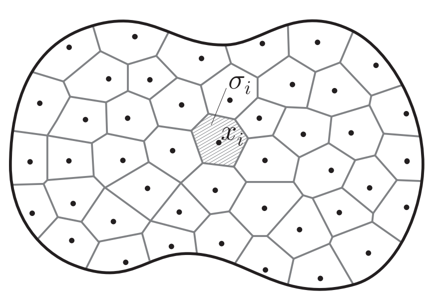

Figure 1.2: The Voronoi decomposition of Ω_H for the particle distribution $X_{N,H}$ in Figure 1.1.

$$r_{\rm c} := \max_{i=1,2,\ldots,N} \max_{x\in\overline{\sigma}_i} |x_i - x|. \tag{1.5}$$

For $i = 1, 2, \ldots, N$, let $\widetilde{V}_i$ be

$$\widetilde{V}_i := \mathrm{meas}(\sigma_i).$$

Let $\omega = \{\omega_i \subset \Omega_H; i = 1, 2, \ldots, N\}$ be a decomposition of Ω_H satisfying

$$\mathrm{meas}(\omega_i) = V_i \quad (i = 1, 2, \ldots, N), \qquad \bigcup_{i=1}^{N} \overline{\omega}_i = \overline{\Omega}_H, \qquad \omega_i \cap \omega_j = \emptyset \quad (i \neq j). \tag{1.6}$$

For $X_{N,H}$ and $V_{N,H}$, the Voronoi deviation $d_{\rm v}$ is defined by

$$d_{\rm v} := \inf_{\omega} \left[\max_{i=1,2,\ldots,N} \left\{ \sum_{j=1}^{N} \frac{\mathrm{meas}(\sigma_i \cap \omega_j) + \mathrm{meas}(\sigma_j \cap \omega_i)}{\mathrm{meas}(\sigma_i)} |x_i - x_j| \right\} \right].$$

Definition 1.1. *A family $\{(X_{N,H}, V_{N,H}, h)\}$ is said to be regular if there exists a constant c_0 (> 0) and m (≥ 1) such that for all the elements in $\{(X_{N,H}, V_{N,H}, h)\}$*

$$h^m \geq c_0(r_{\rm c} + d_{\rm v}). \tag{1.7}$$

In addition, m in (1.7) is said to be a regular order of $\{(X_{N,H}, V_{N,H}, h)\}$.

Proposition 1.2. *If $V_i = \widetilde{V}_i$ $(i = 1, 2, \ldots, N)$, then $d_{\rm v} = 0$.*

Proof. From the definition of $d_{\rm v}$, we have $d_{\rm v} \geq 0$. Since $V_i = \widetilde{V}_i$ $(i = 1, 2, \ldots, N)$, taking $\omega_i = \sigma_i$ $(i = 1, 2, \ldots, N)$, we find that ω $(= \{\omega_i\})$ satisfies (1.6). Then, since $\mathrm{meas}(\sigma_i \cap \omega_j) = \widetilde{V}_i$ $(i = j)$, 0 $(i \neq j)$, we obtain $d_{\rm v} = 0$. □

Remark 1.3. *Being able to compute the covering radius $r_{\rm c}$ and the Voronoi deviation $d_{\rm v}$, we can numerically confirm whether $(X_{N,H}, V_{N,H}, h)$ satisfies (1.7) or not for given c_0 and m.*

We can compute the covering radius $r_{\rm c}$ as follows: By using construction methods of the Voronoi decomposition such as the increment method [10], we first decompose Ω_H by the Voronoi decomposition. Next, for each particle, we compute the maximum distances from the particle to the boundary of its Voronoi cell. Finally, we obtain $r_{\rm c}$ by computing the maximum of the distances.

We can compute the Voronoi deviation $d_{\rm v}$ as follows: Let $A = \{a_{ij} \in \mathbb{R}_0^+;\ i, j = 1, 2, \ldots, N\}$ be a matrix satisfying

$$\sum_{j=1}^{N} a_{ij} = \widetilde{V}_i, \qquad \sum_{j=1}^{N} a_{ji} = V_i, \qquad i = 1, 2, \ldots, N. \tag{1.8}$$

For $X_{N,H}$, $V_{N,H}$, and A, let q and s_i $(i = 1, 2, \ldots, N)$ be positive numbers satisfying

$$q = s_i + \sum_{j=1}^{N} \frac{a_{ij} + a_{ji}}{\widetilde{V}_i} |x_i - x_j|, \qquad i = 1, 2, \ldots, N. \tag{1.9}$$

Then, d_{v} *is equivalent to the minimum of* q*. Let* $b \in \mathbb{R}^{N^2+N+1}$*,* $z \in \mathbb{R}^{N^2+N+1}$*, and* $v \in \mathbb{R}^{3N}$ *be*

$$
\begin{aligned}
b &:= (0, 0, \ldots, 0, 1)^T, \\
z &:= (a_{11}, a_{12}, \ldots, a_{NN}, s_1, s_2, \ldots, s_N, q)^T, \\
\zeta &:= (\widetilde{V}_1, \widetilde{V}_2, \ldots, \widetilde{V}_N, V_1, V_2, \ldots, V_N, 0, 0, \ldots, 0)^T,
\end{aligned}
$$

respectively. Let $M \in \mathbb{R}^{(N^2+N+1)\times 3N}$ *be a matrix such that the equation* $Mz = \zeta$ *replaces* (1.8) *and* (1.9)*. Then, we consider the following minimizing problem:*

$$
\text{Minimize} \quad b^T z \quad \text{Subject to} \quad Mz = \zeta, \; z \geq 0. \tag{1.10}
$$

Since b*,* M*, and* ζ *are unique for* $(X_{N,H}, V_{N,H}, h)$*, the minimizing problem is a linear programing problem. Since the solution* (1.10) *is agree with* d_{v}*, by using numerical methods for linear programing problems such as the simplex method* [18]*, we can compute* d_{v}*.*

1.3.2 Conditions of weight functions

Now we prepare four hypotheses of weight functions as follows:

Hypothesis 1.1. *There exists a positive integer* k *such that for all multi-index* α *such that* $1 \leq |\alpha| \leq k$*,*

$$
\int_{\mathbb{R}^d} x^\alpha w(|x|) dx = 0. \tag{1.11}
$$

Hypothesis 1.2. *There exists* $\widehat{w} \in C^1(\mathbb{R}_0^+)$ *such that*

$$
\widehat{w}(r) = \frac{1}{r} w(r), \qquad r \in \mathbb{R}^+.
$$

Hypothesis 1.3. *There exists* $\widehat{w} \in C^1(\mathbb{R}_0^+)$ *such that*

$$
\widehat{w}(r) = \frac{1}{r^2} w(r), \qquad r \in \mathbb{R}^+.
$$

Hypothesis 1.4. w *satisfies* $w(r) > 0, \; r \in (0, 1)$*.*

We call k in Hypothesis 1.1 an order of w. Now we show some results.

Proposition 1.4. *Any weight function* w *satisfies Hypothesis* 1.1 *with at least* $k = 1$*. Moreover, Hypothesis 1.1 with* $k \geq 2$ *is equivalent to*

$$
\int_0^1 r^{d-1+l} w(r) dr = 0, \qquad \forall l \in \{2n; \; n \in \mathbb{N}, \; 2n \leq k\}. \tag{1.12}
$$

Proof. We consider $\mathcal{T} = (\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_d) : [0, \pi]^{d-2} \times [0, 2\pi) \to \{x \in \mathbb{R}^d; \; |x| = 1\}$ such that

$$
\mathcal{T}_1(\vartheta) := \cos\theta_1,
$$

$$\mathcal{T}_i(\vartheta) := \sin\theta_1 \sin\theta_2 \cdots \sin\theta_{i-1}\cos\theta_i, \qquad i = 2, 3, \ldots, d-1,$$
$$\mathcal{T}_d(\vartheta) := \sin\theta_1 \sin\theta_2 \cdots \sin\theta_{d-2}\sin\theta_{d-1},$$

where $\vartheta = (\theta_1, \theta_2, \ldots, \theta_{d-1})$. Then $r\mathcal{T}(\theta_1, \theta_2, \ldots, \theta_{d-1})$ represents the polar coordinates with respect to $(r, \theta_1, \theta_2, \ldots, \theta_{d-1}) \in \mathbb{R}_0^+ \times [0, \pi]^{d-2} \times [0, 2\pi)$. By considering the coordinate transformation $x = r\mathcal{T}$, since the Jacobian is

$$r^{d-1} \sin^{d-2}\theta_1 \sin^{d-3}\theta_2 \cdots \sin^2\theta_{d-3}\sin\theta_{d-2},$$

we obtain

$$\begin{aligned}\int_{\mathbb{R}^d} x^\alpha w(|x|)dx &= \int_0^1 \int_{[0,\pi]^{d-2}\times[0,2\pi)} \mathcal{T}(\vartheta)^\alpha J(\vartheta) r^{d-1+|\alpha|} w(r) d\vartheta dr \\ &= \int_{[0,\pi]^{d-2}\times[0,2\pi)} \mathcal{T}(\vartheta)^\alpha J(\vartheta) d\vartheta \int_0^1 r^{d-1+|\alpha|} w(r) dr.\end{aligned}$$

Here J is

$$J(\vartheta) := \sin^{d-2}\theta_1 \sin^{d-3}\theta_2 \cdots \sin^2\theta_{d-3}\sin\theta_{d-2}.$$

For all multi index α such that $|\alpha|$ is odd, we have

$$\int_{[0,\pi]^{d-2}\times[0,2\pi)} \mathcal{T}(\vartheta)^\alpha J(\vartheta) d\vartheta = 0. \tag{1.13}$$

Therefore the first statement of the proposition holds. On the other hand, when $|\alpha|$ is even, (1.13) is not always true. Therefore, if

$$\int_0^1 r^{d-1+k} w(r) dr = 0 \tag{1.14}$$

for the even integer k, then (1.11) holds for all α such that $|\alpha| = k$. Since (1.14) is required if and only if k is even, the second statement of the proposition is obtained. □

Lemma 1.5. *If w satisfies Hypothesis 1.4, then w can not satisfy Hypothesis 1.1 with $k \geq 2$.*

Proof. For $k \geq 2$, assume that w satisfies both Hypothesis 1.1 with k and Hypothesis 1.4. By Proposition 1.4, w at least satisfies

$$\int_0^1 r^{d+1} w(r) dr = 0.$$

Then w needs some negative part in $(0, 1)$. However, since $w(r)$ satisfies Hypothesis 1.4, the assumption does not hold. Therefore we obtain this lemma. □

Lemma 1.6. *Suppose that w satisfies Hypothesis 1.1 with k. Then, for all even integer l and all multi-index α such that $1 + l \leq |\alpha| \leq k + l$, we have*

$$\int_{\mathbb{R}^d} |x|^{-l} x^\alpha w(|x|) dx = 0. \tag{1.15}$$

Proof. Since $|\alpha| \geq 1 + l$, the left side of (1.15) is integrable. In case that $k = 1$, since the integrand of the left side of (1.15) is even with respect to the origin, then (1.15) is true.

In case that $k \geq 2$, by considering the coordinate transformation, we have

$$\int_{\mathbb{R}^d} |x|^{-l} x^\alpha w(|x|) dx = \int_{[0,\pi]^{d-2}\times[0,2\pi)} \mathcal{T}(\vartheta)^\alpha J(\vartheta) d\vartheta \int_0^1 r^{d-1+|\alpha|-l} w(r) dr. \tag{1.16}$$

Here r, ϑ, $\mathcal{T}$, J are same as in the proof of Proposition 1.4. In case that $|\alpha|$ is odd, since

$$\int_{[0,\pi]^{d-2}\times[0,2\pi)} \mathcal{T}(\vartheta)^\alpha J(\vartheta) d\vartheta = 0,$$

(1.16) equals zero. In case that $|\alpha|$ is even, by Proposition 1.4, if $1 \leq |\alpha| - l \leq k$, then

$$\int_0^1 r^{d-1+|\alpha|-l} w(r) dr = 0.$$

Therefore (1.15) holds. □

For any $k \in \mathbb{N}$, we can construct weight functions satisfying Hypothesis 1.1 with k. Now, we show some example of the weight functions.

Example 1.7. *Let us construct weight functions satisfying Hypothesis* 1.1 *with k by polynomial functions in $d = 2, 3$. When $k = 1$, since $w \in W$, w requires*

$$w(1) = 0, \qquad \frac{d}{dr} w(1) = 0, \qquad \int_{\mathbb{R}^d} w(|x|) dx = 1. \tag{1.17}$$

Then the weight function with minimum degree is constructed by the quadric function:

$$w(r) := \gamma_d \begin{cases} (1-r)^2, & 0 \leq r < 1, \\ 0, & r \geq 1. \end{cases}$$

Here $\gamma_d = 6/\pi$ $(d = 2)$, $15/2\pi$ $(d = 3)$.

When $k \geq 2$, in addition of (1.17)*, w requires* (1.12)*. Then, for example, the weight function satisfying Hypothesis* 1.1 *with $k = 3$ is construct by the cubic function:*

$$w(r) := \frac{35}{7\pi} \begin{cases} (1-r)^2(4-7r), & 0 \leq r < 1, \\ 0, & r \geq 1, \end{cases}$$

in $d = 2$ and

$$w(r) := \frac{15}{2\pi} \begin{cases} (1-r)^2(5-8r), & 0 \leq r < 1, \\ 0, & r \geq 1, \end{cases}$$

in $d = 3$.

Similarly, we can construct the weight functions 1.1 *with $k \geq 4$.*

For Hypothesis 1.2 and Hypothesis 1.3, we obtain the following propositions.

1.3.3 Connectivity

Definition 1.8. *For the influence radius h, we call that a particle distribution $X_{N,H}$ satisfies the h-connectivity if for all $x_i \in X_{N,H} \cap \Omega$, there exists an integer m and a sequence $\{x_{i_j}\}_{j=1}^{m} \subset X_{N,H}$ such that*

$$x_{i_1} = x_i, \quad |x_{i_j} - x_{i_{j+1}}| < h \quad (j = 1, 2, \ldots, m-1), \quad x_{i_m} \in \Gamma \cup \Gamma_H. \tag{1.18}$$

Now, we consider the graph $G = (\mathcal{V}, \mathcal{E})$ such that

$$\mathcal{V} = X_{N,H}, \qquad \mathcal{E} = \{(x_i, x_j);\ |x_i - x_j| < h,\ i, j = 1, 2, \ldots, N,\ i \neq j\}.$$

By Definition 1.8, we notice that if the particle distribution $X_{N,H}$ satisfies the h-connectivity, then all the vertex of G on Ω has a path to a vertex of G on $\Gamma \cup \Gamma_H$.

Example 1.9. *Figures 1.3–1.4 show examples of the particle distributions satisfying and not satisfying the h-connectivity. In each figure, the left part shows an example of the particle distribution $X_{N,H}$, the center bottom shows the bulk of the influence h, and the right part shows the graph G for $X_{N,H}$ and h. In case of G in Figure 1.3, all the vertex on Ω has a path to the vertex on $\Gamma \cup \Gamma_H$. Therefore the particle distribution $X_{N,H}$ in Figure 1.3 satisfies the h-connectivity. On the other hand, in case of G in Figure 1.4, since there exists an isolated sub-graph on Ω in the left-center of G, the vertex on the sub-graph does not have a path to any vertex on $\Gamma \cup \Gamma_H$. Therefore the particle distribution $X_{N,H}$ in Figure 1.4 does not satisfy the h-connectivity.*

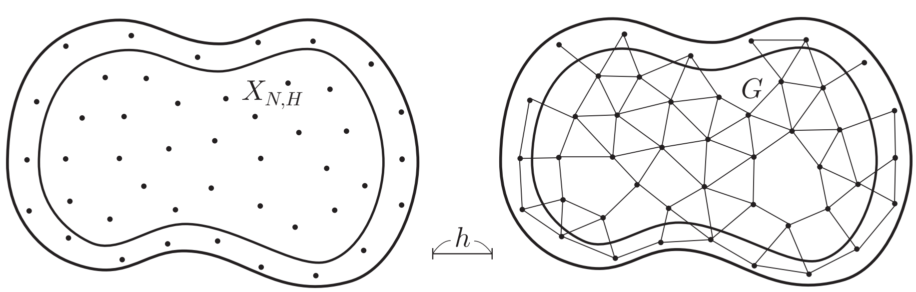

Figure 1.3: An example the particle distribution $X_{N,H}$ satisfying the h-connectivity.

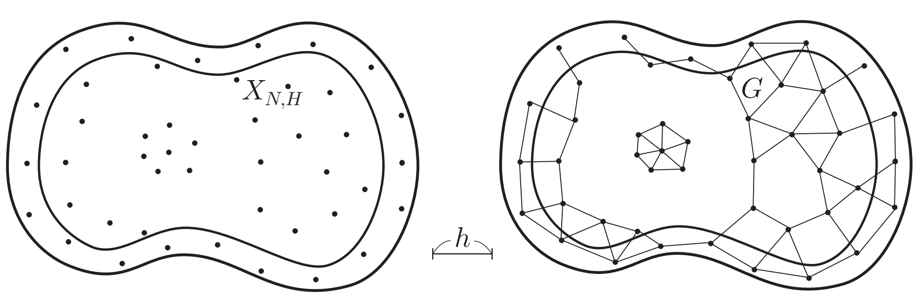

Figure 1.4: An example the particle distribution $X_{N,H}$ not satisfying the h-connectivity.

Lemma 1.10. *If a particle distribution $X_{N,H}$ and an influence radius h satisfy*

$$h > 2r_{\mathrm{c}}, \tag{1.19}$$

then the particle distribution $X_{N,H}$ satisfies the h-connectivity

Proof. Because Ω_H is connected, by the definition of Voronoi decomposition, for all $x_i \in X_{N,H}$, there exists a sequence $\{x_{i_j}\}_{j=1}^{m} \subset X_{N,H}$ such that

$$x_{i_1} = x_i, \quad \overline{\sigma}_{i_j} \cap \overline{\sigma}_{i_{j+1}} \neq \emptyset \quad (j = 1, 2, \ldots, m-1), \quad x_{i_m} \in \Gamma \cup \Gamma_H.$$

By the definition of r_{c}, we find $|x_{i_j} - x_{i_{j+1}}| \leq 2r_{\mathrm{c}}$ $(j = 1, 2, \ldots, m-1)$. Therefore, if $X_{N,H}$ and h satisfy (1.19), then $\{x_{i_j}\}_{j=1}^{m}$ satisfies (1.18). Therefore this concludes the result. □

1.4 Truncation error estimates

In this section, let c be a generic positive constant independent of h and N.

1.4.1 Interpolant

First, we state the theorem with respect to a truncation error of the interpolant (1.2).

Theorem 1.11. *Suppose that $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ is a regular family with order m (≥ 1) and w satisfies Hypothesis 1.1 with k. Then there exists a positive constant c independent of h and N such that for all $v \in C^{k+1}(\overline{\Omega}_H)$,*

$$\|v - \Pi_h v\|_{C(\overline{\Omega})} \leq c\left(h^{k+1}\,|v|_{C^{k+1}(\overline{\Omega}_H)} + h^{m-1}\,\|v\|_{C^{k+1}(\overline{\Omega}_H)}\right). \tag{1.20}$$

Next, before beginning the proof of Theorem 1.11, we show the following lemma.

Lemma 1.12. *There exists a positive constant c independent of h and N such that for all multi-index α,*

$$\|\mathscr{M}_{1,\alpha}\|_{C(\overline{\Omega})} \leq c\left(1 + 2\frac{r_{\mathrm{c}}}{h}\right)^{d}\left(r_{\mathrm{c}} + d_{\mathrm{v}} + \frac{r_{\mathrm{c}} + d_{\mathrm{v}}}{h}\right). \tag{1.21}$$

Here,

$$\mathscr{M}_{1,\alpha}(x) := \sum_{i=1}^{N} V_i (x_i - x)^{\alpha} w_h(|x - x_i|) - \int_{\mathbb{R}^d} y^{\alpha} w(|y|)dy.$$

Proof. Fix $x \in \overline{\Omega}$. Fix any $\omega (= \{\omega_i\})$ satisfying (1.6). Let $\xi_{ij} := \mathrm{meas}(\sigma_i \cap \omega_j)$ $(i, j = 1, 2, \ldots, N)$. Set $E_k(x)$ $(k = 1, 2, 3)$ by

$$E_1(x) := \sum_{i=1}^{N}\sum_{j=1}^{N}(x_j - x)^{\alpha}\int_{\sigma_i \cap \omega_j}\{w_h(|x - x_i|) - w_h(|x - y|)\}\,dy,$$

$$E_2(x) := \sum_{i=1}^{N}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}\{(x_j-x)^\alpha-(y-x)^\alpha\}\,w_h(|x-y|)dy,$$
$$E_3(x) := \sum_{i=1}^{N}\sum_{j=1}^{N}\xi_{ij}(x_j-x)^\alpha\{w_h(|x-x_j|)-w_h(|x-x_i|)\},$$

respectively. Since

$$|\mathscr{M}_{1,\alpha}(x)| = \left|\sum_{k=1}^{3}E_k(x)\right| \le \sum_{k=1}^{3}|E_k(x)|,$$

we estimate each E_k.

First, we consider E_1. For $y\in\mathbb{R}^d$ and $r\in\mathbb{R}^+$, let $B_r(y)$ be an open ball with center y and radius r:

$$B_r(y) := \left\{z\in\mathbb{R}^d;\ |z-y|<r\right\}.$$

If $i \in \Lambda_{B_{h+r_c}(x)}$, then we have

$$w_h(|x-y|) = 0, \qquad \forall y\in\sigma_i. \tag{1.22}$$

Then we can write

$$E_1(x) = \sum_{i\in\Xi}\sum_{j=1}^{N}(x_j-x)^\alpha\int_{\sigma_i\cap\omega_j}\{w_h(|x-x_i|)-w_h(|x-y|)\}\,dy.$$

Here Ξ denotes $\Lambda_{B_{h+r_c}(x)}$. By Taylor expansion, we have

$$\begin{aligned}
|E_1(x)| &\le \sum_{i\in\Xi}\sum_{j=1}^{N}|(x_j-x)^\alpha|\int_{\sigma_i\cap\omega_j}|w_h(|x-x_i|)-w_h(|x-y|)|\,dy \\
&\le \mathrm{diam}(\Omega_H)^{|\alpha|}\sum_{i\in\Xi}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}|w_h(|x-x_i|)-w_h(|x-y|)|\,dy \\
&\le \mathrm{diam}(\Omega_H)^{|\alpha|}\,|w_h|_{C^1(\mathbb{R}_0^+)}\sum_{i\in\Xi}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}|x_i-y|dy \\
&\le \mathrm{diam}(\Omega_H)^{|\alpha|}\frac{r_c}{h^{d+1}}\,|w|_{C^1(\mathbb{R}_0^+)}\sum_{i\in\Xi}\int_{\sigma_i}dy \\
&\le \mathrm{meas}(B)\mathrm{diam}(\Omega_H)^{|\alpha|}\left(1+2\frac{r_c}{h}\right)^d\frac{r_c}{h}\,|w|_{C^1(\mathbb{R}_0^+)}.
\end{aligned}$$

Here, $\mathrm{diam}(S)$ denotes the diameter of $S\subset\mathbb{R}^d$:

$$\mathrm{diam}(S) := \sup_{x,y\in S}|x-y|$$

and $B := B_1(0)$.

