Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 286 (2015) 216–229
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

# Integral approximations to classical diffusion and smoothed particle hydrodynamics[☆]

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Received 11 September 2014; received in revised form 2 December 2014; accepted 12 December 2014
Available online 31 December 2014

**Abstract**

The contribution of the paper is the approximation of a classical diffusion operator by an integral equation with a volume constraint. A particular focus is on classical diffusion problems associated with Neumann boundary conditions. By exploiting this approximation, we can also approximate other quantities such as the flux out of a domain. Our analysis of the model equation on the continuum level is closely related to the recent work on nonlocal diffusion and peridynamic mechanics. In particular, we elucidate the role of a volumetric constraint as an approximation to a classical Neumann boundary condition in the presence of physical boundary. The volume-constrained integral equation then provides the basis for accurate and robust discretization methods. An immediate application is to the understanding and improvement of the Smoothed Particle Hydrodynamics (SPH) method.


*Keywords:* Smooth Particle Hydrodynamics; Classical diffusion; Nonlocal diffusion; Nonlocal operator; Nonlocal Neumann condition; Numerical approximation

## 1. Introduction

Let $\zeta = \zeta(|x|)$ be a compactly supported and absolutely integrable function on the ball $B_\rho(0)$ of radius $\rho$ at the origin satisfying the normalization condition

$$\int_{B_\rho(0)\subset\mathbb{R}^d} \zeta(|x|)\, dx = d, \tag{1}$$

☆ Research of Q. Du was supported in part by US NSF DMS-1318586, and AFOSR MURI center for material failure prediction through peridynamics. Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly subsidiary of Lockheed Martin Corporation, for the US Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. A. Tartakovsky was supported by the US Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Applied Mathematics program. Pacific Northwest National Laboratory is operated by Battelle for the US Department of Energy under Contract DE-AC05-76RL01830.
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http://dx.doi.org/10.1016/j.cma.2014.12.019
0045-7825/

where $|x| = \sqrt{x \cdot x}$ denotes the Euclidean length of $x$. Then for a function $u = u(x)$, a formal Taylor series analysis grants that

$$\begin{aligned}\mathcal{L}_\delta u(x) &:= \frac{1}{\delta^d} \int_{\mathbb{R}^d} \frac{u(y) - u(x)}{|x-y|^2} \big(\kappa(x) + \kappa(y)\big) \zeta \left(\frac{1}{\delta}|x-y|\right) dy \\ &= \nabla \cdot \kappa(x) \nabla u(x) + O(\delta^2) \quad x \in \mathbb{R}^d, \end{aligned} \tag{2}$$

for a positive smooth scalar field $\kappa = \kappa(x)$, which may be identified with a diffusion coefficient. In so many words, a local function (depending only on $x$) is approximated by a nonlocal function (depending on a neighborhood of points $y \neq x$). This is a well-known, often rediscovered approximation of the inhomogeneous diffusion operator, and has been exploited for various problems [1,2]. In particular, Cleary and Monaghan [2] employed the above integral approximation to introduce a Smoothed Particle Hydrodynamics (SPH) discretization for classical heat conduction. However, replacing the infinite domain $\mathbb{R}^d$ with a finite domain $\Omega$ proves to be a challenge for SPH and other approaches attempting to exploit an integral approximation. At root is that constraints on $u$ near the boundary of $\Omega$ need to be provided. However, it is not at all clear what the relevance is of boundary conditions for the above integral operator.

The purpose of our paper is to demonstrate that augmenting the above integral operator with a constraint over a domain of nonzero volume in $\Omega$, rather than $\partial\Omega$, allows us to conclude that a suitable "problem with a volumetric constraint" or "volume constrained problem" associated with the integral operator converges to a boundary value problem involving the diffusion operator. This is accomplished by appealing to recent work in nonlocal diffusion [3,4] and peridynamic mechanics [5–8] where the introduction of volumetric constraints and a variational formulation proved crucial in demonstrating that volume constrained problems are well-posed. Moreover the solution of a volume constrained problem converges with a diminishing modeling error to standard variational formulations of boundary value problems associated with the inhomogeneous diffusion operator.

An important consequence of our analyses is that we may use the nonlocal integral equation as an intermediate or a bridge between classical diffusion problems and their SPH approximations. Although it is a common practice to approximate differential operators by nonlocal operators in the SPH construction, little attention has been paid to the mathematical properties of these nonlocal equations. The analytical framework developed in this work allows us to both distinguish and connect two key limiting processes in the construction of SPH approximations, namely, the use of

1. an integral operator with a diminishing model parameter $\delta$ to approximate the differential operator, and
2. a numerical quadrature with a diminishing mesh size $h$ approximating the integral operator.

We emphasize that it is this two-step process of discretizing the integral operator and letting both the mesh size $h$ and modeling parameter $\delta$ decrease that proves critical in understanding carefully the underlying approximations, see [9] for extended discussions. An immediate application is that the analysis of various SPH discretization schemes become possible including discretizations in the presence of a physical boundary. Such SPH like discretization can therefore be shown to converge to the solution of the appropriate problem defined in a finite domain in a suitable limit. Connecting these two limiting processes can also be extend to consider discretizations of peridynamic mechanics to build upon and extend the work in [10,11].

The conventional SPH discretization is often realized as a discretization of the integral operator where the mesh size and $\delta$ are coupled. The numerical analysis of such discretizations (including the development of higher order methods) and the presence of a boundary adds to the challenges. Meanwhile, the numerical analysis of nonlocal diffusion problems explains that the mesh size must decrease at a faster rate than $\delta$ when using some conventional low order discretizations in order to recover the correct local limit. Otherwise, convergence of the volume constrained problem may mistakenly converge to a boundary value problem different from that anticipated [12]. Moreover, the variational formulation of a volume constrained problem associated with the integral nonlocal operator suggests naturally how higher-order, more robust, discretizations are constructed. For instance, a discontinuous finite element method with linear basis functions leads to a second order accurate conforming discretization where the mesh size does not need to decrease faster than $\delta$ to attain convergence to the boundary value problem of interest involving the inhomogeneous diffusion operator [9]. By appealing to recent work in nonlocal diffusion and peridynamic mechanics, we can demonstrate that the diffusion equation $u_t = \mathcal{L}_\delta u$ conserves the density $u$ and identify the nonlocal flux [13]. This suggests that compatible discretizations of the nonlocal diffusion equation may automatically conserve density at the discrete level. This underscores our contention that focus must be placed on the continuum model, the integral operator, before any discretization.

The organization of the paper is as follows: Section 2 provides the basic mathematical formulations of the classical diffusion problem and nonlocal integral equations. The main ingredients of SPH discretization are also introduced. Section 3 focuses on nonlocal problems with volumetric constraints defined on a finite domain. Various properties of the nonlocal problems are examined along with the analysis on the order of approximations for some illustrative examples. Section 4 considers mass conservation. Section 5 complements the modeling and analytical findings with numerical experiments. Section 6 provides summary and conclusions.

## 2. Mathematical formulation

### 2.1. Classical diffusion equation

Assume that $\Omega \subset \mathbb{R}^d$ is a domain with a suitably regular boundary $\Gamma = \partial\Omega$. Consider the classical mixed boundary value problem

$$\begin{cases} u_t = \nabla \cdot \kappa \nabla u, & \Omega \times (0, T) \\ \kappa \dfrac{\partial u}{\partial n} = g, & \Gamma_1 \times (0, T) \\ u = h, & \Gamma_2 \times (0, T) \\ u(x, 0) = u_0(x), & x \in \Omega. \end{cases} \tag{3}$$

where $g = g(x, u(x, t))$ is a prescribed flux function (that may depend on the solution $u$), and $\Gamma_1 \cap \Gamma_2 = \emptyset$, $\Gamma_1 \cup \Gamma_2 = \partial\Omega$.

In order to focus on the approximation of (3) with a volume constrained nonlocal problem, much of our analyses considers the steady-state problem for (3) with diffusion coefficient $\kappa$ set to one to focus on the key issues and to set $\Gamma_2 = \emptyset$. This leads to the inhomogeneous Neumann boundary value problem

$$\begin{cases} -\Delta u = 0, & \text{on } \Omega \\ \dfrac{\partial u}{\partial n} = g, & \text{on } \partial\Omega \end{cases} \tag{4a}$$

where we assume that the solvability condition

$$\int_{\partial\Omega} g dx = 0, \tag{4b}$$

is satisfied.