Next we consider E_2. Since $E_2 = 0$ when $|\alpha| = 0$, then we estimate when $|\alpha| \geq 1$. By (1.22), we can write

$$E_2(x) = \sum_{i\in\Xi}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}\left\{(x_j - x)^\alpha - (y - x)^\alpha\right\} w_h(|x - y|)dy.$$

Fix a multi-index α. Let $\{\beta_k\}_{k=1}^{|\alpha|}$ be multi-indexes such that

$$|\beta_k| = 1 \quad (k = 1, 2, \ldots, |\alpha|), \qquad \alpha = \sum_{k=1}^{|\alpha|}\beta_k.$$

Then, for all $x, y, z \in \mathbb{R}^d$, we have

$$\begin{aligned}
|(y-x)^\alpha - (z-x)^\alpha| &\leq \left|(y-x)^{\beta_1}\prod_{k=2}^{|\alpha|}(y-x)^{\beta_k} - (z-x)^{\beta_1}\prod_{k=2}^{|\alpha|}(y-x)^{\beta_k}\right| \\
&\quad + \left|(z-x)^{\beta_1}\prod_{k=2}^{|\alpha|}(y-x)^{\beta_k} - (z-x)^{\beta_1}\prod_{k=2}^{|\alpha|}(z-x)^{\beta_k}\right| \\
&\leq |y-z||y-x|^{|\alpha|-1} + |z-x|\left|\prod_{k=2}^{|\alpha|}(y-x)^{\beta_k} - \prod_{k=2}^{|\alpha|}(z-x)^{\beta_2}\right| \\
&\ \ \vdots \\
&\leq |y-z|\sum_{l=1}^{|\alpha|}|z-x|^{l-1}|y-x|^{|\alpha|-l}.
\end{aligned} \tag{1.23}$$

Therefore, we have

$$\begin{aligned}
|E_2(x)| &\leq \sum_{i\in\Xi}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}|(x_j-x)^\alpha - (y-x)^\alpha|\,|w_h(|x-y|)|dy \\
&\leq \sum_{i\in\Xi}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}|y-x_j|\sum_{l=1}^{|\alpha|}|x_j-x|^{l-1}|y-x|^{|\alpha|-l}|w_h(|x-y|)|dy \\
&\leq |\alpha|\mathrm{diam}(\Omega_H)^{|\alpha|}\sum_{i\in\Xi}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}|y-x_j||w_h(|x-y|)|dy \\
&\leq |\alpha|\mathrm{diam}(\Omega_H)^{|\alpha|}\sum_{i\in\Xi}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}(|y-x_i| + |x_i-x_j|)|w_h(|x-y|)|dy \\
&\leq |\alpha|\mathrm{diam}(\Omega_H)^{|\alpha|}h^{-d}\,\|w\|_{C(\mathbb{R}_0^+)}\sum_{i\in\Xi}\sum_{j=1}^{N}\xi_{ij}(r_\mathrm{c} + |x_i - x_j|)
\end{aligned}$$

$$\le |\alpha| \mathrm{diam}(\Omega_H)^{|\alpha|} h^{-d} \|w\|_{C(\mathbb{R}_0^+)} \left(\sum_{i\in\Xi} \widetilde{V}_i \right) \left\{ r_\mathrm{c} + \max_{i=1,2,\dots,N} \left(\sum_{j=1}^{N} \frac{\xi_{ij}}{\widetilde{V}_i} |x_i - x_j| \right) \right\}$$
$$\le |\alpha| \mathrm{meas}(B) \mathrm{diam}(\Omega_H)^{|\alpha|} \left(1 + 2\frac{r_\mathrm{c}}{h}\right)^d \|w\|_{C(\mathbb{R}_0^+)}$$
$$\times \left\{ r_\mathrm{c} + \max_{i=1,2,\dots,N} \left(\sum_{j=1}^{N} \frac{\xi_{ij} + \xi_{ji}}{\widetilde{V}_i} |x_i - x_j| \right) \right\}.$$

Since ω is arbitrary, we obtain

$$|E_2(x)| \le |\alpha| \mathrm{meas}(B) \mathrm{diam}(\Omega_H)^{|\alpha|} \left(1 + 2\frac{r_\mathrm{c}}{h}\right)^d (r_\mathrm{c} + d_\mathrm{v}) \|w\|_{C(\mathbb{R}_0^+)}.$$

Finally, we consider E_3. We estimate

$$|E_3(x)| \le \sum_{i=1}^{N} \sum_{j=1}^{N} \xi_{ij} |(x_j - x)^\alpha| \, |w_h(|x - x_j|) - w_h(|x - x_i|)|$$
$$\le \mathrm{diam}(\Omega_H)^{|\alpha|} \sum_{i=1}^{N} \sum_{j=1}^{N} \xi_{ij} \left| w_h(|x - x_j|) - w_h(|x - x_i|) \right|.$$

By Taylor expansion, we have

$$\sum_{i=1}^{N} \sum_{j=1}^{N} \xi_{ij} \left| w_h(|x - x_i|) - w_h(|x - x_j|) \right|$$
$$\le \sum_{x_i \in B_h(x)} \sum_{j=1}^{N} \xi_{ij} \left| w_h(|x - x_i|) - w_h(|x - x_j|) \right|$$
$$+ \sum_{i=1}^{N} \sum_{x_j \in B_h(x)} \xi_{ij} \left| w_h(|x - x_i|) - w_h(|x - x_j|) \right|$$
$$\le |w_h|_{C^1(\mathbb{R}_0^+)} \left(\sum_{x_i \in B_h(x)} \sum_{j=1}^{N} \xi_{ij} |x_i - x_j| + \sum_{i=1}^{N} \sum_{x_j \in B_h(x)} \xi_{ij} |x_i - x_j| \right)$$
$$= \frac{1}{h^{d+1}} |w|_{C^1(\mathbb{R}_0^+)} \sum_{x_i \in B_h(x)} \sum_{j=1}^{N} (\xi_{ij} + \xi_{ji}) |x_i - x_j|$$
$$= \frac{1}{h^{d+1}} |w|_{C^1(\mathbb{R}_0^+)} \sum_{x_i \in B_h(x)} \widetilde{V}_i \sum_{j=1}^{N} \frac{\xi_{ij} + \xi_{ji}}{\widetilde{V}_i} |x_i - x_j|$$
$$\le \left(1 + \frac{r_\mathrm{c}}{h}\right)^d \frac{1}{h} |w|_{C^1(\mathbb{R}_0^+)} \max_{i=1,2,\dots,N} \left(\sum_{j=1}^{N} \frac{\xi_{ij} + \xi_{ji}}{\widetilde{V}_i} |x_i - x_j| \right).$$

Since ω is arbitrary, we obtain

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\xi_{ij}\,|w_h(|x-x_i|)-w_h(|x-x_j|)| \le \left(1+\frac{r_{\mathrm{c}}}{h}\right)^d \frac{d_{\mathrm{v}}}{h}|w|_{C^1(\mathbb{R}_0^+)}. \tag{1.24}$$

Therefore, we estimate

$$|E_3(x)| \le \mathrm{meas}(B)\mathrm{diam}(\Omega_H)^{|\alpha|}\left(1+\frac{r_{\mathrm{c}}}{h}\right)^d \frac{d_{\mathrm{v}}}{h}|w|_{C^1(\mathbb{R}_0^+)}.$$

By estimates of E_k $(k=1,2,3)$, we obtain (1.21). □

Finally, using the lemma above, we obtain the following proof of Theorem 1.11.

Proof of Theorem 1.11. Fix $x \in \overline{\Omega}$. By $h < H$, we have $B_h(x) \subset \Omega_H$. Then, for all $x_i \in X_{N,H} \cap B_h(x)$, we obtain Taylor expansion of $v \in C^{k+1}(\overline{\Omega}_H)$:

$$v(x_i) = \sum_{0\le|\alpha|\le k}\frac{D^\alpha v(x)}{\alpha!}(x_i-x)^\alpha + \sum_{|\alpha|=k+1}(x_i-x)^\alpha R_\alpha[v](x_i;x). \tag{1.25}$$

Here, R_α is defined by

$$R_\alpha[v](y;x) := \frac{|\alpha|}{\alpha!}\int_0^1 (1-t)^{|\alpha|-1}D^\alpha v(ty+(1-t)x)dt.$$

We multiply both side of (1.25) by $V_i w_h(|x-x_i|)$ and take the sum of these over $i \in \Lambda_{B_h(x)}$. Then, we have

$$\begin{aligned}\Pi_h v(x) = &\sum_{0\le|\alpha|\le k}\frac{D^\alpha v(x)}{\alpha!}\sum_{i\in\Lambda_{B_h(x)}}V_i(x_i-x)^\alpha w_h(|x-x_i|)\\ &+\sum_{|\alpha|=k+1}R_\alpha[v](x_i;x)\sum_{i\in\Lambda_{B_h(x)}}V_i(x_i-x)^\alpha w_h(|x-x_i|).\end{aligned}$$

By Hypotheses 1.1, we obtain

$$\begin{aligned}\Pi_h v(x) - v(x) = &\sum_{0\le|\alpha|\le k}\frac{D^\alpha v(x)}{\alpha!}\mathscr{M}_{1,\alpha}(x)\\ &+\sum_{|\alpha|=k+1}R_\alpha[v](x_i;x)\left(\mathscr{M}_{1,\alpha}(x)+\int_{\mathbb{R}^d}y^\alpha w(|y|)dy\right).\end{aligned}$$

Since

$$\begin{aligned}|D^\alpha v(x)| &\le |v|_{C^{|\alpha|}(\overline{\Omega}_H)},\\ |R_\alpha[v](x_i;x)| &\le |v|_{C^{|\alpha|}(\overline{\Omega}_H)},\end{aligned}$$

we have

$$|\Pi_h v(x) - v(x)| \le \sum_{0\le|\alpha|\le k+1}|\mathscr{M}_{1,\alpha}(x)|\,|v|_{C^{|\alpha|}(\overline{\Omega}_H)} + \sum_{|\alpha|=k+1}\left|\int_{\mathbb{R}^d}y^\alpha w_h(|y|)dy\right||v|_{C^{k+1}(\overline{\Omega}_H)}.$$

Moreover, since

$$\left|\int_{\mathbb{R}^d} y^\alpha w_h(|y|)dy\right| = h^{|\alpha|}\left|\int_B y^\alpha w(|y|)dy\right|,$$

we estimate

$$|\Pi_h v(x) - v(x)| \le c\left(\sum_{0\le|\alpha|\le k+1} |\mathscr{M}_{1,\alpha}(x)|\,|v|_{C^{|\alpha|}(\overline{\Omega}_H)} + h^{k+1}|v|_{C^{k+1}(\overline{\Omega}_H)}\right). \tag{1.26}$$

Applying (1.7) into Lemma 1.12, we have

$$\|\mathscr{M}_{1,\alpha}\|_{C(\overline{\Omega})} \le ch^{m-1}.$$

Therefore, applying this into (1.26), we obtain (1.20). □

1.4.2 Approximate gradient operator

First, we state the theorem with respect to a truncation error of the approximate gradient operator (1.3).

Theorem 1.13. *Suppose that* $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ *is a regular family with order* m (≥ 1) *and* w *satisfies Hypothesis* 1.1 *with* k *and Hypothesis* 1.2. *Set* $k \in \mathbb{N}_0$ *by* k_0 *or less if* w *satisfies Hypothesis 1.1 with order* k. *Then there exists a positive constant* c *independent of* h *and* N *such that for all* $v \in C^{k+2}(\overline{\Omega}_H)$,

$$\|\nabla v - \nabla_h v\|_{[C(\overline{\Omega})]^d} \le c\left(h^{k+1}|v|_{C^{k+2}(\overline{\Omega}_H)} + h^{m-1}\|v\|_{C^{k+2}(\overline{\Omega}_H)}\right). \tag{1.27}$$

Next, before beginning the proof of Theorem 1.13, we show the following lemma.

Lemma 1.14. *Suppose that* w *satisfies Hypothesis* 1.2. *Then there exists a positive constant* c *independent of* h *and* N *such that for all multi-index* α *such that* $|\alpha| \ge 2$,

$$\|\mathscr{M}_{2,\alpha}\|_{C(\overline{\Omega})} \le c\left(1 + 2\frac{r_{\mathrm{c}}}{h}\right)^d \frac{r_{\mathrm{c}} + d_{\mathrm{v}}}{h}. \tag{1.28}$$

Here,

$$\mathscr{M}_{2,\alpha}(x) := \sum_{i\in\Lambda_x^*} V_i \frac{(x_i - x)^\alpha}{|x_i - x|^2} w_h(|x - x_i|) - \int_{\mathbb{R}^d} \frac{y^\alpha}{|y|^2} w_h(|y|)dy.$$

Proof. Fix $x \in \overline{\Omega}$. Fix any $\omega(= \{\omega_i\})$ satisfying (1.6). Let $\xi_{ij} := \mathrm{meas}(\sigma_i \cap \omega_j)$ $(i, j = 1, 2, \ldots, N)$. For a multi-index α, let $\psi_\alpha : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be

$$\psi_\alpha(y, z) := \begin{cases} \dfrac{(y - z)^\alpha}{|y - z|^2}, & y \ne z, \\ 0, & y = z. \end{cases}$$

Set $E_k(x)$ $(k=1,2,3)$ by

$$E_4(x) := \sum_{i=1}^{N}\sum_{j=1}^{N}\psi_\alpha(x_j,x)\int_{\sigma_i\cap\omega_j}\{w_h(|x-x_i|)-w_h(|x-y|)\}\,dy,$$

$$E_5(x) := \sum_{i=1}^{N}\sum_{j=1}^{N}\psi_\alpha(x_j,x)\int_{\sigma_i\cap\omega_j}w_h(|x-y|)dy-\int_{\mathbb{R}^d}\frac{y^\alpha}{|y|^2}w_h(|y|)dy,$$

$$E_6(x) := \sum_{i=1}^{N}\sum_{j=1}^{N}\xi_{ij}\psi_\alpha(x_j,x)\left\{w_h(|x-x_j|)-w_h(|x-x_i|)\right\},$$

respectively. Since

$$|\mathscr{M}_{2,\alpha}(x)| = \left|\sum_{k=4}^{6}E_k(x)\right| \le \sum_{k=4}^{6}|E_k(x)|,$$

we estimate each E_k.

First, we consider E_4. By (1.22), we have

$$\begin{aligned}|E_4(x)| &= \left|\sum_{i\in\Xi}\sum_{j=1}^{N}\psi_\alpha(x_j,x)\int_{\sigma_i\cap\omega_j}\{w_h(|x-x_i|)-w_h(|x-y|)\}\,dy\right|\\ &\le \sum_{i\in\Xi}\sum_{j=1}^{N}|\psi_\alpha(x_j,x)|\int_{\sigma_i\cap\omega_j}|w_h(|x-x_i|)-w_h(|x-y|)|\,dy\\ &\le \operatorname{diam}(\Omega_H)^{|\alpha|-2}\sum_{i\in\Xi}\sum_{j=1}^{N}\int_{\sigma_i\cap\omega_j}|w_h(|x-x_i|)-w_h(|x-y|)|\,dy.\end{aligned}$$

Here, Ξ denotes $\Lambda_{B_{h+r_\mathrm{c}}(x)}$. By Taylor expansion and (1.5), we estimate

$$\begin{aligned}|E_4(x)| &\le \operatorname{diam}(\Omega_H)^{|\alpha|-2}\,|w_h|_{C^1(\mathbb{R}_0^+)}\sum_{i\in\Xi}\int_{\sigma_i}|x_i-y|dy\\ &\le \operatorname{meas}(B)\operatorname{diam}(\Omega_H)^{|\alpha|-2}\left(1+2\frac{r_\mathrm{c}}{h}\right)^d\frac{r_\mathrm{c}}{h}\,|w|_{C^1(\mathbb{R}_0^+)}\\ &\le c\left(1+2\frac{r_\mathrm{c}}{h}\right)^d\frac{r_\mathrm{c}}{h}.\end{aligned}$$

Next, we consider E_5. By (1.23), for all $x,y,z\in\mathbb{R}^d$ such that $x\ne y$ and $x\ne z$, we have

$$\begin{aligned}&|\psi_\alpha(y,x)-\psi_\alpha(z,x)|\\ &\quad\le \left|\frac{(y-x)^\alpha}{|y-x|^2}-\frac{(z-x)^\alpha}{|y-x|^2}\right|+\left|\frac{(z-x)^\alpha}{|y-x|^2}-\frac{(z-x)^\alpha}{|y-x||z-x|}\right|+\left|\frac{(z-x)^\alpha}{|y-x||z-x|}-\frac{(z-x)^\alpha}{|z-x|^2}\right|\\ &\quad\le |y-z|\sum_{l=1}^{|\alpha|}|z-x|^{l-1}|y-x|^{|\alpha|-l-2}+|y-z||z-x|^{|\alpha|-1}|y-x|^{-2}+|y-z||z-x|^{|\alpha|-2}|y-x|^{-1}\end{aligned}$$

$$\leq 2|y-z| \sum_{l=1}^{|\alpha|} |z-x|^{l-1} |y-x|^{|\alpha|-l-2}$$

Moreover, for all $x, y, z \in \mathbb{R}^d$ such that $x \neq y$ and $x = z$, we get

$$|\psi_\alpha(y,x) - \psi_\alpha(z,x)| = |\psi_\alpha(y,x)| \leq |y-x|^{|\alpha|-2} = |y-z| \sum_{l=1}^{|\alpha|-1} |z-x|^{l-1} |y-x|^{|\alpha|-l-2}.$$

Therefore, by using these estimates and (1.5), we obtain

$$\begin{aligned}
|E_5(x)| &\leq \sum_{i\in\Xi} \sum_{j=1}^{N} \int_{\sigma_i\cap\omega_j} |\psi_\alpha(x_j,y) - \psi_\alpha(x_j,x)| w_h(|x-y|) dy \\
&\leq 2 \sum_{i\in\Xi} \sum_{j=1}^{N} \int_{\sigma_i\cap\omega_j} |y-x_j| \sum_{l=1}^{|\alpha|-1} |x_j-x|^{l-1} |y-x|^{|\alpha|-1-l} \frac{|w_h(|x-y|)|}{|x-y|} dy \\
&\leq 2|\alpha| \mathrm{diam}(\Omega_H)^{|\alpha|} \sum_{i\in\Xi} \sum_{j=1}^{N} \int_{\sigma_i\cap\omega_j} |y-x_j| \frac{|w_h(|x-y|)|}{|x-y|} dy \\
&\leq 2|\alpha| \mathrm{diam}(\Omega_H)^{|\alpha|} \sum_{i\in\Xi} \sum_{j=1}^{N} \int_{\sigma_i\cap\omega_j} (|y-x_i| + |x_i-x_j|) \frac{|w_h(|x-y|)|}{|x-y|} dy \\
&\leq 2|\alpha| \mathrm{diam}(\Omega_H)^{|\alpha|} \left(\frac{r_{\mathrm{c}}}{h} \int_B \frac{|w(|y|)|}{|y|} dy + \sum_{i\in\Xi} \sum_{j=1}^{N} |x_i-x_j| \int_{\sigma_i\cap\omega_j} \frac{|w_h(|x-y|)|}{|x-y|} dy \right).
\end{aligned}$$

By Hypothesis 1.2, we have

$$\int_B \frac{|w(|y|)|}{|y|} dy \leq c$$

and

$$\begin{aligned}
\sum_{i\in\Xi} \sum_{j=1}^{N} |x_i-x_j| \int_{\sigma_i\cap\omega_j} \frac{|w_h(|x-y|)|}{|x-y|} dy &\leq c \frac{1}{h^{d+1}} \sum_{i\in\Xi} \sum_{j=1}^{N} \xi_{ij} |x_i-x_j| \\
&\leq c \frac{1}{h^{d+1}} \sum_{i\in\Xi} \widetilde{V}_i \sum_{j=1}^{N} \frac{\xi_{ij}+\xi_{ji}}{\widetilde{V}_i} |x_i-x_j| \\
&\leq c \left(1 + 2\frac{r_{\mathrm{c}}}{h}\right)^d \frac{1}{h} \max_{i=1,2,\ldots,N} \left(\sum_{j=1}^{N} \frac{\xi_{ij}+\xi_{ji}}{\widetilde{V}_i} |x_i-x_j| \right).
\end{aligned}$$

Since ω is arbitrary, we obtain

$$|E_5(x)| \leq c \left(1 + 2\frac{r_{\mathrm{c}}}{h}\right)^d \frac{r_{\mathrm{c}} + d_{\mathrm{v}}}{h}.$$

Finally, we have

$$|E_6(x)| \le \sum_{i=1}^N \sum_{j=1}^N \xi_{ij} |\psi_\alpha(x_j, x)| \{w_h(|x - x_j|) - w_h(|x - x_i|)\}$$
$$\le \operatorname{diam}(\Omega_H)^{|\alpha|-2} \sum_{i=1}^N \sum_{j=1}^N \xi_{ij} \left| w_h(|x - x_j|) - w_h(|x - x_i|) \right|.$$

By (1.24), we estimate

$$|E_6(x)| \le \operatorname{diam}(\Omega_H)^{|\alpha|-2} \left(1 + \frac{r_{\mathrm{c}}}{h}\right)^d \frac{d_{\mathrm{v}}}{h} |w|_{C^1(\mathbb{R}_0^+)}$$
$$\le c \left(1 + \frac{r_{\mathrm{c}}}{h}\right)^d \frac{d_{\mathrm{v}}}{h}.$$

By estimates of E_k ($k = 4, 5, 6$), we obtain (1.28). □

Finally, using the lemma above, we prove Theorem 1.13.

Proof of Theorem 1.13. Fix $x \in \overline{\Omega}$. By $h < H$, we have $B_h(x) \subset \Omega_H$. Then, for all $x_i \in X_{N,H} \cap B_h(x)$, we obtain Taylor expansion of $v \in C^{k+2}(\overline{\Omega}_H)$:

$$v(x_i) = \sum_{0 \le |\alpha| \le k+1} \frac{D^\alpha v(x)}{\alpha!} (x_i - x)^\alpha + \sum_{|\alpha| = k+2} (x_i - x)^\alpha R_\alpha[v](x_i; x). \tag{1.29}$$

Multiplying both side of (1.29) by $dV_i(x - x_i)|x - x_i|^{-2} w_h(|x - x_i|)$ and taking the sum of these over $i \in \Lambda_x^*$, we have

$$\nabla_h v(x) = d \sum_{1 \le |\alpha| \le k+1} (-1)^{|\alpha|+1} \frac{D^\alpha v(x)}{\alpha!} \sum_{i \in \Lambda_x^*} V_i \frac{(x - x_i)(x - x_i)^\alpha}{|x - x_i|^2} w_h(|x - x_i|)$$
$$+ d \sum_{|\alpha| = k+2} (-1)^{|\alpha|+1} R_\alpha[v](x_i; x) \sum_{i \in \Lambda_x^*} V_i \frac{(x - x_i)(x - x_i)^\alpha}{|x - x_i|^2} w_h(|x - x_i|).$$

For all multi-indexes α_1, α_2 such that $|\alpha_1| = |\alpha_2| = 1$, we have

$$d \int_{\mathbb{R}^d} \frac{y^{\alpha_1} y^{\alpha_2}}{|y|^2} w_h(|y|) dy = \begin{cases} 1, & \alpha_1 = \alpha_2, \\ 0, & \alpha_1 \ne \alpha_2. \end{cases}$$

Then we obtain

$$d \sum_{|\alpha| = 1} D^\alpha v(x) \int_{\mathbb{R}^d} \frac{y y^\alpha}{|y|^2} w_h(|y|) dy = \nabla v(x).$$

Moreover, by Lemma 1.6, for all α such that $3 \le |\alpha| \le k + 2$, we have

$$\int_{\mathbb{R}^d} \frac{y^\alpha}{|y|^2} w_h(|y|) dy = 0.$$

Therefore, we obtain

$$|\nabla v(x) - \nabla_h v(x)| \leq d \sum_{2\leq|\alpha|\leq k+3} |\mathscr{M}_{2,\alpha}(x)|\, |v|_{C^{|\alpha|-1}(\overline{\Omega}_H)} + d \sum_{|\alpha|=k+2} \left| \int_{\mathbb{R}^d} \frac{yy^\alpha}{|y|^2} w(|y|)dy \right| |v|_{C^{k+2}(\overline{\Omega}_H)}.$$

Since

$$\left| \int_{\mathbb{R}^d} \frac{yy^\alpha}{|y|^2} w(|y|)dy \right| = h^{|\alpha|-1} \int_B |y|^{|\alpha|-1} |w(|y|)| dy,$$

we estimate

$$|\nabla v(x) - \nabla_h v(x)| \leq c \left(\sum_{2\leq|\alpha|\leq k+2} |\mathscr{M}_{2,\alpha}(x)|\, |v|_{C^{|\alpha|-1}(\overline{\Omega}_H)} + h^{k+1}\, |v|_{C^{k+2}(\overline{\Omega}_H)} \right). \quad (1.30)$$

Applying (1.7) into Lemma 1.14, for all multi-index α such that $2 \leq |\alpha| \leq k+2$, we have

$$\|\mathscr{M}_{2,\alpha}\|_{C(\overline{\Omega})} \leq ch^{m-1}.$$

Applying this into (1.30), we obtain (1.27). □

1.4.3 Approximate Laplace operator

First, we state the theorem with respect to a truncation error of the approximate Laplace operator (1.4).