### 2.2. Volume constrained problem

To study the nonlocal analog of the problem (4a), we begin with the discussion of a nonlocal diffusion operator defined by

$$2 \int_{\mathbb{R}^d} \frac{u(y) - u(x)}{|x - y|^2} \zeta(|x - y|)\, dy, \quad x \in \mathbb{R}^d \tag{5}$$

for a real-valued function $u = u(x)$ given a compactly supported and absolutely integrable kernel function $\zeta$ satisfying (1). In general, the integral operator is understood in the sense of principle value [14,15].

The nonlocal analogue of the Neumann problem (4a) may now be written in the following general form

$$-2 \int_{\Omega} \frac{u(y) - u(x)}{|y - x|^2} \zeta(|x - y|)\, dy = \tilde{f}(x), \quad \text{in } x \in \Omega, \tag{6a}$$

for a function $\tilde{f}$ that also satisfies the solvability condition

$$-2 \int_{\Omega} \int_{\Omega} \frac{u(y) - u(x)}{|y - x|^2} \zeta(|x - y|)\, dy\, dx + \int_{\Omega} \tilde{f}\, dx = \int_{\Omega} \tilde{f}\, dx = 0, \tag{6b}$$

where the first equality follows because the integrand is antisymmetric in the variables $x$ and $y$.

The expansion (2) explained that we may view the integral operator as an approximation to the classical diffusion operator and the discussion that followed (2) also explained that a finite domain complicates the approximation. The subject of Section 3 will be to analyze a myriad of choices for $\tilde{f}$ representing possible nonlocal analogues of the inhomogeneous Neumann problem (4a). When $\tilde{f}$ is given by an integral operator, a volumetric extension of the flux $g$ is determined representing a volume-constraint for the nonlocal problem.

### 2.3. SPH discretization

The SPH discretization of the inhomogeneous diffusion operator was introduced by Cleary and Monaghan [2]. We first relate the integral approximation that inspired their SPH discretization to the general operator defined in (2). Given a smooth and compactly supported function $W = W(r)$ satisfying the normalization condition

$$\int_{\mathbb{R}^d} W(|x|)dx = 1, \tag{7a}$$

we let $\zeta(r) = -rW_r(r)$ which satisfies

$$\int_{\mathbb{R}^d} \zeta(|x|)dx = d, \tag{7b}$$

by doing an integration by parts. Let us define the scaled functions

$$W^\delta(|x|) = \frac{1}{\delta^d} W\Big(\frac{|x|}{\delta}\Big), \qquad \zeta_\delta(|x|) = \frac{1}{\delta^d}\zeta\Big(\frac{|x|}{\delta}\Big). \tag{7c}$$

For $r = |x - y|$, we have

$$\nabla_x W^\delta(r) = \frac{x-y}{r} W_r^\delta(r) = (y-x)\,\frac{\zeta_\delta(r)}{r^2}, \tag{7d}$$

and

$$(x-y)\cdot\nabla_x W^\delta\,(r) = -\,\zeta_\delta(r). \tag{7e}$$

The SPH discretization of $\Delta u(x)$ introduced in [2], for constant $\kappa$, can be written as

$$\Delta\, u(x_i) \approx 2\sum_j \big(u(x_i) - u(x_j)\big)\,\frac{(x_i - x_j)\cdot\nabla_x W^\delta(|x_i - x_j|)}{|x_i - x_j|^2}\,|V_j| \tag{8a}$$

where $|V_j|$ is the volume associated with some volume element about $x_j$ and can be related to the number density. The relations given by (7) can then explain how the integral operator $\mathcal{L}_\delta$ defined by (2) with the kernel $\zeta$ or $\zeta_\delta$ can be related to the SPH discretization in terms of $W$ (or $W^\delta$). Indeed, we have

$$\begin{aligned}\mathcal{L}_\delta\, u(x_i) &\approx 2\sum_j \big(u(x_j) - u(x_i)\big)\,\frac{\zeta_\delta(|x_i - x_j|)}{|x_i - x_j|^2}\,|V_j| \\ &= 2\sum_j \big(u(x_i) - u(x_j)\big)\,\frac{(x_i - x_j)\cdot\nabla_x W^\delta(|x_i - x_j|)}{|x_i - x_j|^2}\,|V_j| \\ &\approx \Delta\, u(x_i).\end{aligned} \tag{8b}$$

Cleary and Monaghan [2] did not provide estimates of the approximation afforded by the above scheme in the absence or presence of boundaries, and the parameter $\delta$ was also not taken to be independent of the spacing of the particles $x_j$ [28–31]. Discretizations of $\mathcal{L}_\delta\, u$ are properly understood as either a finite element, finite volume, or quadrature based collocation discretization of the nonlocal system (6); see [12] for more details including error estimates. For instance, the discretization $\mathcal{L}_\delta\, u$ given in (8b) is a finite volume method with asymptotic accuracy of order $h$.

Our perspective is that the SPH discretization (8a) is first a discretization of $\mathcal{L}_\delta$ defined by (2) with a given $\delta$, and second the integral operator approximates the diffusion operator as $\delta \to 0$. In other words, the nonlocal operator $\mathcal{L}_\delta$ serves as a link between the diffusion operator and the SPH discretization.

In many applications of SPH, $W = W(r)$ is taken to be a decreasing function in $r$ for $r \geq 0$, which implies that $\zeta$ is also nonnegative. In this case, for a scalar function $u = u(x)$, (8) leads to an $M$-matrix representation for the discretized operator; this is a useful property in practice. We note however that the operator $\mathcal{L}_\delta$ remains positive for a certain class of $\zeta$ that take both positive and negative values so as to incorporate more general nonlocal interactions; see [14] for further discussions. In Section 4, we discuss the mass conservation; see also the analysis in [16].

## 3. Nonlocal formulation of Neumann problems

We now move to consider in more detail the nonlocal analogue (6) of the classical Neumann problem (4). It is in these settings that we see the significance of the recent work on volume constrained problems for nonlocal operators as the latter shed light on how to properly pose and interpret constraints in the presence of physical boundary.

### 3.1. Geometry

We introduce some geometric notation and assumptions, following [17]. We note that most of the discussions are for convenience of analysis, and are not needed for numerical implementations.

We assume that $\Gamma$ can be represented globally by some oriented distance function (level set function)

$$d_\Gamma(x) = \text{dist}(x, \Gamma)$$

defined in an open subset $U \subset \mathbb{R}^d$ as

$$\Gamma = \{x \in U \mid d_\Gamma(x) = 0\}.$$

Moreover, for a constant $\sigma > 0$, we assume that in the band:

$$\Omega_\sigma = \{x \in \mathbb{R}^d \mid d_\Gamma(x) < \sigma\} \subset U$$

around $\Gamma$, there is a unique decomposition for any $x \in \Omega_\sigma$,

$$x = p(x) \pm d_\Gamma(x) n(p(x)) \tag{9}$$

with $p(x) \in \Gamma$ and $n(p(x))$ the unit outward normal to the surface $\Gamma$ at $p(x)$. For $x \in \Omega_\sigma$, the projection $p(x)$ is also the so-called closest point of $x$ since $|x - p(x)| = d_\Gamma(x) = \min_{y\in\Gamma}\{|y - x|\}$. The parameter $\sigma$ is usually determined by the surface curvatures if $\Gamma$ is sufficiently smooth. Without loss of generality, we assume that $|\nabla d_\Gamma(x)| \equiv 1$ in $\Omega_\sigma$.

In addition, if we introduce a coordinate transformation in $\Omega_\sigma$ from $x$ to $(p, r)$ with $p = p(x)$ and $r = d_\Gamma(x)$ as in (9), then it is useful to note that when doing volume integration in $\Omega_\sigma$, the volume element $dx$ may be rewritten as $dx = |J(p, r)| dp dr$, with $|J(p, r)|$ being the Jacobian of the transformation. For points close to $\Gamma$, that is, for $p \in \Gamma$ and small $r = d_\Gamma(x)$, we have $|J(p, r)| - 1 = O(r)$.