Theorem 1.15. *Suppose that* $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ *is a regular family with order* m (≥ 1) *and* w *satisfies Hypothesis* 1.1 *with* k *and Hypothesis* 1.3*. Then there exists a positive constant* c *independent of* h *and* N *such that for all* $v \in C^{k+3}(\overline{\Omega}_H)$,

$$\|\Delta v - \Delta_h v\|_{C(\overline{\Omega})} \leq c \left(h^{k+1}\, |v|_{C^{k+3}(\overline{\Omega}_H)} + h^{m-2}\, \|v\|_{C^{k+3}(\overline{\Omega}_H)} \right). \quad (1.31)$$

Next, before beginning the proof of Theorem 1.15, we show the following lemma.

Lemma 1.16. *Suppose that* w *satisfies Hypothesis* 1.3*. Then there exists a positive constant* c *independent of* h *and* N *such that for all multi-index* α *such that* $|\alpha| \geq 1$,

$$\|\mathscr{M}_{2,\alpha}\|_{C(\overline{\Omega})} \leq c \left(1 + 2\frac{r_{\mathrm{c}}}{h}\right)^d \frac{r_{\mathrm{c}} + d_{\mathrm{v}}}{h^2}. \quad (1.32)$$

Proof. If w satisfies Hypothesis 1.3, then w satisfies also Hypothesis 1.2. Therefore, by Lemma 1.14, for all α such that $|\alpha| \geq 2$, we have

$$\|\mathscr{M}_{2,\alpha}\|_{C(\overline{\Omega})} \leq c \left(1 + 2\frac{r_{\mathrm{c}}}{h}\right)^d \frac{r_{\mathrm{c}} + d_{\mathrm{v}}}{h}.$$

Moreover, by $h \in (0, H)$, we obtain

$$\|\mathscr{M}_{2,\alpha}\|_{C(\overline{\Omega})} \leq c\left(1 + 2\frac{r_{\mathrm{c}}}{h}\right)^d \frac{r_{\mathrm{c}} + d_{\mathrm{v}}}{h^2}.$$

Hereafter, we prove the case of $|\alpha| = 1$. Fix $x \in \overline{\Omega}$. Fix any $\omega(= \{\omega_i\})$ satisfying (1.6). Let $\xi_{ij} := \mathrm{meas}(\sigma_i \cap \omega_j)$ $(i, j = 1, 2, \ldots, N)$. For a multi-index α, let ψ_α be a function on $\mathbb{R}^d \times \mathbb{R}^d$ defined by

$$\psi_\alpha(y, z) := \begin{cases} \dfrac{(y - z)^\alpha}{|y - z|}, & y \neq z, \\ 0, & y = z. \end{cases}$$

Since w satisfies Hypothesis 1.2, we can take $\widehat{w} \in C^1(\mathbb{R}_0^+)$ such that

$$\widehat{w}(r) = \frac{1}{r} w(r), \qquad r \in \mathbb{R}^+.$$

For $\widehat{w}$ and h, let $\widehat{w}_h$ be

$$\widehat{w}_h(r) := \frac{1}{h^d}\widehat{w}\left(\frac{r}{h}\right), \qquad r \in \mathbb{R}_0^+.$$

Set $E_k(x)$ $(k = 7, 8, 9)$ by

$$\begin{aligned} E_7(x) &:= \frac{1}{h}\sum_{i=1}^N \sum_{j=1}^N \psi_\alpha(x_j, x) \int_{\sigma_i \cap \omega_j} \{\widehat{w}_h(|x - x_i|) - \widehat{w}_h(|x - y|)\}\, dy, \\ E_8(x) &:= \frac{1}{h}\sum_{i=1}^N \sum_{j=1}^N \psi_\alpha(x_j, x) \int_{\sigma_i \cap \omega_j} \widehat{w}_h(|x - y|) dy - \int_{\mathbb{R}^d} \frac{y^\alpha}{|y|}\widehat{w}_h(|y|) dy, \\ E_9(x) &:= \frac{1}{h}\sum_{i=1}^N \sum_{j=1}^N \xi_{ij}\psi_\alpha(x_j, x)\left\{\widehat{w}_h(|x - x_j|) - \widehat{w}_h(|x - x_i|)\right\}, \end{aligned}$$

respectively. Since

$$|\mathscr{M}_{2,\alpha}(x)| = \left|\sum_{k=7}^9 E_k(x)\right| \leq \sum_{k=7}^9 |E_k(x)|,$$

we estimate each E_k.

First, we consider E_7. By (1.22), we have

$$\begin{aligned} |E_7(x)| &\leq \frac{1}{h}\sum_{i \in \Xi} \sum_{j=1}^N |\psi_\alpha(x_j, x)| \int_{\sigma_i \cap \omega_j} |\widehat{w}_h(|x - x_i|) - \widehat{w}_h(|x - y|)|\, dy \\ &\leq \frac{1}{h}\sum_{i \in \Xi} \sum_{j=1}^N \int_{\sigma_i \cap \omega_j} |\widehat{w}_h(|x - x_i|) - \widehat{w}_h(|x - y|)|\, dy. \end{aligned}$$

Here, Ξ denotes $\Lambda_{B_{h+r_c}(x)}$. By Taylor expansion, we estimate

$$\begin{aligned}|E_7(x)| &\le \frac{1}{h}\,|\widehat{w}_h|_{C^1(\mathbb{R}_0^+)}\sum_{i\in\Xi}\int_{\sigma_i}|x_i-y|dy\\ &\le \operatorname{meas}(B)\left(1+2\frac{r_c}{h}\right)^d\frac{r_c}{h^2}\,|\widehat{w}|_{C^1(\mathbb{R}_0^+)}\\ &\le c\left(1+2\frac{r_c}{h}\right)^d\frac{r_c}{h^2}.\end{aligned}$$

Next, we consider E_8. For all $x,y,z\in\mathbb{R}^d$ such that $x\neq y$ and $x\neq z$, we have

$$\begin{aligned}|\psi_\alpha(y,x)-\psi_\alpha(z,x)| &\le \left|\frac{(y-x)^\alpha-(z-x)^\alpha}{|y-x|}\right|+\left|\left(\frac{1}{|y-x|}-\frac{1}{|z-x|}\right)(z-x)^\alpha\right|\\ &\le 2\frac{|y-z|}{|y-x|}.\end{aligned}$$

Moreover, for all $x,y,z\in\mathbb{R}^d$ such that $x\neq y$ and $x=z$, we get

$$|\psi_\alpha(y,x)-\psi_\alpha(z,x)|=|\psi_\alpha(y,x)|\le 1=\frac{|y-z|}{|y-x|}.$$

Therefore, by using these estimates, we obtain

$$\begin{aligned}|E_8(x)| &\le \frac{1}{h}\sum_{i\in\Xi}\sum_{j=1}^N\int_{\sigma_i\cap\omega_j}|\psi_\alpha(x_j,x)-\psi_\alpha(x_j,y)|\widehat{w}_h(|x-y|)dy\\ &\le \frac{2}{h}\sum_{i\in\Xi}\sum_{j=1}^N\int_{\sigma_i\cap\omega_j}|y-x_j|\frac{|\widehat{w}_h(|x-y|)|}{|x-y|}dy\\ &\le \frac{2}{h}\sum_{i\in\Xi}\sum_{j=1}^N\int_{\sigma_i\cap\omega_j}(|y-x_i|+|x_i-x_j|)\frac{|\widehat{w}_h(|x-y|)|}{|x-y|}dy\\ &\le \frac{2}{h}\left(\frac{r_c}{h}\int_B\frac{|\widehat{w}(|y|)|}{|y|}dy+\sum_{i\in\Xi}\sum_{j=1}^N|x_i-x_j|\int_{\sigma_i\cap\omega_j}\frac{|\widehat{w}_h(|x-y|)|}{|x-y|}dy\right).\end{aligned}$$

By Hypothesis 1.3, for all $y\in\mathbb{R}^d$, we have

$$\frac{|\widehat{w}(|y|)|}{|y|}\le c.$$

Then we estimate

$$\begin{aligned}|E_8(x)| &\le c\left(\frac{r_c}{h^2}+\frac{1}{h^{d+2}}\sum_{i\in\Xi}\sum_{j=1}^N\xi_{ij}|x_i-x_j|\right)\\ &\le c\left\{\frac{r_c}{h^2}+\left(1+2\frac{r_c}{h}\right)^d\frac{1}{h^2}\max_{i=1,2,\dots,N}\left(\sum_{j=1}^N\frac{\xi_{ij}+\xi_{ji}}{\widetilde{V}_i}|x_i-x_j|\right)\right\}\end{aligned}$$

Since ω is arbitrary, we obtain

$$|E_8(x)| \le c\left(1+2\frac{r_\mathrm{c}}{h}\right)^d \frac{r_\mathrm{c}+d_\mathrm{v}}{h^2}.$$

Finally, we consider E_9. We have

$$\begin{aligned}|E_9(x)| &\le \frac{1}{h}\sum_{i=1}^{N}\sum_{j=1}^{N}\xi_{ij}|\psi_\alpha(x_j,x)|\left\{\widehat{w}_h(|x-x_j|)-\widehat{w}_h(|x-x_i|)\right\}\\ &\le \frac{1}{h}\sum_{i=1}^{N}\sum_{j=1}^{N}\xi_{ij}\left|\widehat{w}_h(|x-x_j|)-\widehat{w}_h(|x-x_i|)\right|.\end{aligned}$$

By (1.24), we estimate

$$\begin{aligned}|E_9(x)| &\le \left(1+\frac{r_\mathrm{c}}{h}\right)^d \frac{d_\mathrm{v}}{h^2}|\widehat{w}|_{C^1(\mathbb{R}_0^+)}\\ &\le c\left(1+\frac{r_\mathrm{c}}{h}\right)^d \frac{d_\mathrm{v}}{h^2}.\end{aligned}$$

By estimates of E_k $(k=7,8,9)$, we obtain (1.32). □

Finally, using the lemma above, we obtain the following proof of Theorem 1.15.
Proof of Theorem 1.15. Fix $x\in\overline{\Omega}$. By $h<H$, we have $B_h(x)\subset\Omega_H$. Then, for all $x_i\in X_{N,H}\cap B_h(x)$, we obtain Taylor expansion of $v\in C^{k+3}(\overline{\Omega}_H)$:

$$v(x_i)=\sum_{0\le|\alpha|\le k+2}\frac{D^\alpha v(x)}{\alpha!}(x_i-x)^\alpha+\sum_{|\alpha|=k+3}(x_i-x)^\alpha R_\alpha[v](x_i;x). \qquad (1.33)$$

Multiplying both side of (1.33) by $2dV_i|x-x_i|^{-2}w_h(|x-x_i|)$ and taking the sum of these over $i\in\Lambda_x^*$, we get

$$\begin{aligned}\Delta_h v(x) &= 2d\sum_{1\le|\alpha|\le k+2}\frac{D^\alpha v(x)}{\alpha!}\sum_{i\in\Lambda_x^*}V_i\frac{(x-x_i)^\alpha}{|x-x_i|^2}w_h(|x-x_i|)\\ &\quad + 2d\sum_{|\alpha|=k+3}R_\alpha[v](x_i;x)\sum_{i\in\Lambda_x^*}V_i\frac{(x_i-x)^\alpha}{|x-x_i|^2}w_h(|x-x_i|).\end{aligned}$$

Since for all multi-index α such that $|\alpha|=2$, we have

$$d\int_{\mathbb{R}^d}\frac{y^\alpha}{|y|^2}w_h(|y|)dy=\begin{cases}1, & \alpha!=2,\\ 0, & \alpha!\ne 2.\end{cases}$$

Then we have

$$d\sum_{|\alpha|=2}D^\alpha v(x)\int_{\mathbb{R}^d}\frac{y^\alpha}{|y|^2}w_h(|y|)dy=\Delta v(x).$$

For all multi-index α such that $|\alpha| = 1$, we get

$$\int_{\mathbb{R}^d} \frac{y^\alpha}{|y|^2} w_h(|y|) dy = 0.$$

Note that the integrand is integrable by Hypothesis 1.3. Moreover, by Lemma 1.6, for all multi-index α such that $3 \le |\alpha| \le k+2$, we have

$$\int_{\mathbb{R}^d} \frac{y^\alpha}{|y|^2} w_h(|y|) dy = 0.$$

Therefore, we obtain

$$\begin{aligned} |\Delta v(x) - \Delta_h v(x)| \le 2d \sum_{1 \le |\alpha| \le k+3} & |\mathscr{M}_{2,\alpha}(x)| \, |v|_{C^{|\alpha|}(\overline{\Omega}_H)} \\ & + 2d \sum_{|\alpha| = k+3} \left| \int_{\mathbb{R}^d} \frac{y^\alpha}{|y|^2} w(|y|) dy \right| |v|_{C^{k+3}(\overline{\Omega}_H)} . \end{aligned}$$

Since

$$\left| \int_{\mathbb{R}^d} \frac{y^\alpha}{|y|^2} w(|y|) dy \right| = h^{|\alpha|-2} \int_B |y|^{|\alpha|-2} |w(|y|)| dy,$$

we estimate

$$|\Delta v(x) - \Delta_h v(x)| \le c \left(\sum_{1 \le |\alpha| \le k+2} |\mathscr{M}_{2,\alpha}(x)| \, |v|_{C^{|\alpha|}(\overline{\Omega}_H)} + h^{k+1} |v|_{C^{k+3}(\overline{\Omega}_H)} \right). \tag{1.34}$$

Applying (1.7) into Lemma 1.16, for all α such that $|\alpha| \ge 1$, we have

$$\|\mathscr{M}_{2,\alpha}\|_{C(\overline{\Omega})} \le c h^{m-2}.$$

Applying this into (1.34), we obtain (1.31). $\square$

Chapter 2

Generalized particle method for the Poisson equation

This chapter considers a generalized particle method for the Poisson equation with Dirichlet boundary conditions. In Section 2.1, the Poisson equation and the discrete Poisson equation are introduced. In Section 2.2, error estimates with a discrete L^∞ norm of the generalized particle method for the Poisson equation are established.

2.1 Formulations

Let Ω be a bounded domain in $\mathbb{R}^d$ ($d \geq 2$) with a piecewise smooth boundary Γ. We consider the Poisson equation with Dirichlet boundary conditions:

$$\left\| \begin{array}{l} \text{Find } u : \Omega \to \mathbb{R} \text{ s.t.} \\ \begin{cases} -\Delta u = f, & \text{in } \Omega, \\ \quad u = g, & \text{on } \Gamma. \end{cases} \end{array} \right. \tag{2.1}$$

Here $f \in C(\overline{\Omega})$ and $g \in C(\Gamma)$ are given functions.

Assume that there exists a unique solution u of the Poisson equation [31]. Now we introduce an expanded solution on Ω_H for the solution u of (2.1). Let Γ_H be $\Gamma_H := \Omega_H \setminus \overline{\Omega}$. Set $\widetilde{g} \in C(\Gamma_H)$ such that $\widetilde{g} = g$ on Γ. Let $\widetilde{u}$ be an expansion of the solution of (2.1) defined by

$$\widetilde{u} = \begin{cases} u, & x \in \Omega, \\ \widetilde{g}, & x \in \Gamma_H. \end{cases}$$

We consider the generalized particle method for the Poisson equation with Dirichlet boundary conditions:

$$\left\| \begin{array}{l} \text{Find } U : X_{N,H} \to \mathbb{R} \text{ s.t.} \\ \begin{cases} -\Delta_h U_i = f_i, & i \in \Lambda_\Omega, \\ \quad U_i = \widetilde{g}_i, & i \in \Lambda_{\Gamma \cup \Gamma_H}. \end{cases} \end{array} \right. \tag{2.2}$$

Here v_i denotes $v(x_i)$.

2.2 Error estimates with a discrete L^∞ norm

In this section, let c be a generic positive constant independent of h and N. For $v : X_{N,H} \to \mathbb{R}$ and $S \subset \mathbb{R}^d$, a discrete L^∞ norm $\|.\|_{\ell^\infty(S)}$ is defined by

$$\|v\|_{\ell^\infty(S)} := \max_{i\in\Lambda_S} |v_i| .$$

Now, we state the theorem of the error estimates by the discrete L^∞ norm.

Theorem 2.1. (**Error estimate of the discrete Poisson equation by the discrete L^∞ norm**) *Let u and U be solutions of* (2.1) *and* (2.2)*, respectively. Suppose that the expanded solution $\widetilde{u}$ satisfies $\widetilde{u} \in C^4(\overline{\Omega}_H)$, $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ is a regular family with order m (> 2), and w satisfies Hypothesis* 1.3 *and Hypothesis* 1.4*. Then there exists a positive constant c and h_0 independent of h and N such that for all $\{(X_{N,H}, V_{N,H}, h)\}$ with $h < h_0$*

$$\|\widetilde{u} - U\|_{\ell^\infty(\Omega_H)} \le c\, h^{\min\{2,m-2\}} \|\widetilde{u}\|_{C^4(\overline{\Omega}_H)} . \tag{2.3}$$

Before beginning the proof of Theorem 2.1, we show some results.

Theorem 2.2. (***Unique solvability***) *Suppose that w satisfies Hypothesis* 1.4*. Then the necessary and sufficient condition that* (2.2) *has a unique solution is that $X_{N,H}$ satisfies the h-connectivity.*

Proof. First, assume $X_{N,H}$ satisfies the h-connectivity. Let N_Ω be a number of particles included in Ω. We renumber the index of particles so that $i \in \Lambda_\Omega$ $(i = 1, 2, \dots, N_\Omega)$ and $i \in \Lambda_{\Gamma\cup\Gamma_H}$ $(i = N_\Omega + 1, N_\Omega + 2, \dots, N)$. Let $b_{ij} \in \mathbb{R}_0^+$ $(i, j = 1, 2, \dots, N)$ be

$$b_{ij} := \begin{cases} 0, & i = j, \\ 2d\dfrac{w_h(|x_i - x_j|)}{|x_i - x_j|^2}, & i \ne j. \end{cases}$$

Let $A, D \in \mathbb{R}^{N_\Omega\times N_\Omega}$ and $\mathbf{f}, \mathbf{u} \in \mathbb{R}^{N_\Omega}$ be

$$\begin{aligned} A_{ij} &:= \begin{cases} \displaystyle\sum_{k=1}^{N} \frac{V_k}{V_i} b_{ik}, & i = j, \\ -b_{ij}, & i \ne j, \end{cases} \\ D &:= \operatorname{diag}(V_i), \\ \mathbf{f}_i &:= f_i - \sum_{j=N_\Omega+1}^{N} V_j \widetilde{g}_j b_{ij}, \qquad i = 1, 2, \dots, N, \\ \mathbf{u}_i &:= U_i, \qquad i = 1, 2, \dots, N, \end{aligned}$$

respectively. Then we can write (2.2) as

$$AD\mathbf{u} = \mathbf{f}.$$

By $V_i \in \mathbb{R}^+$ $(i = 1, 2, \dots, N)$, D is the regular matrix. Then it is sufficient to prove that A is a regular matrix. Since A is symmetric, we prove that A is a positive definite. For all $a \in \mathbb{R}^{N_\Omega} \setminus \{0\}$, we have

$$\begin{aligned}\sum_{i,j=1}^{N_\Omega} a_i a_j A_{ij} &= 2 \sum_{1 \le i < j \le N_\Omega} a_i a_j A_{ij} + \sum_{1 \le i \le N_\Omega} a_i^2 A_{ii} \\ &= -2 \sum_{1 \le i < j \le N_\Omega} a_i a_j b_{ij} + \sum_{i=1}^{N_\Omega} a_i^2 \sum_{k=1}^{N} \frac{V_k}{V_i} b_{ik} \\ &= \sum_{1 \le i < j \le N_\Omega} \frac{\left(V_j a_i - V_i a_j\right)^2}{V_i V_j} b_{ij} + \sum_{i=1}^{N_\Omega} a_i^2 \sum_{k=N_\Omega+1}^{N} \frac{V_k}{V_i} b_{ik} \end{aligned} \tag{2.4}$$

Since b_{ij} is nonnegative, (2.4) is nonnegative. For $a \in \mathbb{R}^{N_\Omega} \setminus \{0\}$, we set i such that $a_i \neq 0$. Since $X_{N,H}$ satisfies the h-connectivity, there exists $i_j \in \mathbb{N}$ $(j = 1, \dots, m)$ such that

$$\begin{cases} i_1 = i, \\ i_j \in \Lambda_\Omega \text{ and } |x_{i_j} - x_{i_{j+1}}| < h \ (j = 1, 2, \dots, m-1), \\ i_m \in \Lambda_{\Gamma \cup \Gamma_H}. \end{cases}$$

Since the all terms of the last equation in (2.4) are nonnegative, for the subsequence, we have

$$\sum_{i,j=1}^{N_\Omega} a_i a_j A_{ij} \ge \sum_{k=1}^{m-1} \frac{\left(V_{i_{k+1}} a_{i_k} - V_{i_k} a_{i_{k+1}}\right)^2}{V_{i_k} V_{i_{k+1}}} b_{i_k i_{k+1}} + \frac{V_{i_m}}{V_{i_{m-1}}} a_{i_m}^2 b_{i_{m-1} i_m}.$$

Since $b_{i_k i_{k+1}}$ $(k = 1, 2, \dots, m)$ is positive, the right hand side of this inequality is positive. Therefore, for all $a \in \mathbb{R}^{N_\Omega} \setminus \{0\}$, we have

$$\sum_{i,j=1}^{N_\Omega} a_i a_j A_{ij} > 0.$$

Consequently, A is the positive definite.

Next, in order to show the proposition that $X_{N,H}$ satisfies the h-connectivity if there exists uniquely the solution of (2.2), we will prove the contrapositive. Suppose that $X_{N,H}$ does not satisfy the h-connectivity. Then there exists $\widehat{\Lambda} \subset \Lambda_\Omega$ such that

$$\forall i \in \widehat{\Lambda}, \quad \forall j \in \Lambda_{\Omega_H} \setminus \widehat{\Lambda}, \quad |x_i - x_j| \ge h.$$

We fix $i \in \widehat{\Lambda}$ and consider the i-th column of the matrix AD. For all $j \in \widehat{\Lambda}$, we have

$$(AD)_{ji} = -\sum_{k \in \widehat{\Lambda}} (AD)_{jk}.$$

Moreover, for all $j \in \Lambda_\Omega \setminus \widehat{\Lambda}$ and $k \in \widehat{\Lambda}$, we get

$$(AD)_{jk} = 0.$$

By these, for all $j \in \Lambda_\Omega$, we have

$$(AD)_{ji} = -\sum_{k\in\widehat{\Lambda}} (AD)_{jk}.$$

Therefore, we find

$$\det(AD) = 0.$$

Then AD is not the regular matrix. Consequently, since the contrapositive are proved, $X_{N,H}$ satisfies the h-connectivity if there exists uniquely the solution of (2.2). □

Lemma 2.3. *Suppose that* $v_i \in \mathbb{R}$ $(i = 1, 2, \dots, N)$ *satisfy*

$$\begin{cases} -\Delta_h v_i \geq 0, & i \in \Lambda_\Omega, \\ \quad v_i \geq 0, & i \in \Lambda_{\Gamma\cup\Gamma_H}, \end{cases} \tag{2.5}$$

w satisfies Hypothesis 1.4*, and $X_{N,H}$ satisfies the h-connectivity. Then, for all $i = 1, 2, \dots, N$, we obtain*

$$v_i \geq 0. \tag{2.6}$$

Proof. Set k by

$$k := \underset{i=1,2,\dots,N}{\arg\min}\; v_i.$$

If $k \in \Lambda_{\Gamma\cup\Gamma_H}$, then (2.6) is obviously true.