### 3.2. Functions used in the formulation

For a general flux function $g$ associated with (6), we introduce a kernel function $\zeta^b = \zeta^b(r)$ (to be specified later) and we define $\tilde{g}(x, u)$ as an extension of $g = g(x, u)$ for $x$ away from $\Gamma$, say $x \in U$, such that $\tilde{g}(x, u)$ is sufficiently regular and satisfies

$$\tilde{g}(x, u) = g(x, u), \quad \forall\, x \in \Gamma \text{ and } \forall\, u.$$

Then the source term for the steady-state nonlocal Neumann problem (6) is given by

$$\tilde{f}(x) = \zeta^b(d_\Gamma(x))\, \tilde{g}(x, u(x)) \quad x \in \Omega. \tag{10}$$

### 3.3. Kernel rescaling and local limit

In order to relate the model problem (6) with the source term given by (10) with the classical problem (4), let us make some assumptions on the kernels $\zeta$ and $\zeta^b$. We assume that they are both non-negative density functions with compact support. Let

$$(0, \rho/2) \subset \text{supp}(\zeta) \subset (0, \rho), \qquad (0, \sigma/2) \subset \text{supp}(\zeta^b) \subset (0, \sigma),$$

for some positive constants $\rho, \sigma$ and

$$\int_{B_\rho(0)} \zeta(|z|)dz = d, \quad \text{and} \quad \int_0^\sigma \zeta^b(r)\,dr = 1,$$

where $B_\rho(0)$ denotes a ball of radius $\rho$ at the origin.

As mentioned before, the nonlocal equation and the local PDE can be linked together by choosing a desired sequence of interaction kernels. We expect the same for the boundary conditions so that two sequences

$$\zeta_\delta(r) = \frac{1}{\delta^d}\zeta\left(\frac{r}{\delta}\right), \quad \text{and} \quad \zeta^b_\varepsilon(r) = \frac{1}{\varepsilon}\zeta^b\left(\frac{r}{\varepsilon}\right)$$

are to be used. We then define the rescaled equation for $0 < \delta, \varepsilon < 1$,

$$-2\int_\Omega \frac{u^{\delta,\varepsilon}(y) - u^{\delta,\varepsilon}(x)}{|y-x|^2}\zeta_\delta(|x-y|)\,dy = \zeta^b_\varepsilon(d_\Gamma(x))\tilde{g}(x, u^{\delta,\varepsilon}(x)), \quad x \in \Omega. \tag{11}$$

The formulation given by (11) is easy to work with and the only dependence on the geometry is through the distance function, in this sense, it is conceptually simpler than some other alternatives such as the one given in [18] that require more explicit tracking of the precise location of boundary points as well as normal and curvature information of the boundary.

We remark that the equation (11) offers a formulation of the Neumann type nonlocal volume constraint. The origin of the volume constraint is because the source term on the right hand side of the equation affects a region with nonzero volume. More specifically, the region is given by a subset in

$$\Omega^i_{\varepsilon\sigma} = \{x \in \Omega \mid d_\Gamma(x) < \varepsilon\sigma\} \subset \Omega,$$

which describes an interior layer around the boundary $\Gamma$ of $\Omega$. The constraint is incorporated as part of the equation rather than the function space for the solution, which is reminiscent of the natural boundary condition for local PDEs.

Moreover, in comparison with the formulation for the case of homogeneous problem, the additional term accounting for the data $g$ or $\tilde{g}$ is local in the sense that it only depends on the instantaneous value of the solution $u$ in space and time.

We now discuss the local limit. Formally, as $\delta$ and $\varepsilon$ decrease to zero, we claim that $u^{\delta,\varepsilon}$ converges to the solution $u$ of (3) in different topologies depending on different choices of $\zeta(\cdot)$ and $\zeta^b(\cdot)$ and under sufficient regularity assumptions on the boundary $\Gamma$ and the function $\tilde{g}$.

In fact, the results in the two papers [4,16] grant that for any pair of functions $v, w \in C^\infty(\Omega)$, we may define the bilinear form

$$\begin{aligned} B_\delta(v, w) &= 2\int_\Omega\int_\Omega \frac{w(x) - w(y)}{|y-x|^2}\zeta_\delta(|x-y|)v(x)\,dy\,dx \\ &= \int_\Omega\int_\Omega \frac{\zeta_\delta(|x-y|)}{|x-y|^2}\big(v(y) - v(x)\big)\big(w(y) - w(x)\big)\,dy\,dx. \end{aligned} \tag{12a}$$

For smooth functions $f = f(z)$ and $b = b(r)$, we have that

$$\lim_{\delta\to 0}\int_{B_{\delta\rho}(0)} f(z)\zeta_\delta(|z|)\,dz = d\,f(0) \quad \text{and} \quad \lim_{\varepsilon\to 0}\int_0^{\varepsilon\sigma} \zeta^b_\varepsilon(r)b(r)\,dr = b(0), \tag{12b}$$

where $B_{\delta\rho}(0)$ denotes a ball of radius $\delta\rho$ at the origin. Thus, we may interpret the limits of $\zeta_\delta(|z|)$ and $\zeta^b_\varepsilon(r)$ as $d$-dimensional and one-dimensional Dirac-delta measures at $z = \{0 \in \mathbb{R}^d\}$ and $r = \{0 \in \mathbb{R}\}$ respectively, in the sense of (12b).

Hence, as shown in [4,16], we have

$$\lim_{\delta\to 0} B_\delta(v, w) = \int_\Omega \nabla v\,\nabla w\,dx = (\nabla v, \nabla w)_\Omega \tag{12c}$$

where $(\cdot,\cdot)_\Omega$ denotes the standard $L^2$ inner product on $\Omega$.

Moreover, we can show that

$$\lim_{\varepsilon\to 0}\int_\Omega \zeta_\varepsilon^b(d_\Gamma(x))\tilde{g}(x,w(x))\,v(x)\,dx = \int_\Gamma g(x,w(x))v(x)dx = (g(x,w(x)),v(x))_\Gamma$$

where $(\cdot,\cdot)_\Gamma$ is the standard duality pairing ($L^2$ inner product) on $\Gamma$.

Indeed, while the limit in (12c) is established in [4,16], the above equation follows from

$$\begin{aligned}\int_\Omega \zeta_\varepsilon^b(d_\Gamma(x))\tilde{g}(x,w(x))\,v(x)\,dx &= \int_{\Omega_{\varepsilon\sigma}} \zeta_\varepsilon^b(d_\Gamma(x))\tilde{g}(x,w(x))\,v(x)\,dx\\ &= \int_\Gamma\int_0^{\varepsilon\sigma} \zeta_\varepsilon^b(r)\tilde{g}(p-rn(p),w(p-rn(p)))v(p-rn(p))\,|J(p,r)|\,dr\,dp\\ &\to \int_\Gamma g(p,w(p))\,v(p)\,dp \quad \text{as } \varepsilon\to 0.\end{aligned} \tag{12d}$$

Let us then examine the weak form of (11): for any suitably smooth test function $v = v(x)$,

$$B_\delta(u^{\delta,\varepsilon}(x),v(x)) = \big(\zeta_\varepsilon^b(d_\Gamma(x))\tilde{g}(x,u^{\delta,\varepsilon}(x)),v(x)\big)_\Omega. \tag{13a}$$

Following the above discussion, under suitable assumption on $\tilde{g}$ that allowing a pass through the limit in its argument as $\delta,\varepsilon\to 0$, we get that the limit $u = \lim_{\delta,\varepsilon\to 0} u^{\delta,\varepsilon}$ satisfies the weak form: for any $v = v(x)$ suitably smooth,

$$(\nabla u,\nabla v)_\Omega = \big(g,v\big)_\Gamma. \tag{13b}$$

Hence, given sufficient regularity on the solution, we recover the boundary value problem (4) in its strong form.

Note that in the above discussion, we have used two separate sets of scaling constants for functions $\zeta$ and $\zeta^b$. While it is fine to set $\varepsilon=\delta$ to reduce the number of different parameters used in the model, the fact that we can take $\varepsilon$ and $\delta$ independently provides us more flexibility in practical implementations.

The convergence in (12d) requires only that the leading order of the Jacobian for the coordinate transformation $|J(r,p)|$ near the boundary approaches 1. When boundary curvature information is easily computable, it is possible to utilize such information to account for the higher order corrections in $|J(r,p)|$, which then may help to improve the accuracy of the approximation.