Suppose that $k \in \Lambda_\Omega$. Since $X_{N,H}$ satisfies the h-connectivity, there exists $\{x_{k_l}\}_{l=1}^m \subset X_{N,H}$ such that

$$x_{k_1} = x_k, \quad |x_{k_l} - x_{i_{l+1}}| < h \ (l = 1, 2, \dots, m-1), \quad x_{k_m} \in \Gamma \cup \Gamma_H.$$

By Hypothesis 1.4, we have

$$-\Delta_h v_{k_1} = 2d \sum_{j\neq k} V_j \frac{v_k - v_j}{|x_k - x_j|^2} w_h(|x_k - x_j|) \leq 2d V_{k_2} \frac{v_{k_1} - v_{k_2}}{|x_{k_1} - x_{k_2}|^2} w_h(|x_{k_1} - x_{k_2}|) \leq 0.$$

After all, by (2.5), we obtain

$$-\Delta_h v_{k_1} = 0.$$

Since $|x_{k_1} - x_{k_2}| < h$, we have $v_{k_1} = v_{k_2}$. By repeating the argument above with $l = 2, 3, \dots, m-1$, we obtain $v_{k_1} = v_{k_2} = \cdots = v_{k_m}$. Since $v_k = v_{k_m} \geq 0$, we find that (2.6) is true. □

Lemma 2.4. (***Discrete maximum principle***) *Suppose that* $v_i \in \mathbb{R}$ $(i = 1, 2, \dots, N)$ *satisfy*

$$-\Delta_h v_i \leq 0, \qquad i \in \Lambda_\Omega,$$

w satisfies Hypothesis 1.4*, and $X_{N,H}$ satisfies the h-connectivity. Then we obtain*

$$v_i \leq \max_{j\in\Lambda_{\Gamma\cup\Gamma_H}} \{v_j\} \quad i = 1, 2, \dots, N. \tag{2.7}$$

Proof. Let φ_i $(i = 1, 2, \ldots, N)$ be

$$\varphi_i := -v_i + \max_{j \in \Lambda_{\Gamma \cup \Gamma_H}} \{v_j\}.$$

Then we have

$$-\Delta_h \varphi_i = \Delta_h v_i \geq 0, \qquad i \in \Lambda_\Omega$$

and

$$\varphi_i \geq 0, \qquad i \in \Lambda_{\Gamma \cup \Gamma_H}.$$

Hence, by Lemma 2.3, we have

$$\varphi_i \geq 0, \qquad i = 1, 2, \ldots, N.$$

Consequently, we obtain (2.7). □

Lemma 2.5. (***Stability***) *Suppose that for* $\phi : X_{N,H} \to \mathbb{R}$*,* $v : X_{N,H} \to \mathbb{R}$ *satisfies*

$$\begin{cases} -\Delta_h v_i = \phi_i, & i \in \Lambda_\Omega, \\ \quad\;\; v_i = \phi_i, & i \in \Lambda_{\Gamma \cup \Gamma_H}, \end{cases}$$

$\{(X_{N,H}, V_{N,H}, h)\}$ *is a regular family with order* m (> 2) *whose* $X_{N,H}$ *satisfies the* h*-connectivity, and* w *satisfies Hypothesis* 1.3 *and Hypothesis* 1.4*. Then there exists a positive constant* c *and* h_0 *independent of* h *and* N *such that for all* $\{(X_{N,H}, V_{N,H}, h)\}$ *with* $h < h_0$*,*

$$\|v\|_{\ell^\infty(\Omega_H)} \leq c \|\phi\|_{\ell^\infty(\Omega_H)}. \tag{2.8}$$

Proof. We first show

$$v_i \leq c \|\phi\|_{\ell^\infty(\Omega_H)}, \quad i = 1, 2, \ldots, N. \tag{2.9}$$

Set $z \in \mathbb{R}^d$ such that

$$|x - z| \leq \mathrm{diam}(\Omega_H), \quad \forall x \in \overline{\Omega}_H.$$

Let $\Phi : \overline{\Omega}_H \to \mathbb{R}$ be

$$\Phi(x) := -\frac{1}{2d}(x - z)^2 + \frac{1}{2d}\mathrm{diam}(\Omega_H)^2 + 1.$$

Since $\Phi \in C^\infty(\overline{\Omega}_H)$ and $|\Phi|_{C^l(\overline{\Omega}_H)} = 0$ $(l \geq 3)$, by Theorem 1.15, there exists a positive constant c_1 independent of $X_{N,H}$, $V_{N,H}$, and h such that

$$\|\Delta\Phi - \Delta_h \Phi\|_{C(\overline{\Omega})} \leq c_1 h^{m-2}.$$

Therefore, by $\Delta\Phi \equiv -1$, we have

$$-\Delta_h \Phi_i \geq 1 - c_1 h^{m-2}, \quad i = 1, 2, \ldots, N. \tag{2.10}$$

Take h_0 satisfying

$$0 < h_0^{m-2} < \frac{1}{c_1}.$$

By (2.10), for all $h < h_0$, we have

$$-\Delta_h \Phi_i \geq 1 - c_1 h_0^{m-2} > 0, \quad i = 1, 2, \ldots, N. \tag{2.11}$$

Let φ_i $(i = 1, 2, \ldots, N)$ be

$$\varphi_i := v_i - (1 - c_1 h_0^{m-2})^{-1} \|\phi\|_{\ell^\infty(\Omega)} \Phi_i.$$

By (2.11), for all $h < h_0$ and $i = 1, \ldots, N_\Omega$, we have

$$\begin{aligned}
-\Delta_h \varphi_i &= -\Delta_h v_i + (1 - c_1 h_0^{m-2})^{-1} \|\phi\|_{\ell^\infty(\Omega)} \Delta_h \Phi_i \\
&\leq \phi_i - \|\phi\|_{\ell^\infty(\Omega)} \\
&\leq 0.
\end{aligned}$$

Since $\Phi \geq 1$ and by Theorem 2.4, we estimate

$$\begin{aligned}
\varphi_i &\leq \max_{j \in \Lambda_{\Gamma \cup \Gamma_H}} \left\{ v_j - (1 - c_1 h_0^{m-2})^{-1} \|\phi\|_{\ell^\infty(\Omega)} \Phi_j \right\} \\
&\leq \max_{j \in \Lambda_{\Gamma \cup \Gamma_H}} \{v_j\} - (1 - c_1 h_0^{m-2})^{-1} \|\phi\|_{\ell^\infty(\Omega)} \min_{j \in \Lambda_{\Gamma \cup \Gamma_H}} \{\Phi_j\} \\
&\leq \|\phi\|_{\ell^\infty(\Gamma \cup \Gamma_H)} - (1 - c_1 h_0^{m-2})^{-1} \|\phi\|_{\ell^\infty(\Omega)}.
\end{aligned}$$

Therefore, since

$$\Phi_i \leq \frac{1}{2d} \mathrm{diam}(\Omega_H)^2 + 1, \quad i = 1, 2, \ldots, N, \tag{2.12}$$

for all $i = 1, 2, \ldots, N$, we obtain

$$\begin{aligned}
v_i &\leq \|\phi\|_{\ell^\infty(\Gamma \cup \Gamma_H)} + \frac{\Phi_i - 1}{1 - c_1 h_0^{m-2}} \|\phi\|_{\ell^\infty(\Omega)} \\
&\leq \|\phi\|_{\ell^\infty(\Gamma \cup \Gamma_H)} + \frac{\mathrm{diam}(\Omega_H)^2}{2d(1 - c_1 h_0^{m-2})} \|\phi\|_{\ell^\infty(\Omega)} \\
&\leq \max \left\{ 1, \frac{\mathrm{diam}(\Omega_H)^2}{2d(1 - c_1 h_0^{m-2})} \right\} \|\phi\|_{\ell^\infty(\Omega_H)}.
\end{aligned}$$

Then (2.9) is proved.

Next, we show

$$v_i \geq -c \|\phi\|_{\ell^\infty(\Omega_H)}, \quad i = 1, 2, \ldots, N. \tag{2.13}$$

Let ψ_i $(i = 1, 2, \ldots, N)$ be

$$\psi_i := -v_i - \left(1 - c h_0^{m-2}\right)^{-1} \|\phi\|_{\ell^\infty(\Omega)} \Phi(x_i).$$

By (2.11), for all $h < h_0,\ i = 1, \ldots, N_\Omega$, we have

$$\begin{aligned}-\Delta_h \psi_i &= \Delta_h v_i + \left(1 - c h_0^{m-2}\right)^{-1} \|\phi\|_{\ell^\infty(\Omega)} \Delta_h \Phi(x_i) \\ &\le -\phi_i - \|\phi\|_{\ell^\infty(\Omega)} \\ &\le 0.\end{aligned}$$

Since $\Phi \ge 1$ and Theorem 2.4, we estimate

$$\begin{aligned}\psi_i &\le \max_{j \in \Lambda_{\Gamma \cup \Gamma_H}} \left\{-v_j - (1 - c_1 h_0^{m-2})^{-1} \|\phi\|_{\ell^\infty(\Omega)} \Phi_j\right\} \\ &\le \max_{j \in \Lambda_{\Gamma \cup \Gamma_H}} \{-v_j\} - (1 - c_1 h_0^{m-2})^{-1} \|\phi\|_{\ell^\infty(\Omega)} \min_{j \in \Lambda_{\Gamma \cup \Gamma_H}} \{\Phi_j\} \\ &\le \|\phi\|_{\ell^\infty(\Gamma \cup \Gamma_H)} - (1 - c_1 h_0^{m-2})^{-1} \|\phi\|_{\ell^\infty(\Omega)}.\end{aligned}$$

Therefore, by (2.12), for all $i = 1, 2, \ldots, N$, we have

$$\begin{aligned}v_i &\ge - \|\phi\|_{\ell^\infty(\Gamma \cup \Gamma_H)} - \frac{\Phi_i - 1}{1 - c_1 h_0^{m-2}} \|\phi\|_{\ell^\infty(\Omega)} \\ &\ge - \|\phi\|_{\ell^\infty(\Gamma \cup \Gamma_H)} - \frac{\operatorname{diam}(\Omega_H)^2}{2d(1 - c_1 h_0^{m-2})} \|\phi\|_{\ell^\infty(\Omega)} \\ &\ge - \max\left\{1, \frac{\operatorname{diam}(\Omega_H)^2}{2d(1 - c_1 h_0^{m-2})}\right\} \|\phi\|_{\ell^\infty(\Omega_H)}.\end{aligned}$$

Then (2.13) is shown. Consequently, we obtain (2.8). □

Utilizing the results above, we prove Theorem 2.1.

Proof of Theorem 2.1. Since $m > 2$, by the definition of the regular (1.7), there exists a positive constant h_1 such that

$$h > 2r_c, \qquad \forall h < h_1.$$

By Lemma 1.10 and Lemma 2.2, for all $h < h_1$, the discrete Poisson equation (2.2) is solvable.

Let e_i $(i = 1, 2, \ldots, N)$ be

$$e_i := \widetilde{u}_i - U_i.$$

For all $i \in \Lambda_\Omega$, we have

$$-\Delta_h e_i = -\Delta_h \widetilde{u}_i + \Delta_h U_i = -\Delta_h \widetilde{u}_i - f_i = \Delta \widetilde{u}_i - \Delta_h \widetilde{u}_i.$$

Moreover, for all $i \in \Lambda_{\Gamma_H}$, we get

$$e_i = 0.$$

Then, by Lemma 2.5, we obtain

$$\begin{aligned}\|u - U\|_{\ell^\infty(\Omega_H)} &= \|e\|_{\ell^\infty(\Omega)} \\ &\le c \, \|\Delta \widetilde{u} - \Delta_h \widetilde{u}\|_{C(\overline{\Omega})}.\end{aligned}$$

By Lemma 1.5 and Theorem 1.15, we have

$$\|\Delta \widetilde{u} - \Delta_h \widetilde{u}\|_{C(\overline{\Omega})} \le c \, h^{\min\{2, m-2\}} \, \|\widetilde{u}\|_{C^4(\overline{\Omega}_H)}.$$

Consequently we obtain (2.3). □

Chapter 3

Generalized particle method for the heat equation

This chapter deals with a heat equation with Dirichlet boundary conditions discretized by a generalized particle method in space and the θ-method in time for the heat equation. In Section 3.1, the heat equation and the discrete heat equation are formulated. In Section 3.2, error estimates with a discrete L^∞ norm in space and time of approximate solutions of the discrete heat equation are established. Moreover, in Section 3.3, error estimates with an discrete L^2 norm in space and the discrete L^∞ norm in time are also obtained.

3.1 Formulations

Let Ω be a bounded domain in $\mathbb{R}^d$ $(d \geq 2)$ with a piecewise smooth boundary Γ. We consider the heat equation with Dirichlet boundary conditions:

$$\left\| \begin{array}{l} \text{Find } u : \Omega \times (0,T) \to \mathbb{R} \text{ s.t.} \\ \begin{cases} \partial_t u + Lu = f, & \text{in } \Omega \times (0,T), \\ u = g, & \text{on } \Gamma \times (0,T), \\ u = a, & \text{in } \Omega, \text{ at } t = 0. \end{cases} \end{array} \right. \tag{3.1}$$

Here, $f \in C(\overline{\Omega} \times [0,T))$ is an external heat source, $g \in C(\Gamma \times (0,T))$ is a boundary temperature, $a \in C(\Omega)$ is an initial temperature. Moreover $\partial_t := \partial/\partial t$, $L := -\kappa\Delta$, and $\kappa \in \mathbb{R}^+$ is the thermal conductivity.

Assume that there exists a unique solution u of the heat equation [31]. Set $\widetilde{g} \in C(\Gamma_H \times (0,T))$ such that $\widetilde{g} = g$ on $\Gamma \times (0,T)$ and $\widetilde{a} \in C(\Omega_H)$ such that $\widetilde{a} = a$ on Ω and $\widetilde{a} = \widetilde{g}|_{t=0}$ on Γ_H. Let $\widetilde{u}$ be an expanded solution on $\Omega_H \times (0,T)$ for the solution u of (3.1) defined by

$$\widetilde{u} := \begin{cases} u, & (x,t) \in \Omega \times (0,T), \\ \widetilde{g}, & (x,t) \in \Gamma_H \times (0,T). \end{cases}$$

Set a positive integer K and time step Δt by $\Delta t := T/K$. For $k = 0, 1, \ldots, K$, let us denote $k\Delta t$ as t^k . Let I_K be $I_K := \{t^k;\ k = 0, 1, \ldots, K\}$. For $v : I_K \to \mathbb{R}$, the approximate operator $D_{\Delta t}$ is defined by

$$D_{\Delta t} v^k := \frac{v^{k+1} - v^k}{\Delta t}, \qquad k = 0, 1, \ldots, K-1.$$

Here we denote $v(t^k)$ as v^k.

Let L_h be $L_h := -\kappa \Delta_h$. Then we consider the generalized particle method for the heat equation with Dirichlet boundary conditions:

$$\left\| \begin{array}{l} \text{Find } U : X_{N,H} \times I_K \to \mathbb{R} \text{ s.t.} \\ \begin{cases} D_{\Delta t} U_i^k + L_h U_i^{k+\theta} = f_i^{k+\theta}, & i \in \Lambda_\Omega, \quad k = 0, 1, \ldots, K-1, \\ U_i^k = \widetilde{g}_i^k, & i \in \Lambda_{\Gamma \cup \Gamma_H}, \quad k = 1, 2, \ldots, K, \\ U_i^0 = \widetilde{a}_i, & i \in \Lambda_{\Omega_H}. \end{cases} \end{array} \right. \tag{3.2}$$

Here $\theta \in [0, 1]$, $v^{k+\theta} = \theta v^{k+1} + (1-\theta) v^k$, and $v_i^k := v(x_i, t^k)$.

3.2 Error estimates with a discrete L^∞ norm

For a set $S \subset \mathbb{R}$ and Banach space X, a discrete L^∞ norm in time $\|.\|_{\ell^\infty(S;X)}$ is defined by

$$\|v\|_{\ell^\infty(S;X)} := \max \left\{ \|v^k\|_X;\ k = 0, 1, \ldots, K,\ t^k \in I_K \cap S \right\}.$$

Now, we state the theorem with respect to the errors between solutions of (3.1) and (3.2) by the maximum norm $\|.\|_{\ell^\infty([0,T];\ell^\infty(\Omega_H))}$.

Theorem 3.1. (***Error estimate of the discrete heat equation by the discrete L^∞ norm***) *Let u and U be solutions of (3.1) and (3.2), respectively. Suppose that the expanded solution $\widetilde{u}$ satisfies $\widetilde{u} \in C^2([0,T]; C^4(\overline{\Omega}_H))$, $\{(X_{N,H}, V_{N,H}, h)\}_{h \downarrow 0}$ is a regular family with order m (> 2), and w satisfies Hypothesis 1.3 and Hypothesis 1.4. Moreover, when $\theta \in [0, 1)$, suppose that for any fixed $\delta \in (0, 1)$, Δt satisfies*

$$\Delta t \le \min \left\{ \frac{\delta}{2 d \kappa (1-\theta)} \left(\int_{\mathbb{R}^d} \frac{1}{|x|^2} w(|x|) dx \right)^{-1} h^2, \frac{1}{1-\theta} \right\}. \tag{3.3}$$

Then there exists a positive constant c and h_0 independent of h, N, and Δt such that for all $\{(X_{N,H}, V_{N,H}, h)\}$ with $h < h_0$,

$$\|\widetilde{u} - U\|_{\ell^\infty([0,T];\ell^\infty(\Omega_H))} \le c \, (\Delta t + h^{\min\{2, m-2\}}) \, \|\widetilde{u}\|_{C^2([0,T];C^4(\overline{\Omega}_H))}. \tag{3.4}$$

Furthermore, if $\widetilde{u} \in C^3([0,T]; C^4(\overline{\Omega}_H))$ and $\theta = 1/2$, then

$$\|\widetilde{u} - U\|_{\ell^\infty([0,T];\ell^\infty(\Omega_H))} \le c \, (\Delta t^2 + h^{\min\{2, m-2\}}) \, \|\widetilde{u}\|_{C^3([0,T];C^4(\overline{\Omega}_H))}. \tag{3.5}$$

Here,

$$\|v\|_{C^m([0,T];C^n(\overline{\Omega}_H))} := \max_{k=0,1,\ldots,m} \max_{t \in [0,T]} \|\partial_t^k v(\cdot, t)\|_{C^n(\overline{\Omega}_H)}.$$

Hereafter, in this section, let c be a generic positive constant independent of h, N, and Δt. Before beginning the proof of Theorem 3.1, we show some results

Theorem 3.2. (***Unique solvability***) *Suppose that w satisfies Hypothesis* 1.4 *if $\theta \in (0,1]$. Then* (3.2) *has a unique solution.*

Proof. Let N_Ω be a number of particles included in Ω. We renumber the index of particles so that $i \in \Lambda_\Omega$ $(i = 1,2,\dots,N_\Omega)$ and $i \in \Lambda_{\Gamma\cup\Gamma_H}$ $(i = N_\Omega+1, N_\Omega+2,\dots,N)$. Let $b_{ij} \in \mathbb{R}_0^+$ $(i,j = 1,2,\dots,N)$ be

$$b_{ij} := \begin{cases} 0, & i = j, \\ 2d\kappa\Delta t \dfrac{w_h(|x_i - x_j|)}{|x_i - x_j|^2}, & i \neq j. \end{cases}$$

Set $A \in \mathbb{R}^{N_\Omega \times N_\Omega}$, $D \in \mathbb{R}^{N_\Omega \times N_\Omega}$, and $\mathbf{f}^{k+\theta} \in \mathbb{R}^{N_\Omega}$ $(k = 0,1,\dots,K,\ \theta \in [0,1])$ by

$$\begin{aligned} A_{ij} &:= \begin{cases} \displaystyle\sum_{k=1}^{N} \frac{V_k}{V_i} b_{ik}, & i = j, \\ -b_{ij}, & i \neq j, \end{cases} \\ D &:= \operatorname{diag}(V_i), \\ \mathbf{f}_i^{k+\theta} &:= \Delta t f_i^{k+\theta} + \sum_{j \in \Lambda_{\Gamma\cup\Gamma_H}} V_j \tilde{g}_j^{k+\theta} b_{ij}, \quad i = 1,2,\dots,N, \end{aligned}$$

respectively. Then we can write (3.2) as

$$\begin{cases} (I + \theta AD)\mathbf{u}^{k+1} = (I - (1-\theta)AD)\mathbf{u}^k + \mathbf{f}^{k+\theta}, \quad k = 0,1,\dots,K-1 \\ \mathbf{u}^0 = \mathbf{u}_0. \end{cases}$$

Here, $\mathbf{u}^k := (U_1^k, U_2^k, \dots, U_{N_\Omega}^k)^T$, $\mathbf{u}_0 := (\tilde{a}_1, \tilde{a}_2, \dots, \tilde{a}_{N_\Omega})^T$, and $I \in \mathbb{R}^{N_\Omega \times N_\Omega}$ is the identity matrix. Therefore, if $(I + \theta AD)$ is the regular matrix, then (3.2) has a unique solution. In case that $\theta = 0$, then $(I + \theta AD)$ is obviously the regular matrix.

Hereafter, we consider case that $\theta \in (0,1]$. Let R be $R := D^{-1} + \theta A$. Then we have $(I + \theta AD) = RD$. Since D is the regular matrix and R is symmetric, it is sufficient to show that R is the positive definite. For all $a \in \mathbb{R}^{N_\Omega}$, we have

$$\begin{aligned} \sum_{i,j=1}^{N_\Omega} a_i a_j R_{ij} &= \sum_{i,j=1}^{N_\Omega} a_i a_j ([D^{-1}]_{ij} + \theta A_{ij}) \\ &= \sum_{i=1}^{N_\Omega} a_i^2 \left(\frac{1}{V_i} + \theta A_{ii} \right) + 2\theta \sum_{1 \le i < j \le N} a_i a_j A_{ij} \\ &= \sum_{i=1}^{N_\Omega} \frac{a_i^2}{V_i} \left(1 + \theta \sum_{l=1}^{N_\Omega} V_l b_{il} + \theta \sum_{l=N_\Omega+1}^{N} V_k b_{ik} \right) - 2\theta \sum_{1 \le i < j \le N} a_i a_j b_{ij} \\ &= \sum_{i=1}^{N_\Omega} \frac{a_i^2}{V_i} \left(1 + \theta \sum_{l=N_\Omega+1}^{N} V_l b_{il} \right) + \theta \sum_{1 \le i < j \le N} \frac{(V_j a_i - V_i a_j)^2}{V_i V_j} b_{ij}. \end{aligned}$$

By Hypothesis 1.4, the equation is 0 if and only if $a = 0$. Then R is the positive definite matrix. Therefore, (3.2) has a unique solution. □

Lemma 3.3. *Suppose that* $v_i^k \in \mathbb{R}$ $(i = 1, 2, \ldots, N,\ k = 0, 1, \ldots, K)$ *satisfy*

$$\begin{cases} D_{\Delta t} v_i^k + L_h v_i^{k+\theta} \geq 0, & i \in \Lambda_\Omega, \quad k = 0, 1, \ldots, K-1, \\ v_i^k \geq 0, & i \in \Lambda_{\Gamma \cup \Gamma_H}, \quad k = 1, 2, \ldots, K, \\ v_i^0 \geq 0, & i \in \Lambda_{\Omega_H} \end{cases} \tag{3.6}$$

and w *satisfies Hypothesis* 1.4*. Moreover, when* $\theta \in [0, 1)$*, suppose that* Δt *satisfies*

$$\Delta t \leq \frac{1}{2d\kappa(1-\theta)} \left[\max_{i \in \Lambda_\Omega} \left\{ \sum_{j \neq i} V_j \frac{w_h(|x_i - x_j|)}{|x_i - x_j|^2} \right\} \right]^{-1}. \tag{3.7}$$

Then for all $i \in \Lambda_{\Omega_H}$ *and* $k = 0, 1, \ldots, K$*, we obtain*

$$v_i^k \geq 0. \tag{3.8}$$

Proof. For $k = 0, 1, \ldots, K$, let α_k be

$$\alpha_k := \min_{i=1,2,\ldots,N} v_i^k.$$

We will prove inductively that

$$\alpha_k \geq 0, \qquad \forall k = 0, 1, \ldots, K. \tag{3.9}$$

By (3.6), we have $\alpha_0 \geq 0$. Let n be a positive integer not greater than K. Suppose that (3.9) holds when $k = n - 1$. Let l be an integer so that $v_l^n = \alpha_n$. For $i, j = 1, 2, \ldots, N$, we set λ_{ij} by

$$\lambda_{ij} := \begin{cases} 0, & i = j, \\ 2d\kappa\Delta t V_j \dfrac{w_h(|x_i - x_j|)}{|x_i - x_j|^2} & i \neq j. \end{cases}$$

In case that $\theta = 1$, by Hypothesis 1.4, we have

$$\begin{aligned} \alpha_{n-1} &\leq v_l^{n-1} \\ &\leq v_l^n + \Delta t L_h v_l^n \\ &= v_l^n \left(1 + \sum_{j \neq l} \lambda_{lj} \right) - \sum_{j \neq l} \lambda_{lj} v_j^n \\ &\leq \alpha_n \left(1 + \sum_{j \neq l} \lambda_{lj} \right) - \alpha_n \sum_{j \neq l} \lambda_{lj} \\ &= \alpha_n. \end{aligned}$$

Moreover, in case that $\theta \in [0,1)$, by Hypothesis 1.4 and (3.7), we get

$$\begin{aligned}
\alpha_{n-1} &= \alpha_{n-1}\left\{1-(1-\theta)\sum_{j\neq l}\lambda_{lj}\right\} + \alpha_{n-1}(1-\theta)\sum_{j\neq l}\lambda_{lj} \\
&\le v_l^{n-1}\left\{1-(1-\theta)\sum_{j\neq l}\lambda_{lj}\right\} + (1-\theta)\sum_{j\neq l}\lambda_{lj}v_j^{n-1} \\
&= v_l^{n-1} - (1-\theta)\Delta t L_h v_l^{n-1} \\
&\le v_l^n + \theta\Delta t L_h v_l^n \\
&= v_l^n\left(1+\theta\sum_{j\neq l}\lambda_{lj}\right) - \theta\sum_{j\neq l}\lambda_{lj}v_j^n \\
&\le \alpha_n\left(1+\theta\sum_{j\neq l}\lambda_{lj}\right) - \alpha_n\theta\sum_{j\neq l}\lambda_{lj} \\
&= \alpha_n.
\end{aligned}$$

Therefore, (3.9) also holds when $k=n$. Consequently, since (3.9) is true, we obtain (3.8). □

Lemma 3.4. (***Discrete maximum principle***) *Suppose that $v_i^k \in \mathbb{R}$ $(i=1,2,\ldots,N,\ k=0,1,\ldots,K)$ satisfies*

$$D_{\Delta t}v_i^k + L_h v_i^{k+\theta} \le 0, \qquad i\in\Lambda_\Omega,\ k=0,1,\ldots,K-1,$$

and w satisfies Hypothesis 1.4. Moreover, suppose (3.7) if $\theta\in[0,1)$. Then for all $i=1,2,\ldots,N$ and $k=0,1,\ldots,K$, we obtain

$$v_i^k \le \|v^0\|_{\ell^\infty(\Omega_H)} + \max_{l=0,1,\ldots,k}\|v^l\|_{\ell^\infty(\Gamma\cup\Gamma_H)}. \tag{3.10}$$

Proof. Let φ_i^k $(i=1,2,\ldots,N,\ k=0,1,\ldots,K)$ be

$$\varphi_i^k := -v_i^k + \|v^0\|_{\ell^\infty(\Omega_H)} + \max_{l=0,1,\ldots,k}\|v^l\|_{\ell^\infty(\Gamma\cup\Gamma_H)}.$$

We prove that $\varphi_i^k \ge 0$ for all $i=1,2,\ldots,N$ and $k=0,1,\ldots,K$. By the definition of φ_i^k, we have

$$\begin{aligned}
\varphi_i^k &\ge 0, \qquad i\in\Lambda_{\Gamma\cup\Gamma_H},\ k=0,1,\ldots,K,\\
\varphi_i^0 &\ge 0, \qquad i\in\Lambda_{\Omega_H}.
\end{aligned}$$

Moreover, for all $i\in\Lambda_\Omega,\ k=0,1,\ldots,K-1$, we get

$$\begin{aligned}
D_{\Delta t}\varphi_i^k &= -D_{\Delta t}v_i^k + \frac{1}{\Delta t}\left(\max_{l=0,1,\ldots,k+1}\|v^l\|_{\ell^\infty(\Gamma\cup\Gamma_H)} - \max_{l=0,1,\ldots,k}\|v^l\|_{\ell^\infty(\Gamma\cup\Gamma_H)}\right)\\
&\ge -D_{\Delta t}v_i^k
\end{aligned}$$

$$\geq L_h v_i^{k+\theta}$$
$$= -L_h \varphi_i^{k+\theta}.$$

Therefore, by Lemma 3.3, for all $i = 1, 2, \dots, N$ and $k = 0, 1, \dots, K$, we obtain

$$\varphi_i^k \geq 0.$$

Then (3.10) holds. □

Lemma 3.5. *Suppose that* $v : X_{N,H} \times I_K \to \mathbb{R}$ *and* $\phi : X_{N,H} \cap \Omega \times I_K \to \mathbb{R}$ *satisfy*

$$\begin{cases} D_{\Delta t} v_i^k + L_h v_i^{k+\theta} = \phi_i^k, & i \in \Lambda_\Omega, \quad k = 0, 1, \dots, K-1, \\ v_i^k = 0, & i \in \Lambda_{\Gamma \cup \Gamma_H}, \quad k = 1, 2, \dots, K, \\ v_i^0 = 0, & i \in \Lambda_{\Omega_H}, \end{cases}$$

$\{(X_{N,H}, V_{N,H}, h)\}_{h \downarrow 0}$ *is a regular family with order* m (> 2), *and* w *satisfies Hypothesis* 1.3 *and Hypothesis* 1.4. *Moreover, when* $\theta \in [0, 1)$, *suppose that* Δt *satisfies* (3.3). *Then there exists a positive constant* c *and* h_0 *independent of* h, N, *and* Δt *such that for all* $\{(X_{N,H}, V_{N,H}, h)\}_{h \downarrow 0}$ *with* $h < h_0$,

$$\|v\|_{\ell^\infty([0,T];\ell^\infty(\Omega_H))} \leq c\,\|\phi\|_{\ell^\infty([0,T);\ell^\infty(\Omega))}. \tag{3.11}$$

Proof. First, we consider the case that $\theta = 1$. Fix any $z \in \mathbb{R}^d$ satisfying

$$|x - z| \leq \operatorname{diam}(\Omega_H), \quad \forall x \in \overline{\Omega}_H.$$

Let $\Phi : \overline{\Omega}_H \to \mathbb{R}$ be

$$\Phi(x) := -\frac{1}{2d\kappa}(x - z)^2 + \frac{1}{2d\kappa}\operatorname{diam}(\Omega_H)^2 + 1.$$

Since $|\Phi|_{C^l(\overline{\Omega}_H)} = 0$ $(l \geq 3)$ and by Theorem 1.15, there exists a positive constant c_2 independent of h and N such that

$$\|\Delta\Phi - \Delta_h\Phi\|_{C(\overline{\Omega})} \leq c_2 h^{m-2}.$$

Therefore, since $\Delta\Phi \equiv -\kappa^{-1}$, we have

$$L_h\Phi_i \geq 1 - c_2\kappa h^{m-2}, \quad i = 1, 2, \dots, N. \tag{3.12}$$

Set $h_0 \in \mathbb{R}^+$ such that

$$h_0 < (c_2\kappa)^{(2-m)^{-1}}.$$

By (3.12), for all $\{(X_{N,H}, V_{N,H}, h)\}_{h \downarrow 0}$ with $h < h_0$, we have

$$L_h\Phi_i \geq 1 - c_2\kappa h_0^{m-2} > 0, \qquad i = 1, 2, \dots, N. \tag{3.13}$$

Let φ_i^k $(i = 1, 2, \dots, N,\ k = 0, 1, \dots, K)$ be

$$\varphi_i^k := v_i^k - (1 - c_2\kappa h_0^{m-2})^{-1} F^k \Phi_i.$$

Here,

$$F^k := \begin{cases} 0, & k = 0, \\ \max_{l=0,1,\ldots,k-1} \|\phi^l\|_{\ell^\infty(\Omega)}, & k = 1, 2, \ldots, K. \end{cases}$$

By (3.13) and $\Phi \geq 1$, for all $i = 1, \ldots, N_\Omega$ and $k = 0, 1, \ldots, K-1$, we have

$$\begin{aligned} D_{\Delta t}\varphi_i^k &= D_{\Delta t}v_i^k - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} \Phi_i D_{\Delta t}F^k \\ &= -L_h v_i^{k+\theta} + \phi_i^k - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} \Phi_i D_{\Delta t}F^k \\ &= -L_h \varphi_i^{k+\theta} + \phi_i^k - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} F^{k+\theta} L_h\Phi_i - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} \Phi_i D_{\Delta t}F^k \\ &\leq -L_h \varphi_i^{k+\theta} + \phi_i^k - F^{k+\theta} - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} \Phi_i D_{\Delta t}F^k \\ &\leq -L_h \varphi_i^{k+\theta} + \phi_i^k - F^{k+\theta} - D_{\Delta t}F^k. \end{aligned}$$

Since $\Delta t \leq (1-\theta)^{-1}$, we find

$$\begin{aligned} F^{k+\theta} + D_{\Delta t}F^k &\geq (\theta + \Delta t^{-1})F^{k+1} + (1 - \theta - \Delta t^{-1})F^k \\ &\geq F^{k+1} \end{aligned} \tag{3.14}$$

Hence we have

$$D_{\Delta t}\varphi_i^k + L_h\varphi_i^{k+\theta} \leq 0.$$

Therefore, by Lemma 3.4, for all $i = 1, 2, \ldots, N$ and $k = 0, 1, \ldots, K$, we obtain

$$\begin{aligned} \varphi_i^k &\leq \|\varphi^0\|_{\ell^\infty(\Omega_H)} + \max_{l=0,1,\ldots,k} \|\varphi^l\|_{\ell^\infty(\Gamma\cup\Gamma_H)} \\ &\leq \|v^0\|_{\ell^\infty(\Omega_H)} + (1 - c_2\kappa h_0^{m-2})^{-1} \max_{l=0,1,\ldots,k-1} F^l \|\Phi\|_{\ell^\infty(\Gamma\cup\Gamma_H)}. \end{aligned}$$

Since

$$\|\Phi\|_{\ell^\infty(\Omega_H)} \leq \frac{\mathrm{diam}(\Omega_H)^2 + 1}{2d\kappa}, \tag{3.15}$$

for all $i = 1, 2, \ldots, N$ and $k = 0, 1, \ldots, K$, we have

$$v_i^k \leq c \max_{l=0,1,\ldots,k-1} \|\phi^l\|_{\ell^\infty(\Gamma\cup\Gamma_H)}. \tag{3.16}$$

Let ψ_i^k $(i = 1, 2, \ldots, N,\ k = 0, 1, \ldots, K)$ be

$$\psi_i^k := -v_i^k - (1 - c_2\kappa h_0^{m-2})^{-1} F^k \Phi_i.$$

Since (3.13) and $\Phi \geq 1$, for all $i = 1, \ldots, N_\Omega$ and $k = 0, 1, \ldots, K-1$, we have

$$\begin{aligned} D_{\Delta t}\psi_i^k &= -D_{\Delta t}v_i^k - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} \Phi_i D_{\Delta t}F^k \\ &= L_h v_i^{k+\theta} - \phi_i^k - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} \Phi_i D_{\Delta t}F^k \end{aligned}$$

$$
\begin{aligned}
&= -L_h\psi_i^{k+\theta} - \phi_i^k - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} F^{k+\theta} L_h\Phi_i - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} \Phi_i D_{\Delta t} F^k \\
&\le -L_h\psi_i^{k+\theta} - \phi_i^k - F^{k+\theta} - \left(1 - c_2\kappa h_0^{m-2}\right)^{-1} \Phi_i D_{\Delta t} F^k \\
&\le -L_h\psi_i^{k+\theta} - \phi_i^k - F^{k+\theta} - \Phi_i D_{\Delta t} F^k.
\end{aligned}
$$

By (3.14) we have

$$D_{\Delta t}\psi_i^k + L_h\psi_i^{k+\theta} \le 0.$$

Therefore, by Lemma 3.4, for all $i = 1, 2, \ldots, N, k = 0, 1, \ldots, K$, we obtain

$$
\begin{aligned}
\psi_i^k &\le \|\psi^0\|_{\ell^\infty(\Omega_H)} + \max_{l=0,1,\ldots,k} \|\psi^l\|_{\ell^\infty(\Gamma\cup\Gamma_H)} \\
&\le \|v^0\|_{\ell^\infty(\Omega_H)} + (1 - c_2\kappa h_0^{m-2})^{-1} \max_{l=0,1,\ldots,k-1} F^l \|\Phi\|_{\ell^\infty(\Gamma\cup\Gamma_H)}.
\end{aligned}
$$

Hence, by (3.15), we obtain

$$-v_i^k \le c \max_{l=0,1,\ldots,k-1} \|\phi^l\|_{\ell^\infty(\Gamma\cup\Gamma_H)}. \tag{3.17}$$

Consequently, by (3.16) and (3.17), we obtain (3.11) when $\theta = 1$.

Next we consider case that $\theta \in [0, 1)$. Since w satisfies Hypothesis 1.3, we can take $\widehat{w} \in W$ such that

$$\widehat{w}(r) = \frac{c_w^{-1}}{r^2} w(r) \qquad \forall r \in \mathbb{R}^+.$$

Here,

$$c_w := \int_{\mathbb{R}^d} \frac{1}{|x|^2} w(|x|) dx.$$

For $\widehat{w}$ and h, let $\widehat{w}_h \in C^1(\mathbb{R}_0^+)$ be

$$\widehat{w}_h(r) := \frac{1}{h^d} \widehat{w}\left(\frac{r}{h}\right), \qquad r \in \mathbb{R}_0^+.$$

By Theorem 1.11, there exists a positive constant c_3 independent of h and N such that for all $x \in \Omega$

$$\left| \sum_{j=1}^N V_j \widehat{w}_h(|x - x_j|) - 1 \right| \le c_3 h^{m-1}.$$

Therefore, since

$$
\begin{aligned}
\sum_{j\neq i} V_j \frac{w_h(|x_i - x_j|)}{|x_i - x_j|^2} &\le \sum_{j=1}^N V_j \frac{w_h(|x_i - x_j|)}{|x_i - x_j|^2} \\
&= \frac{c_w}{h^2} \sum_{j=1}^N V_j \widehat{w}_h(|x - x_j|)
\end{aligned}
$$

$$\le \frac{c_w}{h^2}(1 + c_3 h^{m-1}),$$

by taking h_1 satisfying

$$0 < h_1^{m-1} < \frac{1-c_1}{c_1 c_3},$$

for all $h < h_1$ and $i = 1, 2, \dots, N$, we have

$$\sum_{j \ne i} V_j \frac{w_h(|x_i - x_j|)}{|x_i - x_j|^2} \le \frac{c_w}{h^2}(1 + c_3 h_1^{m-1})$$
$$\le \frac{c_w}{c_1 h^2}.$$

Hence, since for all $h < h_1$

$$\frac{1}{2d\kappa(1-\theta)} \left[\max_{i \in \Lambda_\Omega} \left\{ \sum_{j \ne i} V_j \frac{w_h(|x_i - x_j|)}{|x_i - x_j|^2} \right\} \right]^{-1} \ge \frac{c_1}{2d\kappa(1-\theta)c_w 1} h^2,$$

(3.7) holds. Consequently, by taking h_0 such that

$$0 < h_0 < \min \left\{ (c_2 \kappa)^{(2-m)^{-1}}, h_1 \right\},$$

Theorem 3.4 is true for $h < h_0$. Then, by the similar arguments the case that $\theta = 1$, we obtain (3.11). □

Utilizing the results above, we prove Theorem 3.1.
Proof of Theorem 3.1. $e : X_{N,H} \times I_K \to \mathbb{R}$ and $R : X_{N,H} \times (I_K \setminus \{t^K\}) \to \mathbb{R}$ are defined by

$$e_i^k := \widetilde{u}_i^k - U_i^k,$$
$$R_i^k := D_{\Delta t} \widetilde{u}_i^k + L_h \widetilde{u}_i^{k+\theta} - \theta \left(\partial_t \widetilde{u}_i^{k+1} - \kappa \Delta \widetilde{u}_i^{k+1} \right) - (1-\theta) \left(\partial_t \widetilde{u}_i^k - \kappa \Delta \widetilde{u}_i^k \right),$$

respectively. Then, by (3.1) and (3.2), we have

$$\begin{cases} D_{\Delta t} e_i^k + L_h e_i^{k+\theta} = R_i^k, & i \in \Lambda_\Omega, \quad k = 0, 1, \dots, K-1, \\ e_i^k = 0, & i \in \Lambda_{\Gamma \cup \Gamma_H}, \quad k = 1, 2, \dots, K, \\ e_i^0 = 0, & i \in \Lambda_{\Omega_H}. \end{cases}$$

Then by Lemma 3.5, we obtain

$$\|e\|_{\ell^\infty([0,T];\ell^\infty(\Omega_H))} \le c \, \|R\|_{\ell^\infty([0,T);\ell^\infty(\Omega))}. \tag{3.18}$$

Now, since

$$|R_i^k| \le \left| D_{\Delta t} \widetilde{u}_i^k - \left\{ \theta \partial_t \widetilde{u}_i^{k+1} + (1-\theta) \partial_t \widetilde{u}_i^k \right\} \right|$$
$$+ \kappa\theta \left| \Delta \widetilde{u}_i^{k+1} - \Delta_h \widetilde{u}_i^{k+1} \right| + (1-\theta)\kappa \left| \Delta \widetilde{u}_i^k - \Delta_h \widetilde{u}_i^k \right|,$$

we estimate the each term. Assume $\widetilde{u} \in C^2([0,T]; C^4(\overline{\Omega}_H))$. By Taylor expansion, we have

$$\begin{aligned} \partial_t \widetilde{u}_i^{k+1} &= \frac{\widetilde{u}_i^{k+1} - \widetilde{u}_i^k}{\Delta t} + \Delta t \int_0^1 (1-t) \frac{\partial^2}{\partial t^2} \widetilde{u}(x_i, (k+s)\Delta t) ds, \\ \partial_t \widetilde{u}_i^{k} &= \frac{\widetilde{u}_i^{k+1} - \widetilde{u}_i^k}{\Delta t} + \Delta t \int_0^1 (1-t) \frac{\partial^2}{\partial t^2} \widetilde{u}(x_i, (k+1-s)\Delta t) ds. \end{aligned}$$

Hence, we find

$$\begin{aligned} \left| D_{\Delta t} \widetilde{u}_i^k - \left\{ \theta \partial_t \widetilde{u}_i^{k+1} + (1-\theta) \partial_t \widetilde{u}_i^k \right\} \right| &\leq \frac{\Delta t}{2} \max_{0 \leq s \leq 1} \left| \frac{\partial^2}{\partial t^2} \widetilde{u}(x_i, (k+s)\Delta t) \right| \\ &\leq c \Delta t \left\| \widetilde{u} \right\|_{C^2([0,T]; C(\overline{\Omega}_H))}. \end{aligned}$$

Since $\{(X_{N,H}, V_{N,H}, h)\}$ is the regular family, by Lemma 1.5 and Theorem 1.15, for all $i \in \Lambda_\Omega$ and $k = 0, 1, \ldots, K$, we have

$$|\Delta \widetilde{u}_i^k - \Delta_h \widetilde{u}_i^k| \leq c h^{\min\{2, m-2\}} \left\| \widetilde{u} \right\|_{C([0,T]; C^4(\overline{\Omega}_H))}.$$

Therefore, for all $i \in \Lambda_\Omega$, $k = 0, 1, \ldots, K-1$, and $\theta \in [0,1]$, we obtain

$$|R_i^k| \leq c(\Delta t + h^{\min\{2, m-2\}}) \left\| \widetilde{u} \right\|_{C^2([0,T]; C^4(\overline{\Omega}_H))}. \tag{3.19}$$

Moreover, when $\widetilde{u} \in C^3([0,T]; C^4(\overline{\Omega}_H))$ and $\theta = 1/2$, by Taylor expansion, we have

$$\begin{aligned} \partial_t \widetilde{u}_i^{k+1} &= \frac{\widetilde{u}_i^{k+1} - \widetilde{u}_i^k}{\Delta t} + \frac{\Delta t}{2} \frac{\partial^2}{\partial t^2} \widetilde{u}_i^{k+1} + \frac{\Delta t^2}{2!} \int_0^1 (1-t)^2 \frac{\partial^3}{\partial t^3} \widetilde{u}(x_i, (k+s)\Delta t) ds, \\ \partial_t \widetilde{u}_i^{k} &= \frac{\widetilde{u}_i^{k+1} - \widetilde{u}_i^k}{\Delta t} - \frac{\Delta t}{2} \frac{\partial^2}{\partial t^2} \widetilde{u}_i^{k} + \frac{\Delta t^2}{2!} \int_0^1 (1-t)^2 \frac{\partial^3}{\partial t^3} \widetilde{u}(x_i, (k+1-s)\Delta t) ds. \end{aligned}$$

Since

$$\frac{\partial^2}{\partial t^2} \widetilde{u}_i^{k+1} - \frac{\partial^2}{\partial t^2} \widetilde{u}_i^{k} = \Delta t \int_0^1 \frac{\partial^3}{\partial t^3} \widetilde{u}(x_i, (k+s)\Delta t) ds,$$

we estimate

$$\begin{aligned} \left| D_{\Delta t} \widetilde{u}_i^k - \frac{1}{2} \left(\partial_t \widetilde{u}_i^{k+1} + \partial_t \widetilde{u}_i^k \right) \right| &\leq \frac{5 \Delta t^2}{12} \max_{0 \leq s \leq 1} \left| \frac{\partial^3}{\partial t^3} \widetilde{u}(x_i, (k+s)\Delta t) \right| \\ &\leq c \, \Delta t^2 \left\| \widetilde{u} \right\|_{C^3([0,T]; C(\overline{\Omega}_H))}. \end{aligned}$$

Therefore, for all $i \in \Lambda_\Omega$, $k = 0, 1, \ldots, K-1$, we estimate

$$|R_i^k| \leq c \, (\Delta t^2 + h^{\min\{2, m-2\}}) \left\| \widetilde{u} \right\|_{C^3([0,T]; C^4(\overline{\Omega}_H))}. \tag{3.20}$$

Consequently, by (3.18), we obtain (3.4) and (3.5). □

3.3 Error estimates with a discrete L^2 norm

For $v : X_{N,H} \to \mathbb{R}$ and $S \subset \mathbb{R}^d$, a discrete L^2 norm $\|.\|_{\ell^2(S)}$ is defined by

$$\|v\|_{\ell^2(S)} := \left(\sum_{i \in \Lambda_S} V_i \, |v_i|^2 \right)^{1/2},$$

and a discrete H^1 semi-norm $|.|_{h^1(S)}$ is defined by

$$|v|_{h^1(S)} := \left(d \sum_{i \in \Lambda_S} V_i \sum_{j \neq i} V_j \frac{|v_i - v_j|^2}{|x_i - x_j|^2} w_h(|x_i - x_j|) \right)^{1/2}.$$

Note that the discrete H^1 semi-norm satisfies the axioms of semi-norm if w satisfies Hypotheses 1.4 and $X_{N,H}$ satisfies the h-connectivity. First, we show an inequality with respect to $\|.\|_{\ell^2(\Omega_H)}$ and $|.|_{h^1(\Omega_H)}$.