### 3.4. Nonlocal extensions

We may also consider a nonlocal source term for the steady-state nonlocal Neumann problem (6) instead of the local source term used in (10). This leads to

$$\tilde{f}(x) = \zeta^b(d_\Gamma(x))\,m(x)\int_\Omega K(|x-y|)\tilde{g}(y,u(y))\,dy, \quad x\in\Omega, \tag{14a}$$

where $K = K(r)$ is a kernel function similar to $\zeta = \zeta(r)$ and

$$m(x) = \left(\int_\Omega K(|x-y|)dy\right)^{-1}.$$

As explained following the nonlocal formulation (6), when the source term $\tilde{f}$ involves an integral operator for imposing an approximation to the flux $g$, a volume constraint has been applied. In particular, when $g=0$, then $\tilde{g}$ may be set to zero implying that $\tilde{f}=0$. In this case, we have a nonlocal approximation to a pure homogeneous Neumann problem.

A rescaled version can also be constructed as

$$\tilde{f}(x) = \zeta_\varepsilon^b(d_\Gamma(x))\,m_\mu(x)\int_\Omega K_\mu(|x-y|)\tilde{g}(y,u(y))\,dy, \quad x\in\Omega, \tag{14b}$$

where $K_\mu$ and $m_\mu$ are given by

$$K_\mu(r) = \frac{1}{\mu^d}K\left(\frac{r}{\mu}\right), \qquad m_\mu(x) = \left(\int_\Omega K_\mu(|x-y|)dy\right)^{-1}.$$

Given that $K_\mu$ in (14b) gives a sequence of functions approaching to the Dirac delta measure at the origin, we recover, in the limit $\mu \to 0$, the equation (10). A few additional remarks are in order. First, in (14b), there are three possible scaling factors $\delta$, $\varepsilon$ and $\mu$. In practice, one can bundle them together in suitable ways, for instance, $\delta = \varepsilon = \mu$. The kernel functions can also be related to each other to avoid complications in the numerical implementation. In such a setting, it is important to develop asymptotically compatible schemes so that the performance and convergence of numerical schemes are insensitive to the changes of the relevant parameters [9]. Secondly, the general formulation (14b) retains the minimal explicit dependence on the domain boundary $\Gamma$ so that only the distance function is needed. It is also possible to replace such a distance function with other order parameters or marker functions (including diffuse interface representations) that changes monotonically with the distance function. Finally, the nonlocal formulations given here no longer use explicit Neumann type conditions at the boundary surface. This is similar in spirit to many existing works. For example, in CFD, it has been a very popular practice to reformulate or approximate the boundary stress in terms of singular or diffused bulk body force in numerical simulations, see for example, discussions on immersed boundary methods by Peskin [19] and their variants like level set based fluid structure interaction methods [20] and phase field type diffuse interface methods [21].

### 3.5. CERW formulation of nonlocal Neumann problems

We next discuss two particular relevant works to the nonlocal formulations presented here. The model (14b) is similar to the choice of source term considered by Cortazar, Elgueta, Rossi and Wolanski in [18], or

$$\tilde{f}(x) = \int_{\mathbb{R}^d \setminus \Omega} G(x, x-y) g(y)\, dy. \tag{15}$$

There is, however, an important distinction in that all integrals in (14b) are taken to be on the domain $\Omega$ while the formulation in (15) presents the second term as an integral from $\mathbb{R}^d \setminus \Omega$. In the case where the data $g$ depends on $u$, the choice (14b) only requires knowledge of $\Omega$. Thus, this minor difference in the formulation can have dramatic impact in numerical implementation. We note that much of the analysis in [18] can be modified to work for the case where the second integral in (15) is defined on $\Omega$ rather than $\mathbb{R}^d \setminus \Omega$.

Another point to be noted is that the choices of $G$ given in [18] involve the explicit use of normal vectors of the boundary $\Gamma$ while in (14b), the boundary is used implicitly through a distance function.

### 3.6. CSR and CBF SPH schemes

The equation (11) is a conduit to understand the SPH formulation of the classical local equation (3) with an inhomogeneous data $g$. A continuum form of a discrete approximation can now be exploited to develop numerical analyses.