Lemma 3.6. *Suppose that $\{(X_{N,H}, V_{N,H}, h)\}_{h \downarrow 0}$ is a regular family with order m (≥ 1) and that w satisfies Hypothesis 1.3 and Hypothesis 1.4. Then there exists a positive constant c_2 independent of h and N such that for all $v : X_{N,H} \to \mathbb{R}$,*

$$|v|_{h^1(\Omega_H)} \leq \frac{c_2}{h} \|v\|_{\ell^2(\Omega_H)}. \tag{3.21}$$

Proof. Set $\widehat{w} \in C(\mathbb{R}_0^+)$ satisfying

$$\widehat{w}(r) = \frac{1}{c_w r^2} w(r), \qquad r \in \mathbb{R}^+.$$

Here

$$c_w := \int_{\mathbb{R}^d} \frac{1}{|x|^2} w(|x|) dx.$$

Then, by Hypothesis 1.3, we have $\widehat{w} \in W$. Then, by Hypothesis 1.4, we estimate

$$\begin{aligned}
|v|^2_{h^1(\Omega_H)} &= d \sum_{i=1}^{N} V_i \sum_{j \neq i} V_j \frac{|v_i - v_j|^2}{|x_i - x_j|^2} w_h(|x_i - x_j|) \\
&= \frac{d c_w}{h^2} \sum_{i=1}^{N} V_i \sum_{j \neq i} V_j |v_i - v_j|^2 \widehat{w}_h(|x_i - x_j|) \\
&\leq \frac{2 d c_w}{h^2} \sum_{i=1}^{N} V_i \sum_{j \neq i} V_j \left(|v_i|^2 + |v_j|^2 \right) \widehat{w}_h(|x_i - x_j|) \\
&\leq \frac{4 d c_w}{h^2} \sum_{i=1}^{N} V_i |v_i|^2 \sum_{j=1}^{N} V_j \widehat{w}_h(|x_i - x_j|).
\end{aligned}$$

Now, fix any $\omega = \{\omega_i\}$ satisfying (1.6) and set ξ_{ij} $(i, j = 1, 2, \ldots, N)$ by $\xi_{ij} := \mathrm{meas}(\sigma_i \cap \omega_j)$. Then we have

$$\sum_{j=1}^{N} V_j \widehat{w}_h(|x_i - x_j|) = \int_{\Omega_H} \widehat{w}_h(|x_i - y|)dy + \sum_{j=1}^{N}\sum_{k=1}^{N} \int_{\sigma_j \cap \omega_k} \{\widehat{w}_h(|x_i - x_j|) - \widehat{w}_h(|x_i - y|)\}dy$$
$$+ \sum_{j=1}^{N}\sum_{k=1}^{N} \xi_{jk}\{\widehat{w}_h(|x_i - x_k|) - \widehat{w}_h(|x_i - x_j|)\}. \tag{3.22}$$

For $i = 1, 2, \ldots, N$, let $\mathcal{N}_i(r)$ $(r \in \mathbb{R}^+)$ be

$$\mathcal{N}_i(r) := \{j;\ j = 1, 2, \ldots, N,\ |x_i - x_j| < r\}.$$

By $\widehat{w} \in W$ and Hypothesis 1.4, the second term of (3.22) is estimated by

$$\int_{\Omega_H} \widehat{w}_h(|x_i - y|)dy \leq 1.$$

By Taylor expansion, the second term of (3.22) is estimated by

$$\begin{aligned}
&\sum_{j=1}^{N}\sum_{k=1}^{N} \int_{\sigma_j \cap \omega_k} \{\widehat{w}_h(|x_i - x_j|) - \widehat{w}_h(|x_i - y|)\}dy \\
&\quad = \sum_{j \in \mathcal{N}_i(h + r_{\mathrm{c}})} \sum_{k=1}^{N} \int_{\sigma_j \cap \omega_k} \{\widehat{w}_h(|x_i - x_j|) - \widehat{w}_h(|x_i - y|)\}dy \\
&\quad \leq \frac{r_{\mathrm{c}}}{h^{d+1}} |\widehat{w}|_{C^1(\mathbb{R}_0^+)} \sum_{j \in \mathcal{N}_i(h + r_{\mathrm{c}})} \int_{\sigma_j} dy \\
&\quad \leq c\left(1 + 2\frac{r_{\mathrm{c}}}{h}\right)^d \frac{r_{\mathrm{c}}}{h}.
\end{aligned}$$

The third term of (3.22) is estimated by

$$\begin{aligned}
&\sum_{j=1}^{N}\sum_{k=1}^{N} \xi_{jk}\{\widehat{w}_h(|x_i - x_k|) - \widehat{w}_h(|x_i - x_j|)\} \\
&\quad \leq \sum_{j \in \mathcal{N}_i(h)} \sum_{k=1}^{N} (\xi_{jk} + \xi_{kj})|\widehat{w}_h(|x_i - x_k|) - \widehat{w}_h(|x_i - x_j|)| \\
&\quad \leq \frac{1}{h^{d+1}} |\widehat{w}|_{C^1(\mathbb{R}_0^+)} \sum_{j \in \Lambda_{\mathcal{N}_i(h)}} \sum_{k=1}^{N} (\xi_{jk} + \xi_{kj})|x_j - x_k| \\
&\quad = \frac{1}{h^{d+1}} |\widehat{w}|_{C^1(\mathbb{R}_0^+)} \sum_{j \in \mathcal{N}_i(h)} \mathrm{meas}(\sigma_j) \sum_{j=1}^{N} \frac{\xi_{jk} + \xi_{kj}}{\mathrm{meas}(\sigma_j)} |x_i - x_j| \\
&\quad \leq \left(1 + \frac{r_{\mathrm{c}}}{h}\right)^d \frac{1}{h} |\widehat{w}|_{C^1(\mathbb{R}_0^+)} \max_{j=1,2,\ldots,N} \left(\sum_{k=1}^{N} \frac{\xi_{jk} + \xi_{kj}}{\mathrm{meas}(\sigma_j)} |x_j - x_k|\right),
\end{aligned}$$

and, since ω is arbitrary, we have

$$\sum_{j=1}^{N}\sum_{k=1}^{N}\xi_{jk}\{\widehat{w}_h(|x_i-x_k|)-\widehat{w}_h(|x_i-x_j|)\}\leq c\left(1+\frac{r_{\rm c}}{h}\right)^d\frac{d_{\rm v}}{h}.$$

Therefore, we have

$$|v|_{h^1(\Omega_H)}^2\leq\frac{4dc_w}{h^2}\left\{1+c\left(1+2\frac{r_{\rm c}}{h}\right)^d\frac{r_{\rm c}+d_{\rm v}}{h}\right\}\|v\|_{\ell^2(\Omega_H)}^2.$$

By the regularity, we therefore obtain (3.21). □

Now, we state error estimates with the discrete L^2 norm in space of the approximate solutions.

Theorem 3.7. *Let u and U be solutions of* (3.1) *and* (3.2)*, respectively. Suppose that the expanded solution $\widetilde{u}$ satisfies $\widetilde{u}\in C^2([0,T];C^4(\overline{\Omega}_H))$, $\{(X_{N,H},V_{N,H},h)\}_{h\downarrow 0}$ is a regular family with order m (>2), and w satisfies Hypothesis* 1.3 *and Hypothesis* 1.4*. Moreover, when $\theta\in[0,1/2)$, suppose that for any fixed $\delta\in(0,1)$, Δt satisfies*

$$\Delta t\leq\frac{\delta}{\kappa\,(1-2\theta)\,c_2^2}h^2. \tag{3.23}$$

Here c_2 is the positive constant in (3.21)*. Then there exists a positive constant c independent of h, N, and Δt such that for all $\{(X_{N,H},V_{N,H},h)\}$*

$$\|\widetilde{u}-U\|_{\ell^\infty([0,T];\ell^2(\Omega_H))}\leq c\,(\Delta t+h^{\min\{2,m-2\}})\,\|\widetilde{u}\|_{C^2([0,T];C^4(\overline{\Omega}_H))}. \tag{3.24}$$

Furthermore, if $\widetilde{u}\in C^3([0,T];C^4(\overline{\Omega}_H))$ and $\theta=1/2$, then

$$\|\widetilde{u}-U\|_{\ell^\infty([0,T];\ell^2(\Omega_H))}\leq c\,(\Delta t^2+h^{\min\{2,m-2\}})\,\|\widetilde{u}\|_{C^3([0,T];C^4(\overline{\Omega}_H))}. \tag{3.25}$$

Hereafter, in this section, let c be a generic positive constant independent of h, N, and Δt. Before beginning the proof of Theorem 3.7, we show the following lemma.

Lemma 3.8. (***Stability***) *Suppose that for $\phi: X_{N,H}\cap\Omega\times I_K\to\mathbb{R}$, $v: X_{N,H}\times I_K\to\mathbb{R}$ satisfies*

$$\begin{cases} D_{\Delta t}v_i^k+L_hv_i^{k+\theta}=\phi_i^k, & i\in\Lambda_\Omega, \quad k=0,1,\ldots,K-1,\\ v_i^k=0, & i\in\Lambda_{\Gamma\cup\Gamma_H}, \quad k=1,2,\ldots,K,\\ v_i^0=0, & i\in\Lambda_{\Omega_H}, \end{cases} \tag{3.26}$$

$\{(X_{N,H},V_{N,H},h)\}_{h\downarrow 0}$ is a regular family with order m (≥ 1), and w satisfies Hypothesis 1.4*. Moreover, if $\theta\in[0,1/2)$, suppose that w satisfies Hypothesis* 1.3 *and Δt satisfies* (3.23)*. Then there exists a positive constant c independent of h, N, and Δt such that*

$$\|v\|_{\ell^\infty([0,T];\ell^2(\Omega_H))}\leq c\,\|\phi\|_{\ell^\infty([0,T);\ell^2(\Omega))}. \tag{3.27}$$

Proof. Multiplying both side of the fist term of (3.26) by $V_i v_i^{k+1/2}$ and taking the sum of these over $i \in \Lambda_\Omega$, we have

$$\sum_{i\in\Lambda_\Omega} V_i v_i^{k+1/2} D_{\Delta t} v_i^k + \sum_{i\in\Lambda_\Omega} V_i v_i^{k+1/2} L_h v_i^{k+\theta} = \sum_{i\in\Lambda_\Omega} V_i v_i^{k+1/2} \phi_i^k. \tag{3.28}$$

The first term of the left hand side of (3.28) yields

$$\begin{aligned}\sum_{i\in\Lambda_\Omega} V_i v_i^{k+1/2} D_{\Delta t} v_i^k &= \frac{1}{2\Delta t}\sum_{i=1}^{N} V_i \{(v_i^{k+1})^2 - (v_i^k)^2\} \\ &= \frac{1}{2\Delta t}(\|v^{k+1}\|^2_{\ell^2(\Omega_H)} - \|v^k\|^2_{\ell^2(\Omega_H)})\end{aligned}$$

and the second term gives

$$\begin{aligned}&\sum_{i\in\Lambda_\Omega} V_i v_i^{k+1/2} L_h v_i^{k+\theta} \\ &= 2\kappa d \sum_{i\in\Lambda_\Omega} V_i v_i^{k+1/2} \sum_{j\neq i} V_j \frac{v_i^{k+\theta} - v_j^{k+\theta}}{|x_i - x_j|^2} w_h(|x_i - x_j|) \\ &= d\kappa \sum_{i=1}^{N}\sum_{j\neq i} V_i V_j \frac{(v_i^{k+1/2} - v_j^{k+1/2})(v_i^{k+\theta} - v_j^{k+\theta})}{|x_i - x_j|^2} w_h(|x_i - x_j|) \\ &= d\kappa \sum_{i=1}^{N}\sum_{j\neq i} V_i V_j \frac{(v_i^{k+1/2} - v_j^{k+1/2})^2}{|x_i - x_j|^2} w_h(|x_i - x_j|) \\ &\quad + \frac{d\kappa}{2}\left(\theta - \frac{1}{2}\right)\sum_{i=1}^{N}\sum_{j\neq i} V_i V_j \frac{(v_i^{k+1} - v_j^{k+1})^2 - (v_i^k - v_j^k)^2}{|x_i - x_j|^2} w_h(|x_i - x_j|) \\ &= \kappa |v^{k+1/2}|^2_{h^1(\Omega_H)} + \frac{\kappa}{2}\left(\theta - \frac{1}{2}\right)(|v^{k+1}|^2_{h^1(\Omega_H)} - |v^k|^2_{h^1(\Omega_H)}).\end{aligned}$$

Therefore we obtain

$$\begin{aligned}&\frac{1}{2\Delta t}(\|v^{k+1}\|^2_{\ell^2(\Omega_H)} - \|v^k\|^2_{\ell^2(\Omega_H)}) + \kappa|v^{k+1/2}|^2_{h^1(\Omega_H)} + \frac{\kappa}{2}\left(\theta - \frac{1}{2}\right)(|v^{k+1}|^2_{h^1(\Omega_H)} - |v^k|^2_{h^1(\Omega_H)}) \\ &= \sum_{i\in\Lambda_\Omega} V_i v_i^{k+1/2}\phi_i^k.\end{aligned} \tag{3.29}$$

For $l = 0, 1, \ldots, K$, let E_l be

$$E_l := \|v^l\|^2_{\ell^2(\Omega_H)} + \kappa\Delta t\left(\theta - \frac{1}{2}\right)|v^l|^2_{h^1(\Omega_H)}.$$

By (3.29), for all $s \in (0, 1)$, we have

$$E_{l+1} - E_l = \|v^{l+1}\|^2_{\ell^2(\Omega_H)} - \|v^l\|^2_{\ell^2(\Omega_H)} + \Delta t\kappa\left(\theta - \frac{1}{2}\right)(|v^{l+1}|^2_{h^1(\Omega_H)} - |v^l|^2_{h^1(\Omega_H)})$$

$$
\begin{aligned}
&= -2\Delta t\kappa|v^{l+1/2}|^2_{h^1(\Omega_H)} + 2\Delta t\sum_{i\in\Lambda_\Omega} V_i v_i^{l+1/2}\phi_i^l \\
&\leq -2\Delta t\kappa|v^{l+1/2}|^2_{h^1(\Omega_H)} + \Delta t\sum_{i\in\Lambda_\Omega} V_i(|v_i^{l+1}| + |v_i^l|)|\phi_i^l| \\
&\leq -2\Delta t\kappa|v^{l+1/2}|^2_{h^1(\Omega_H)} + s\|v^{l+1}\|^2_{\ell^2(\Omega_H)} + (1-s)\|v^l\|^2_{\ell^2(\Omega_H)} + \frac{\Delta t^2}{4s(1-s)}\|\phi^l\|^2_{\ell^2(\Omega)}
\end{aligned}
$$

By Hypothesis 1.4, we have $|v^{l+1/2}|_{h^1(\Omega_H)} \geq 0$. Then we obtain

$$
E_{l+1} - E_l \leq s\|v^{l+1}\|^2_{\ell^2(\Omega_H)} + (1-s)\|v^l\|^2_{\ell^2(\Omega_H)} + \frac{\Delta t^2}{4s(1-s)}\|\phi^l\|^2_{\ell^2(\Omega)}.
$$

Taking the sum of the both side with respect to l from 0 to $k-1$, since $\|v^0\|^2_{\ell^2(\Omega_H)} = 0$, we have

$$
E_k - E_0 \leq s\|v^k\|^2_{\ell^2(\Omega_H)} + \sum_{l=0}^{k-1}\|v^l\|^2_{\ell^2(\Omega_H)} + \frac{\Delta t^2}{4s(1-s)}\sum_{l=0}^{k-1}\|\phi^l\|^2_{\ell^2(\Omega)}.
$$

Since $E_0 = 0$, we obtain

$$
\|v^k\|^2_{\ell^2(\Omega_H)} + \frac{\kappa\Delta t}{1-s}\left(\theta - \frac{1}{2}\right)|v^k|^2_{h^1(\Omega_H)} \leq \frac{s}{1-s}\sum_{l=0}^{k-1}\|v^l\|^2_{\ell^2(\Omega_H)} + \frac{\Delta t^2}{4s(1-s)^2}\sum_{l=0}^{k-1}\|\phi^l\|^2_{\ell^2(\Omega)}.
$$

Taking $s = \Delta t/(2T)$, we have

$$
\begin{aligned}
&\|v^k\|^2_{\ell^2(\Omega_H)} + \frac{2\kappa T\Delta t}{2T-\Delta t}\left(\theta - \frac{1}{2}\right)|v^{k-1}|^2_{h^1(\Omega_H)} \\
&\quad\leq \frac{\Delta t}{2T-\Delta t}\sum_{k=0}^{k-1}\|v^k\|^2_{\ell^2(\Omega_H)} + \frac{2T^3\Delta t}{(2T-\Delta t)^2}\sum_{l=0}^{k-1}\|\phi^l\|^2_{\ell^2(\Omega)} \\
&\quad\leq \frac{\Delta t}{T}\sum_{l=0}^{k-1}\|v^l\|^2_{\ell^2(\Omega_H)} + 2T\sum_{l=0}^{k-1}\Delta t\|\phi^l\|^2_{\ell^2(\Omega)} \qquad (3.30)
\end{aligned}
$$

When $\theta \in [1/2, 1]$, since

$$
\|v^k\|^2_{\ell^2(\Omega_H)} + \frac{2\kappa T\Delta t}{2T-\Delta t}\left(\theta - \frac{1}{2}\right)|v^k|^2_{h^1(\Omega_H)} \geq \|v^k\|^2_{\ell^2(\Omega_H)},
$$

for all $k = 0, 1, \dots, K$, we have

$$
\|v^k\|^2_{\ell^2(\Omega_H)} \leq \frac{\Delta t}{T}\sum_{l=0}^{k-1}\|v^l\|^2_{\ell^2(\Omega_H)} + 2T\sum_{l=0}^{k-1}\Delta t\|\phi^l\|^2_{\ell^2(\Omega)}.
$$

Since $\|v^0\|^2_{\ell^2(\Omega_H)} = 0$, by applying Gronwall's lemma into the inequality, for all $k = 0, 1, \dots, K$, we have

$$
\|v^k\|^2_{\ell^2(\Omega_H)} \leq 2eT\sum_{l=0}^{k-1}\Delta t\|\phi^l\|^2_{\ell^2(\Omega)}.
$$

Therefore we obtain

$$\|v\|_{\ell^\infty([0,T];\ell^2(\Omega_H))} \le \sqrt{2e}T\,\|\phi\|_{\ell^\infty([0,T);\ell^2(\Omega))}.$$

When $\theta \in [0,1/2)$, by (3.21) and (3.23), we have

$$\begin{aligned}\|v^k\|^2_{\ell^2(\Omega_H)} + \frac{2\kappa T\Delta t}{2T-\Delta t}\left(\theta - \frac{1}{2}\right)|v^k|^2_{h^1(\Omega_H)} &\ge \|v^k\|^2_{\ell^2(\Omega_H)} + \kappa\Delta t\,(2\theta-1)\,|v^k|^2_{h^1(\Omega_H)}\\ &\ge \left\{1 + \frac{c_2^2\kappa\Delta t\,(2\theta-1)}{h^2}\right\}\|v^k\|^2_{\ell^2(\Omega_H)}\\ &\ge (1-\delta)\|v^k\|^2_{\ell^2(\Omega_H)}.\end{aligned}$$

Therefore, by (3.30), we have

$$\|v^k\|^2_{\ell^2(\Omega_H)} \le \frac{\Delta t}{(1-\delta)T}\sum_{l=0}^{k-1}\|v^l\|^2_{\ell^2(\Omega_H)} + \frac{2T}{1-\delta}\sum_{l=0}^{k-1}\Delta t\|\phi^l\|^2_{\ell^2(\Omega)}.$$

By applying Gronwall's lemma into the inequality, for all $k = 0, 1, \ldots, K$, we have

$$\|v^k\|^2_{\ell^2(\Omega_H)} \le \frac{2e^{1/(1-\delta)}T}{1-\delta}\sum_{l=0}^{k-1}\Delta t\|\phi^l\|^2_{\ell^2(\Omega)}.$$

Therefore we obtain

$$\|v\|_{\ell^\infty([0,T];\ell^2(\Omega_H))} \le \sqrt{\frac{e^{1/(1-\delta)}}{1-\delta}}T\,\|\phi\|_{\ell^\infty([0,T);\ell^2(\Omega))}$$

Consequently, (3.27) holds. □

Finally, using the lemma above, we prove Theorem 3.7.

Proof of Theorem 3.7. $e : X_{N,H} \times I_K \to \mathbb{R}$ and $R : X_{N,H} \times (I_K \setminus \{t^K\}) \to \mathbb{R}$ are defined by

$$\begin{aligned}e_i^k &:= \widetilde{u}_i^k - U_i^k,\\ R_i^k &:= D_{\Delta t}\widetilde{u}_i^k + L_h\widetilde{u}_i^{k+\theta} - \theta\left(\partial_t\widetilde{u}_i^{k+1} - \kappa\Delta\widetilde{u}_i^{k+1}\right) - (1-\theta)\left(\partial_t\widetilde{u}_i^k - \kappa\Delta\widetilde{u}_i^k\right),\end{aligned}$$

respectively. By (3.1) and (3.2), we find

$$\begin{cases} D_{\Delta t}e_i^k + L_h e_i^{k+\theta} = R_i^k, & i \in \Lambda_\Omega, \quad k = 0,1,\ldots,K-1,\\ e_i^k = 0, & i \in \Lambda_{\Gamma\cup\Gamma_H}, \quad k = 1,2,\ldots,K,\\ e_i^0 = 0, & i \in \Lambda_{\Omega_H}.\end{cases}$$

By Lemma 3.8, for $k = 1, 2, \ldots, K$, we have

$$\|e\|_{\ell^\infty([0,T];\ell^2(\Omega_H))} \le c\,\|R\|_{\ell^\infty([0,T);\ell^2(\Omega))}.$$

Therefore, by (3.19) and (3.20), we obtain (3.24) and (3.25). □

Chapter 4

Numerical results

The purpose of this chapter is to confirm theoretical results obtained in previous chapters numerically. After preparations of particle distributions, Section 4.1 shows some numerical results corresponding to the truncation error estimates of the approximate operators shown in Section 1.4 and confirm the convergence rates for some weight functions of SPH and unconventional ones. Section 4.2 presents some numerical results corresponding to the error estimates of the generalized particle method for the Poisson equation mentioned in Section 2.2 and confirm the convergence rates. Section 4.3 gives some numerical results corresponding to the error estimates of the generalized particle method for the heat equation mentioned in Section 3.3 and confirm the convergence rates and the stability conditions with respect to the time step.

In this chapter, we set particle distributions as follows: Set $\Omega = (0,1)^2$ and $H = 0.1$. Let $G_{\Delta x}$ be a grid distribution with size Δx defined by

$$G_{\Delta x} := \{(i\Delta x, j\Delta x) \in \Omega_H;\ i,j \in \mathbb{Z}\}.$$

We set $X_{N,H}$ by a distribution constructed to disturb $G_{\Delta x}$ at random:

$$X_{N,H} = \{((i+\eta_{ij}^{(1)})\Delta x, (j+\eta_{ij}^{(2)})\Delta x) \in \Omega_H;\ i,j \in \mathbb{Z}\}.$$

Here $\eta_{ij}^{(n)}$ $(i,j \in \mathbb{Z}, n = 1,2)$ are random numbers in $(-0.25, 0.25)$. Then we have $N \simeq \Delta x^{-2}$ and $1.4\Delta x \le r_{\mathrm{c}} \le 1.8\Delta x$. Figure 4.1 shows a particle distribution with $\Delta x = 2^{-5}$.

We will state how to give a grid size Δx, a weight function w, an influence radius h, and particle volume V_i in each section.

4.1 Truncation errors

We compute truncation error for two cases of functions v as follows:

$$\text{Case 1}: \quad v(x,y) = (x-0.5)^4 + (y-0.5)^4,$$
$$\text{Case 2}: \quad v(x,y) = \sin(2\pi(x+y)).$$

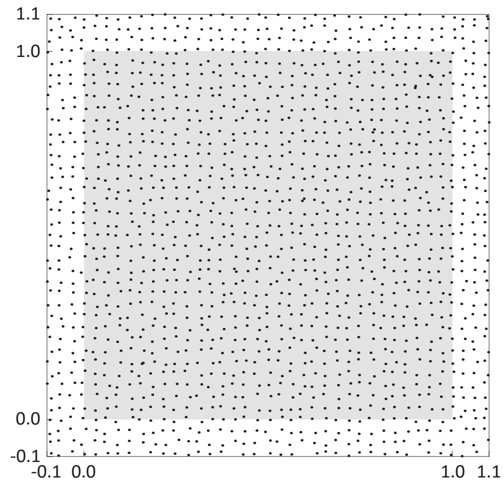

Figure 4.1: A particle distribution $X_{N,H}$ with $\Delta x = 2^{-5}$ ($N = 1,521$). A gray area shows Ω.

4.1.1 Interpolants

We compute truncation errors of interpolants. First, we consider three weight functions: the cubic B-spline

$$w^{\mathrm{CB}}(r) := \frac{40}{7\pi} \begin{cases} 1 - 6r^2 + 6r^3, & 0 \le r < \dfrac{1}{2}, \\ 2(1-r)^2, & \dfrac{1}{2} \le r < 1, \\ 0, & r \ge 1 \end{cases}$$

and the quintic B-spline

$$w^{\mathrm{QB}}(r) := \frac{63}{578\pi} \begin{cases} (3-3r)^5 + 6(2-3r)^5 + 15(1-3r)^5, & 0 \le r < \dfrac{1}{3}, \\ (3-3r)^5 + 6(2-3r)^5, & \dfrac{1}{3} \le r < \dfrac{2}{3}, \\ (3-3r)^5, & \dfrac{2}{3} \le r < 1, \\ 0, & r \ge 1 \end{cases}$$

used in SPH [38] and a quadratic spike function defined by

$$w^{\mathrm{QS}}(r) := \frac{6}{\pi} \begin{cases} (1-r)^2, & 0 \le r < 1, \\ 0, & r \ge 1. \end{cases} \tag{4.1}$$

These weight functions satisfy Hypothesis 1.1 with order $k = 1$. Figure 4.2 shows the graph of weight functions.

Set Δx by $2^{-5}, 2^{-6}, \dots, 2^{-11}$. For Δx, set h by $h = \{(3.1^3 \times 2^{-10})\Delta x\}^{1/3}$. Set particle volumes by $V_i = \widetilde{V}_i$ ($i = 1, 2, \dots, N$). Under the settings above, Theorem 1.11 is valid with $O(h^2)$.

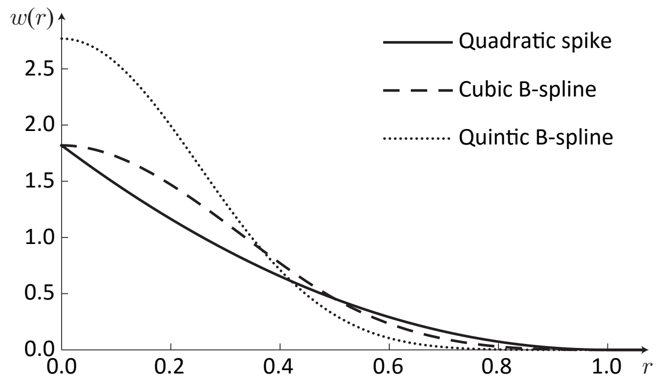

Figure 4.2: The graph of weight functions: the cubic B-spline, the quintic B-spline, and the quadratic spike function.

Figure 4.3 shows graphs of the relative errors

$$\frac{\|v - \Pi_h v\|_{\ell^\infty(\Omega)}}{\|v\|_{\ell^\infty(\Omega)}}$$

versus the influence radius h. The slopes of triangles show the theoretical convergence rates derived from Theorem 1.11. Table 4.1 shows numerical convergence rates obtained from the slopes of the relative errors between $\Delta x = 2^{-10}$ and 2^{-11}. Figure 4.3 and Table 4.1 show that the numerical convergence rates agree well with theoretical ones.

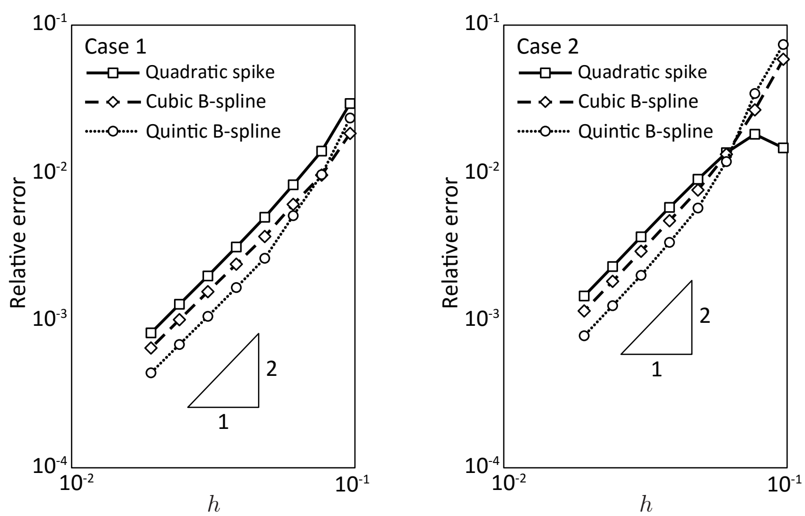

Figure 4.3: The graphs of the relative errors of interpolants versus h.

Next, we consider a cubic spike function defined by

$$w(r) := \frac{5}{\pi}\begin{cases}(1-r)^2(4-7r), & 0 \le r < 1,\\ 0, & r \ge 1,\end{cases}$$

Table 4.1: Numerical convergence rates of interpolants obtained from $\Delta x = 2^{-10}$ and 2^{-11} in Figure 4.3.

Weight function	Case 1	Case 2
Quadratic spike	1.93	2.00
Cubic B-spline	1.91	2.01
Quintic B-spline	1.91	2.02

in addition of the previous weight functions. The cubic spike function satisfies Hypothesis 1.1 with order $k = 3$. Figure 4.4 shows the graph of the quadratic spike function and the cubic spike function.

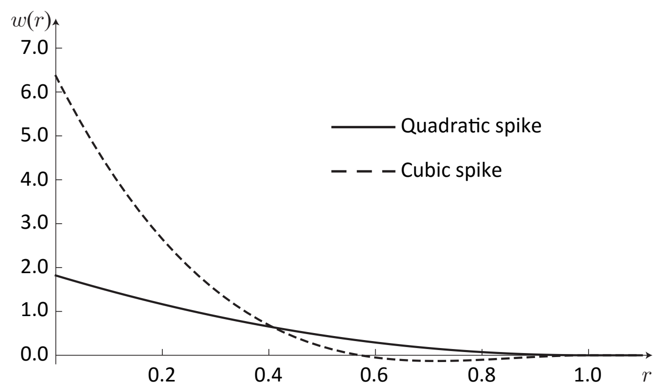

Figure 4.4: The graphs of the weight functions: the quadratic spike and the cubic spike.

Set Δx by $2^{-5}, 2^{-6}, \ldots, 2^{-12}$. For Δx, set h by $h = \{(3.1^3 \times 2^{-10})\Delta x\}^{1/5}$. Set particle volumes by $V_i = \widetilde{V_i}$ $(i = 1, 2, \ldots, N)$. Under the settings above, Theorem 1.11 is valid with $O(h^4)$ in case of the cubic spike function (4.1) and with $O(h^2)$ in case of the other functions.

Figure 4.5 shows graphs of the relative errors 4.1.1 versus the influence radius h. The slopes of triangles show the theoretical convergence rates derived from Theorem 1.11. Table 4.2 shows numerical convergence rates obtained from the slopes of the relative errors between $\Delta x = 2^{-11}$ and 2^{-12}. Figure 4.5 and Table 4.2 show that the numerical convergence rates agree well with theoretical ones.

Table 4.2: Numerical convergence rates of interpolants obtained from $\Delta x = 2^{-11}$ and 2^{-12} in Figure 4.5.

Weight function	Case 1	Case 2
Cubic B-spline	2.00	2.00
Quintic B-spline	2.00	2.00
Quadratic spike	2.00	2.00
Cubic spike	4.00	4.26

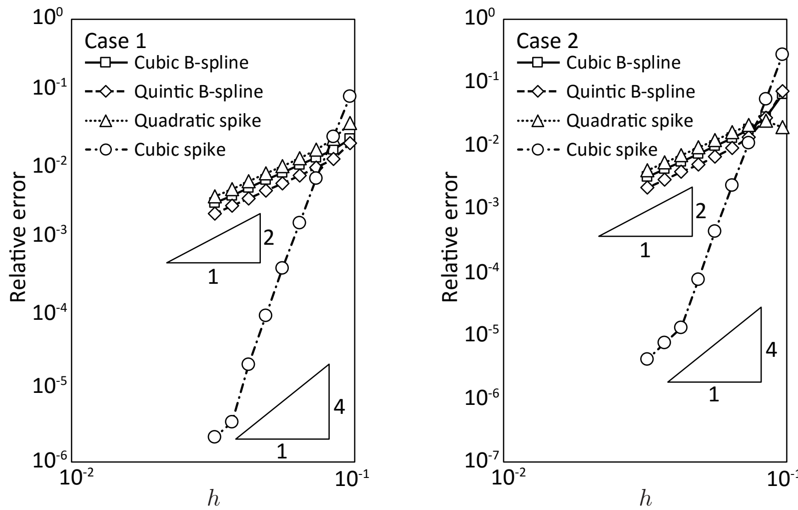

Figure 4.5: The graphs of the relative errors of interpolants versus h.

4.1.2 Approximate gradient and Laplace operators

We compute truncation errors of approximate differential operators. We consider the following weight functions: the quartic polynomial

$$w^{\mathrm{QP}}(r) := \frac{60}{2\pi}\begin{cases} r^2(1-r)^2, & 0 \le r < 1, \\ 0, & r \ge 1, \end{cases}$$

the piecewise cubic polynomial

$$w^{\mathrm{PCP}}(r) := -\frac{r}{2}\frac{d}{dr}w^{\mathrm{CB}}(r), \qquad r \in \mathbb{R}_0^+,$$

and the piecewise quintic polynomial

$$w^{\mathrm{PQP}}(r) := -\frac{r}{2}\frac{d}{dr}w^{\mathrm{QB}}(r), \qquad r \in \mathbb{R}_0^+,$$

The approximate differential operators using the quartic polynomial, the piecewise cubic polynomial, and the piecewise quintic polynomial agree with the approximate differential operators in SPH using the bell-shaped function, the cubic B-spline, and the quintic B-spline [38], respectively; see Appendix A.1. Set Δx by $2^{-5}, 2^{-6}, \ldots, 2^{-11}$. For Δx, set h by $h = \{(3.1^4 \times 2^{-10})\Delta x\}^{1/4}$. Set particle volumes by $V_i = \widetilde{V}_i$ $(i = 1, 2, \ldots, N)$. Under the settings above, Theorem 1.13 and Theorem 1.15 are valid with $O(h^2)$.

Figure 4.6 shows graphs of the relative errors

$$\frac{\|\nabla v - \nabla_h v\|_{[\ell^\infty(\Omega)]^2}}{\|\nabla v\|_{[\ell^\infty(\Omega)]^2}}$$

versus the influence radius h and Figure 4.7 shows graphs of the relative errors

$$\frac{\|\Delta v - \Delta_h v\|_{\ell^\infty(\Omega)}}{\|\Delta v\|_{\ell^\infty(\Omega)}}$$

versus the influence radius h. The slopes of triangles show the theoretical convergence rates derived from Theorem 1.13 and Theorem 1.15. Table 4.3 shows numerical convergence rates obtained from the slopes of the relative errors between $\Delta x = 2^{-10}$ and 2^{-11}. Figures 4.6–4.7 and Table 4.3 show that the numerical convergence rates agree well with theoretical ones.

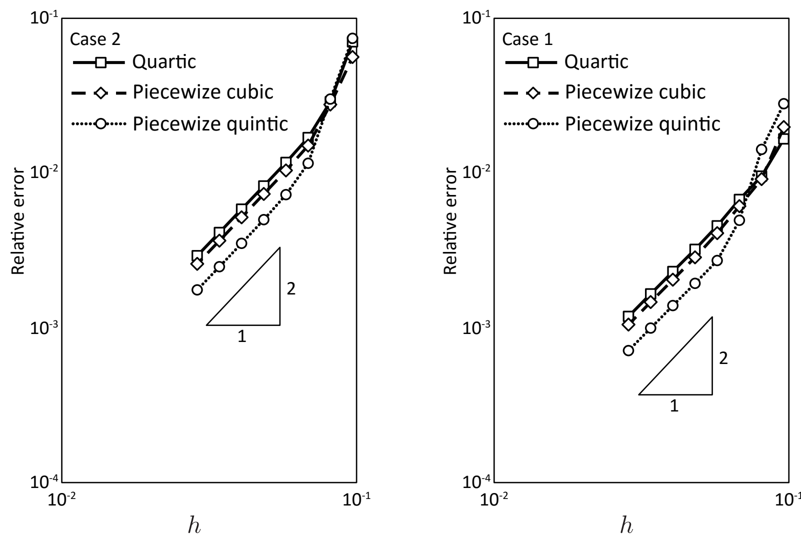

Figure 4.6: The graphs of the relative errors of approximate gradient operators versus h.

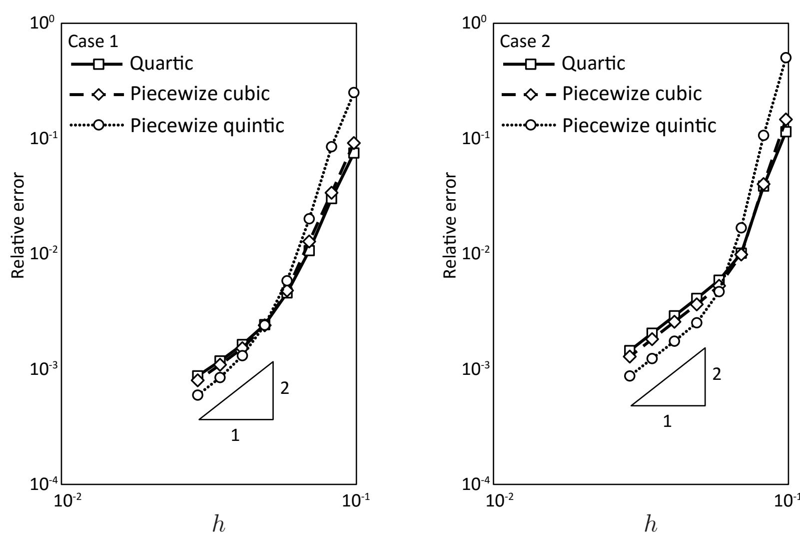

Figure 4.7: The graphs of the relative errors of approximate Laplace operators versus h.

Table 4.3: Numerical convergence rates of approximate gradient operators and approximate Laplace operators obtained from $\Delta x = 2^{-10}$ and 2^{-11} in Figures 4.6–4.7.

	gradient operators		Laplace operators	
Weight function	Case 1	Case 2	Case 1	Case 2
Quartic polynomial	2.00	2.16	2.00	1.93
	2.00	2.25	2.00	1.93
Piecewise quintic polynomial	2.00	2.52	2.00	1.93

4.2 Poisson equation

Set a manufactured solution of Poisson equation (2.1) by

$$u(x,y) = \sin(2\pi(x+y)), \qquad (x,y) \in \Omega.$$

Set $\widetilde{g}$ by $\widetilde{g}(x,y) = \sin(2\pi(x+y))$, $(x,y) \in \Gamma \cup \Gamma_H$.

We consider the weight functions w^{bell}, w^{cubic}, and w^{quintic}. Set Δx by $2^{-5}, 2^{-6}, \ldots, 2^{-9}$. For Δx, set h by $h = \{(2.6^4 \times 2^{-10})\Delta x\}^{1/4}$. Set particle volumes by (A.10). Under the setting above, Theorem 2.1 is valid with $O(h^2)$.

Figure 4.8 shows graphs of the relative errors

$$\frac{\|\widetilde{u} - U\|_{\ell^\infty(\Omega)}}{\|\widetilde{u}\|_{\ell^\infty(\Omega)}}$$

versus the influence radius h. The slopes of triangles show the theoretical convergence rates derived from Theorem 2.1. Table 4.4 shows numerical convergence rates obtained from the slopes of the relative errors between $\Delta x = 2^{-8}$ and 2^{-9}. Figure 4.8 and Table 4.4 show that the numerical convergence rates agree well with theoretical ones.

Table 4.4: Numerical convergence rates of the discrete Poisson equation.

Weight function	convergence rates
Quartic polynomial	1.95
Piecewise cubic polynomial	1.99
Piecewise quintic polynomial	2.00

4.3 Heat equation

Set $T = 0.1$ and $\kappa = 0.5$. Set a manufactured solution of the heat equation (2.1) by

$$u(x,y,t) = \exp(-2\kappa\pi^2 t)\sin(\pi x)\sin(\pi y), \qquad (x,y) \in \Omega,\ t \in (0,T).$$

Set $\widetilde{g}$ and $\widetilde{a}$ by

$$\begin{aligned} \widetilde{g}(x,y,t) &= \exp(-2\kappa\pi^2 t)\sin(\pi x)\sin(\pi y), \quad && (x,y) \in \Gamma \cup \Gamma_H,\ t \in (0,T), \\ \widetilde{a}(x,y,t) &= \sin(\pi x)\sin(\pi y), && (x,y) \in \Omega_H, \end{aligned}$$

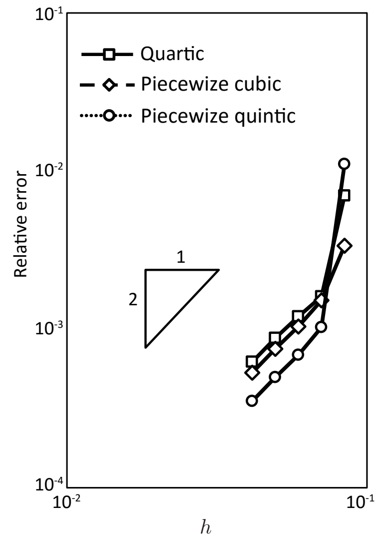

Figure 4.8: The graphs of the relative errors of the discrete Poisson equation versus h.

respectively. We consider the weight functions w^{bell}, w^{cubic}, and w^{quintic}. Set particle volumes by (A.10).

First, setting Δt to satisfy (3.23), we confirm convergence of errors in case that $\theta = 0, 1/2$, and 1. Set $\Delta x = 2^{-5}, 2^{-6}, \ldots, 2^{-8}$, $h = \{(2.6^4 \times 2^{-10})\Delta x\}^{1/4}$, and $\Delta t = 0.0025h^2$. Figure 4.9 shows graphs of the relative errors

$$\frac{\|\widetilde{u} - U\|_{\ell^\infty([0,T];\ell^2(\Omega_H))}}{\|\widetilde{u}\|_{\ell^\infty([0,T];\ell^2(\Omega_H))}} \tag{4.2}$$

versus the influence radius h in case that $\theta = 0, 1/2$, and 1. The slopes of triangles show the theoretical convergence rates derived from Theorem 3.7. Table 4.5 shows numerical convergence rates obtained from the slopes of the relative errors between $\Delta x = 2^{-7}$ and 2^{-8}. Though the convergences of errors are obtained, the numerical rates are not agree with ones of Theorem 3.7. It is conjectured that we can not enough compute asymptotic estimates for the limit of calculation environments.

Table 4.5: Numerical convergence rates of the discrete heat equation in case that $\Delta t = 0.0025h^2$.

Weight function	$\theta = 0$	$\theta = 1/2$	$\theta = 1$
Quartic polynomial	6.63	4.92	4.62
Piecewise cubic polynomial	6.64	5.43	5.66
Piecewise quintic polynomial	6.67	6.81	7.17

Next, in order to confirm unconditional stabilities when $\theta \in [1/2, 1]$, we compute under a sufficiently large time step $\Delta t = 0.5h^2$. Set $\Delta x = 2^{-5}, 2^{-6}, \ldots, 2^{-9}$, $h = \{(2.6^4 \times 2^{-10})\Delta x\}^{1/4}$, and $\theta = 0, 1/2, 1$.

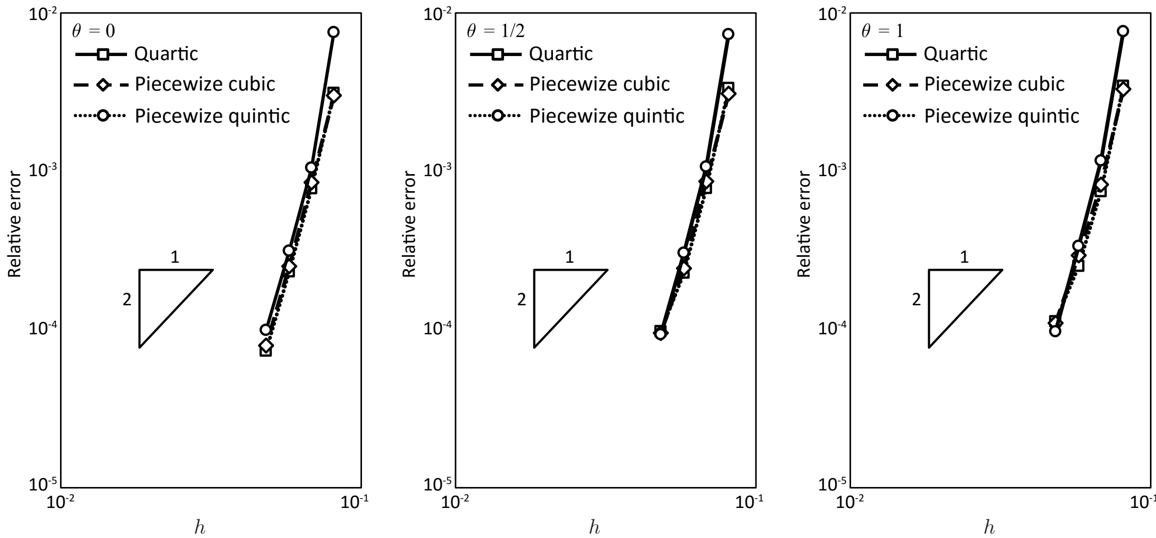

Figure 4.9: The graphs of the relative errors of the discrete heat equation versus h in case that $\Delta t = 0.0025h^2$ and $\theta = 0, 1/2, 1$.

Figure 4.10 shows graphs of the relative errors (4.2) versus the influence radius h in case that $\theta = 1/2$ and 1. The slopes of triangles show the theoretical convergence rates derived from Theorem 3.7. Table 4.6 shows numerical convergence rates obtained from the slopes of the relative errors between $\Delta x = 2^{-8}$ and 2^{-9}. From Table 4.6, we can confirm that the stability conditions are valid when $\theta = 0$. Moreover, Figure 4.6 and Table 4.6 show, in case that $\theta = 1$, the numerical convergence rates agree with ones of Theorem 3.7. On the other hand, in case that $\theta = 1/2$, the numerical convergence rates do not agree with ones of Theorem 3.7, although the errors convergence. In case that $\theta = 1/2$, it is also conjectured that we can not enough compute asymptotic estimates for the limit of calculation environments.

Table 4.6: Numerical convergence rates of the discrete heat equation in case that $\Delta t = 0.5h^2$

Weight function	$\theta = 0$	$\theta = 1/2$	$\theta = 1$
Quartic polynomial	−281	4.31	1.94
Piecewise cubic polynomial	−314	4.39	2.02
Piecewise quintic polynomial	−416	4.55	2.06

Finally, setting Δt by a first order of h, we confirm differences of convergence rates in case that $\theta = 1/2$ and 1. Set $\Delta x = 2^{-5}, 2^{-6}, \ldots, 2^{-9}$, $h = \{(2.6^4 \times 2^{-10})\Delta x\}^{1/4}$, and $\Delta t = 0.5h$. Figure 4.11 shows graphs of the relative errors (4.2) versus the influence radius h in case that $\theta = 1/2$ and 1. The slopes of triangles show the theoretical convergence rates derived from Theorem 3.7. Table 4.7 shows numerical convergence rates obtained from the slopes of the relative errors between $\Delta x = 2^{-8}$ and 2^{-9}. Figure 4.11 and Table 4.7 shows that the numerical convergence rates agree with theoretical ones.

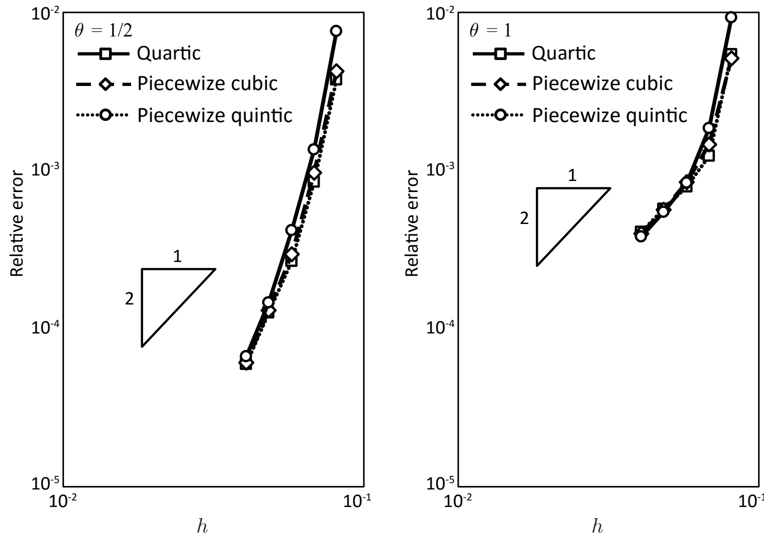

Figure 4.10: The graphs of the relative errors of the discrete heat equation versus h in case that $\Delta t = 0.5h^2$ and $\theta = 1/2, 1$.

Table 4.7: Numerical convergence rates of the discrete heat equation in case that $\Delta t = 0.5h$.

Weight function	$\theta = 1/2$	$\theta = 1$
Quartic polynomial	2.01	0.84
Piecewise cubic polynomial	2.02	0.84
Piecewise quintic polynomial	2.03	0.83

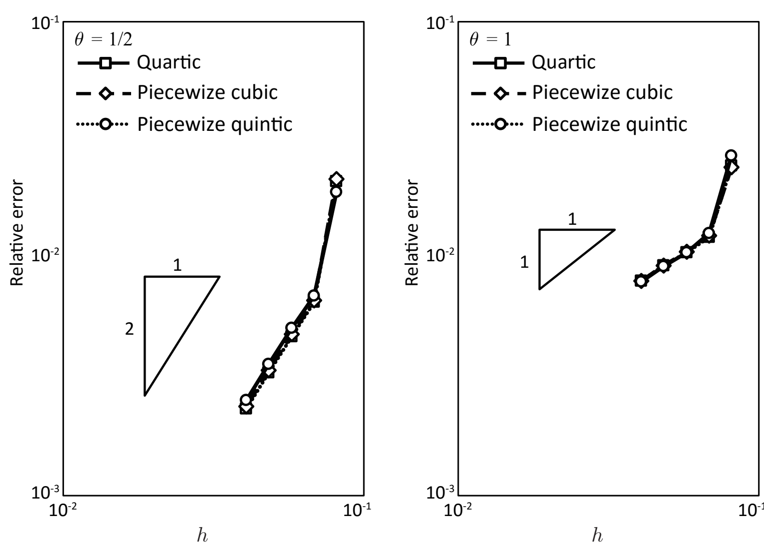

Figure 4.11: The graphs of the relative errors of the discrete heat equation versus h in case that $\Delta t = 0.5h$ and $\theta = 1/2, 1$.

Conclusion

A generalized particle method has been introduced for discretizing partial differential equations described by strong formulations and error estimates of the generalized particle method have been established for the Poisson and heat equations.

At first we have introduced the generalized particle method and have made preparations for subsequent analysis. The generalized particle method have been defined as a class of particle methods that discretize the partial differential equations that can describe conventional particle methods such as SPH and MPS. For discrete parameters of the generalized particle method, we have introduced a regularity, hypotheses of weight functions, and a connectivity condition. The regularity has been a condition of a family of particle distribution, particle volumes, and influence radii defined by a ratio among the influence radius and two indicators of the particle distributions and the particle volumes. The one of the indicators, which is called a covering radius, has been defined by a radius of circles whose centers are particles when an union of the circles just covers the spatial domain. The another indicator, which is called a Voronoi deviation, has been defined by a weighted deviation between the particle volume and Voronoi volumes. Also we have been defined a regular order of the regularity by this ratio. The hypotheses of weight functions have been given by four conditions; the first condition is that an integration of the weight functions multiplied by polynomials vanishes; the second and third conditions are properties around the origin; and the last condition is a positivity within the support of the weight function. In the first condition, we call the maximum degree of polynomial an order of weight function. The connectivity condition, which is called h-connectivity condition, has been defined by a property of a graph with respect to the particle distributions and the influence radius h. After the introduction of the conditions of the parameters, we have obtained truncation errors of the interpolant and the approximate differential operators. Under the regularity and the some hypotheses of the weight functions, we have established the truncation error estimates with the maximum norm that are $O(h^{\min\{k+1,m-1\}})$ in case of the interpolant and the approximate gradient operator and $O(h^{\min\{k+1,m-2\}})$ in case of the approximate Laplace operator for the regular order m and the order of weight function k.

Next we have introduced the Poisson equation discretized by the generalized particle method and have proved its error estimates. By using the connectivity condition, we have shown the unique solvability and the discrete maximum principle of the discrete Poisson equation. Utilizing the truncation error estimates and the discrete maximum principle, we have established the stability and the error estimates with a discrete L^∞ norm that are $O(h^{\min\{2,m-2\}})$.

Furthermore we have introduced the heat equation discretized by the generalized particle method in space and by the θ-method in time and have established its error estimates. We first have proved the unique solvability and the discrete maximum principle of the discrete heat equation. Utilizing the truncation error estimates and the discrete maximum principle, we have established the stability with a condition of the time step in case of $\theta \in [0, 1)$ and without in case of $\theta = 1$ (backward Euler method), where θ is a discretize parameter of the θ-method. Under the conditions of the stability, we have obtained the error estimates with the discrete L^∞ norm in space and time that are $O(\Delta t + h^{\min\{2,m-2\}})$ in case of $\theta \neq 1/2$ and $O(\Delta t^2 + h^{\min\{2,m-2\}})$ in case that $\theta = 1/2$ (Crank-Nicolson method). Furthermore, by introducing a discrete L^2 norm in space, we have obtained a stability with a condition of the time step in case of $\theta \in [0, 1/2)$ and without in case of $\theta \in [1/2, 1]$. Then we have established the error estimates with the discrete L^2 norm in space and the discrete L^∞ norm in time, which are same orders of the error estimates with the discrete L^∞ norm.

Finally, we have shown some numerical results corresponding to the above results. Under each condition derived from the theorems, we have confirmed that the errors have converged and the convergence rates almost agree with theoretical ones.

In future work, as aiming to further establish mathematical framework of the generalized particle method, we will investigate error estimates of the generalized particle method for the partial differential equations including convections such as the convection-diffusion equation and Navier-Stokes equations. Moreover, by utilizing knowledge obtained from numerical analysis, we will try to solve some problems in practical computations, for example, redistribution methods of the particles and finding appropriate weight functions.

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Appendix A

Conventional particle methods

This appendix introduces conventional particle methods: Smoothed Particle Hydrodynamics (in Section A.1) and Moving Particle Semi-implicit (in Section A.2) and shows numerical analysis of these particle methods by utilizing the theoretical results in this thesis.

A.1 Smoothed Particle Hydrodynamics

Smoothed Particle Hydrodynamics (SPH) is a particle method developed for computing astrophysics in 1977 [26, 40]. Later on, SPH has been used for various problems, including the fluid dynamics [42, 43]. In SPH, various types of approximate operators have been proposed [12, 26, 38]. In this section, we introduce approximate operators used in SPH for incompressible flow problems (Incompressible SPH) [3, 17, 53].

Let us define $w^{\mathrm{S}} : \mathbb{R}_0^+ \to \mathbb{R}$ as a weight function of SPH (also called a smoothing function). The weight functions satisfying the following conditions are often used [19, 25].

$$w^{\mathrm{S}}(r) \begin{cases} > 0, & 0 \le r < 1, \\ = 0, & r \ge 1, \end{cases} \tag{A.1}$$

$$\int_{\mathbb{R}^d} w^{\mathrm{S}}(|x|)dx = 1, \tag{A.2}$$

$$w^{\mathrm{S}} \in C^2(\mathbb{R}_0^+), \tag{A.3}$$

$$\lim_{r \downarrow 0} \left| \frac{1}{r} \frac{d}{dr} w^{\mathrm{S}}(r) \right| < \infty, \tag{A.4}$$

$$\frac{d}{dr} w^{\mathrm{S}}(r) < 0, \qquad 0 < r < 1. \tag{A.5}$$

For example, the bell-shaped function, the cubic B-spline, the quartic B-spline, and the quintic B-spline [37, 38] satisfy the conditions. For the weight function w^{S} and the influence radius h (also called a smoothing length), set $w_h^{\mathrm{S}} : \mathbb{R}_0^+ \to \mathbb{R}$ by

$$w_h^{\mathrm{S}}(r) := \frac{1}{h^d} w^{\mathrm{S}} \left(\frac{r}{h} \right).$$

Then, in SPH, the interpolant $\Pi_h^{\mathrm{S}} : C(\overline{\Omega}_H) \to C(\overline{\Omega}_H)$, the approximate gradient operator $\nabla_h^{\mathrm{S}} : C(\overline{\Omega}_H) \to C(\overline{\Omega}_H)$, and the approximate Laplace operator $\Delta_h^{\mathrm{S}} : C(\overline{\Omega}_H) \to C(\overline{\Omega}_H)$ are defined by

$$\Pi_h^{\mathrm{S}} v(x) := \sum_{i=1}^{N} V_i v(x_i) w_h^{\mathrm{S}}(|x - x_i|), \tag{A.6}$$

$$\nabla_h^{\mathrm{S}} v(x) := \sum_{i=1}^{N} V_i \left\{v(x_i) - v(x)\right\} \nabla w_h^{\mathrm{S}}(|x - x_i|), \tag{A.7}$$

$$\Delta_h^{\mathrm{S}} v(x) := 2 \sum_{i\in\Lambda_x^*} V_i \frac{v(x) - v(x_i)}{|x - x_i|} \frac{x - x_i}{|x - x_i|} \cdot \nabla w_h^{\mathrm{S}}(|x - x_i|), \tag{A.8}$$

respectively.

Remark A.1. *The approximate operators of the generalized particle method* (1.2), (1.3), (1.4) *can describe ones of SPH* (A.6), (A.7), (A.8) *by substituting the weight functions of the generalized particle method. For example, by substituting $w = w^{\mathrm{S}}$, it holds that $\Pi_h = \Pi_h^{\mathrm{S}}$. Moreover, by substituting*

$$w(r) = -\frac{r}{d}\frac{d}{dr} w^{\mathrm{S}}(r), \qquad r \in \mathbb{R}_0^+, \tag{A.9}$$

it holds that $\nabla_h = \nabla_h^{\mathrm{S}}$ and $\Delta_h = \Delta_h^{\mathrm{S}}$.

Remark A.2. *In SPH, $V_{N,H}$ is well used such as*

$$V_{N,H} = \left\{ V_i;\ V_i = \frac{\mathrm{meas}(\Omega_H)}{N},\ i = 1, 2, \ldots, N \right\} \tag{A.10}$$

or

$$V_{N,H} = \left\{ V_i;\ V_i = \frac{1}{\sum_{j=1}^{N} w_h(|x_i - x_j|)},\ i = 1, 2, \ldots, N \right\}. \tag{A.11}$$

(A.10) *obviously satisfies* (1.1)*. On the other hand,* (A.11) *approximately satisfies* (1.1).

Corollary A.3. *Suppose that $V_{N,H}$ satisfies* (1.1)*, $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ is a regular family, and w^{S} satisfies* (A.1)–(A.3)*. Then, for the interpolant of SPH* (A.6)*, truncation error estimates as same as Theorem* 1.11 *are obtained.*

Proof. It is sufficient to prove that w^{S} satisfies conditions of Theorem 1.11. Since w^{S} satisfies (A.1)–(A.3), we have $w^{\mathrm{S}} \in W$. Moreover, by Proposition 1.4, w^{S} satisfies Hypothesis 1.1 with at least $k = 1$. Therefore the corollary is proved. □

Corollary A.4. *Suppose that $V_{N,H}$ satisfies* (1.1)*, $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ is a regular family, and w^{S} satisfies* (A.1)–(A.4)*. Then, for the approximate gradient operator* (A.7) *and the approximate Laplace operator* (A.8)*, truncation error estimates as same as Theorem* 1.13 *and Theorem* 1.15 *are valid.*

Proof. The weight function w is set by (A.9). It is sufficient to show that w satisfies conditions of Theorem 1.13 and Theorem 1.15. By (A.1), (A.2), and using the integration by parts, we have

$$\begin{aligned}\int_{\mathbb{R}^d} w(|x|)dx &= -\frac{1}{d}\int_{\mathbb{R}^d} |x|\frac{d}{dr}w^{\mathrm{S}}(|x|)dx\\ &= -\frac{1}{d}\int_{\mathbb{R}^d} x\cdot\nabla w^{\mathrm{S}}(|x|)dx\\ &= \frac{1}{d}\int_{\mathbb{R}^d}(\nabla\cdot x)w^{\mathrm{S}}(|x|)dx\\ &= \int_{\mathbb{R}^d} w^{\mathrm{S}}(|x|)dx\\ &= 1.\end{aligned}$$

Therefore we find $w \in W$. By (A.3) and (A.4), w satisfies Hypothesis 1.2 and Hypothesis 1.3. Moreover, by Proposition 1.4, w satisfies Hypothesis 1.1 with at least $k = 1$. Therefore the corollary is true. □

Corollary A.5. *Suppose that* $V_{N,H}$ *satisfies* (1.1), $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ *is a regular family with order* m (> 2), *and* w^{S} *satisfies* (A.1)–(A.5). *Then, for Poisson equation discretized by the approximate Laplace operator* (A.8), *error estimates as same as Theorem* 2.1 *are derived.*

Moreover, for the heat equation discretized by the approximate Laplace operator (A.8) *in space, error estimates as same as Theorem* 3.7 *are obtained under appropriate conditions with respect to the time step.*

Proof. The weight function w is set by (A.9). It is sufficient to prove that w satisfies conditions of Theorem 2.1 and Theorem 3.7. By (A.5), w satisfies Hypothesis 1.4. Therefore, by Corollary A.4, w satisfies assumptions of Theorem 2.1 and Theorem 3.7. Consequently the corollary is obtained. □

A.2 Moving Particle Semi-implicit

Moving Particle Semi-implicit (MPS) is a particle method developed for computing incompressible flow in 1996 [33] and has been applied into various problems as same as SPH. Now we introduce approximate differential operators of MPS. We define a weight function of MPS by $w^{\mathrm{M}} : \mathbb{R}_0^+ \to \mathbb{R}$ satisfying

$$w^{\mathrm{M}}(r)\begin{cases} > 0, & 0 < r < 1,\\ = 0, & r \geq 1.\end{cases} \tag{A.12}$$

For example, the following unbounded weight function [19, 25] is often used.

$$w^{\mathrm{M}}(r) = \begin{cases} \dfrac{1}{r} - 1, & 0 < r < 1,\\ 0, & r = 0,\ r \geq 1.\end{cases} \tag{A.13}$$

For the weight function w^{M} and the influence radius h, set $w_h^{\mathrm{M}} : \mathbb{R}_0^+ \to \mathbb{R}$ by

$$w_h^{\mathrm{M}}(r) := \frac{1}{h^d} w^{\mathrm{M}}\left(\frac{r}{h}\right).$$

Then, in MPS, the approximate gradient operator $\nabla_h^{\mathrm{M}} : C(\overline{\Omega}_H) \to C(\overline{\Omega}_H)$ and the approximate Laplace operator $\Delta_h^{\mathrm{M}} : C(\overline{\Omega}_H) \to C(\overline{\Omega}_H)$ are defined by

$$\nabla_h^{\mathrm{M}} v(x) := \frac{d}{n_0} \sum_{i \in \Lambda_x^*} \frac{v(x) - v(x_i)}{|x - x_i|} \frac{x - x_i}{|x - x_i|} w_h^{\mathrm{M}}(|x - x_i|), \tag{A.14}$$

$$\Delta_h^{\mathrm{M}} v(x) := -\frac{2d}{\lambda_0} \sum_{i \in \Lambda_x^*} \{v(x) - v(x_i)\}\, w_h^{\mathrm{M}}(|x - x_i|), \tag{A.15}$$

respectively, where an interpolant is not introduced in MPS. Here n_0 and λ_0 are regularized parameters for each operator. For example, by setting a representative particle $x_{i'} \in X_{N,H}$, these regularized parameters are given by

$$n_0 = \sum_{i=1}^{N} w_h^{\mathrm{M}}(|x_{i'} - x_i|),$$

$$\lambda_0 = \sum_{i=1}^{N} |x_{i'} - x_i|^2 w_h^{\mathrm{M}}(|x_{i'} - x_i|).$$

Remark A.6. *The approximate differential operators of the generalized particle method* (1.3), (1.4) *can describe ones of MPS* (A.14), (A.15) *by substituting the particle volumes and the weight functions. For example, substituting $V_{N,H}$ by* (A.10) *and w by*

$$w(r) = \left\{ \int_{\mathbb{R}^d} w^{\mathrm{M}}(|x|) dx \right\}^{-1} w^{\mathrm{M}}(r), \quad r \in \mathbb{R}_0^+, \tag{A.16}$$

we have ∇_h that is equivalent to ∇_h^{M} with n_0 given by

$$n_0 = \left(\frac{\mathrm{meas}(\Omega_H)}{N} \right)^{-1} \int_{\mathbb{R}^d} w^{\mathrm{M}}(|x|) dx. \tag{A.17}$$

Also, by substituting $V_{N,H}$ by (A.10) *and w by*

$$w(r) = \left\{ \int_{\mathbb{R}^d} |x|^2 w^{\mathrm{M}}(|x|) dx \right\}^{-1} r^2 w^{\mathrm{M}}(r), \quad r \in \mathbb{R}_0^+, \tag{A.18}$$

we get Δ_h that equals Δ_h^{M} with λ_0 given by

$$\lambda_0 = \left(\frac{\mathrm{meas}(\Omega_H)}{N} \right)^{-1} \int_{\mathbb{R}^d} |x|^2 w^{\mathrm{M}}(|x|) dx. \tag{A.19}$$

Corollary A.7. *Set $V_{N,H}$ by* (A.10) *and n_0 by* (A.17)*. Suppose that $\{(X_{N,H}, V_{N,H}, h)\}_{h \downarrow 0}$ is a regular family and w^{M} satisfies $w^{\mathrm{M}} \in C^1(\mathbb{R}_0^+)$ and Hypothesis* 1.2*. Then, for the approximate gradient operator of MPS* (A.14)*, truncation error estimates as same as Theorem* 1.13 *with $k = 1$ are obtained.*

Proof. The weight function w is set by (A.16). It is sufficient to prove that w satisfies conditions of Theorem 1.13. Since w^{M} satisfies $w^{\mathrm{M}} \in C^1(\mathbb{R}_0^+)$ and Hypothesis 1.2, w satisfies $w \in W$ and Hypothesis 1.2. Moreover, by Lemma 1.5, w satisfies Hypothesis 1.1 with $k = 1$. Therefore the corollary is true. □

Corollary A.8. *Set* $V_{N,H}$ *by* (A.10) *and* λ_0 *by* (A.19). *Suppose that* $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ *is a regular family and* w^{M} *satisfies* $w^{\mathrm{M}} \in C^1(\mathbb{R}_0^+)$. *Therefore, for the approximate Laplace operator of MPS* (A.15), *truncation error estimates as same as Theorem* 1.15 *with* $k = 1$ *are obtained.*

Proof. The weight function w is set by (A.18). It is sufficient to prove that w satisfies conditions of Theorem 1.15. Since $w^{\mathrm{M}} \in C^1(\mathbb{R}_0^+)$, w satisfies $w \in W$ and Hypothesis 1.3. Moreover, by Lemma 1.5, w satisfies Hypothesis 1.1 with $k = 1$. Therefore the corollary is proved. □

Corollary A.9. *Set* $V_{N,H}$ *by* (A.10) *and* λ_0 *by* (A.19). *Suppose that* $\{(X_{N,H}, V_{N,H}, h)\}_{h\downarrow 0}$ *is a regular family with order* m (> 2) *and* w^{M} *satisfies* $w^{\mathrm{M}} \in C(\mathbb{R}_0^+)$. *Then, for Poisson equation discretized by the approximate Laplace operator* (A.15), *error estimates as same as Theorem* 2.1 *are derived.*

Moreover, for the heat equation discretized by the approximate Laplace operator (A.15) *in space, error estimates as same as Theorem* 3.7 *are established under appropriate conditions with respect to the time step.*

Proof. The weight function w is set by (A.18). It is sufficient to prove that w satisfies conditions of Theorem 2.1 and Theorem 3.7. By (A.12), w satisfies Hypothesis 1.4. Therefore, by Corollary A.8, w satisfies conditions Theorem 2.1 and Theorem 3.7. Therefore the corollary is obtained. □

Remark A.10. *In case of using* (A.13) *as the weight function, since the weight function does not belong to* $C(\mathbb{R}_0^+)$, *the corollaries above are not obtained.*