We may take $\delta \to 0$ first while keeping $\varepsilon$ fixed. In this case, the weak form of the limiting equation of (11) becomes

$$\left(\nabla u^\varepsilon, \nabla v\right)_\Omega = \left(\zeta_\varepsilon^b(d_\Gamma(x))\, \tilde{g}(x, u^\varepsilon), v\right)_\Omega.$$

Under suitable solution regularity assumptions, we obtain the strong form of the above equation

$$\begin{cases} -\Delta u^\varepsilon(x) = \zeta_\varepsilon^b(d_\Gamma(x)) \tilde{g}(x, u^\varepsilon(x)), & x \in \Omega \\ \dfrac{\partial u^\varepsilon(x)}{\partial n} = 0, & x \in \Gamma. \end{cases} \tag{16a}$$

This is similar to the Continuum Surface Reaction SPH (CSR-SPH) method [22–24] and Continuum Boundary Force SPH (CBF-SPH) method [25] to approximate Neumann/Robin boundary conditions for the diffusion and Navier–Stokes equations, respectively.

Note that in the CSR-SPH approach, we have that

$$\zeta^b(x) = n(x) \cdot \nabla(\phi(x)), \quad \text{and} \quad \tilde{g}(x, u^\varepsilon(x)) = g(x, u^\varepsilon(x)) \tag{16b}$$

where $\phi(x)$ is a differentiable approximation of the indicator function $\chi$ of the domain $\Omega$ such as $\chi(x) = 0$ in $\Omega$ and $\chi(x) = 1$ outside $\Omega$. In [24], the (*inward*) normal $n$ was found as

$$n(x) = \frac{\nabla\phi(x)}{|\nabla\phi(x)|}. \tag{16c}$$

When the distance function is known analytically, the normal can be computed more accurately as

$$n(x) = \nabla d_\Gamma(x).$$

The advantage of using the indicator function approximation is that it can be trivially defined for boundaries with arbitrary complex geometry. It was numerically demonstrated in [24] that the SPH discretization of (16) results in $u^{\varepsilon\xi}$ that converges to $u$ as $\varepsilon \to 0$ and $\xi \to 0$ for both linear and non-linear Robin boundary conditions. Based upon the analysis in Section 3.3, as $\varepsilon \to 0$, we get the limit of (16a) to be the same as the solution of (13b).

We note that the construction in [24] requires the extension of normal vectors and a smoothly defined diffuse interface marker, which, as discussed earlier, can also be incorporated in (16a). The use of distance function can be more convenient computationally.

### 3.7. DDM scheme

Similar to discussions above, we may consider spatially inhomogeneous nonlocal operators and relate such studies with the DDM approach developed for solving PDEs on complicated domains [26]. For Neumann problems, a special DDM (Diffuse-Domain Method) formulation can be simply written as

$$-\nabla \cdot (\phi_\varepsilon \nabla u) = |\nabla \phi_\varepsilon| \tilde{g}(x, u(x)) \quad x \in \Omega, \tag{17}$$

where $\phi_\varepsilon = \phi_\varepsilon(x)$ is an approximation of the indicator function. Such techniques are popular in many numerical studies of interface problems such as diffuse-interface/phase-field approaches that substitute the effect of stress on the sharp interface boundary by the action of body force in the diffuse interfacial layer [27].

The nonlocal approximation to $\nabla \cdot \phi_\varepsilon \nabla u$ can be given by (2) or more generally by

$$\mathcal{L}_\delta u(x) = \int_{\mathbb{R}^d} \frac{u(y) - u(x)}{|y - x|^2} \psi_\varepsilon(x, y)\, \zeta_\delta(|y - x|)\, dy \tag{18}$$

for a smooth symmetric function $\psi_\varepsilon(x, y) = \psi_\varepsilon(y, x)$ which is chosen to satisfy that as $\delta \to 0$,

$$\int_{\mathbb{R}^d} \frac{y - x}{|y - x|^2} \psi_\varepsilon(x, y)\, \zeta_\delta(|y - x|)\, dy \to \nabla \phi_\varepsilon(x), \tag{19a}$$

and

$$\int_{\mathbb{R}^d} \frac{(y_n - x_n)(y_m - x_m)}{2|y - x|^2} \psi_\varepsilon(x, y)\, \zeta_\delta(|y - x|)\, dy \to \begin{cases} \phi_\varepsilon(x), & m = n, \\ 0 & m \neq n, \end{cases} \tag{19b}$$

as $\delta \to 0$, where $x_n$ and $y_n$ denote the $n$th coordinate of $x$ and $y$ respectively.

A particular choice of $\psi_\varepsilon$ is given by

$$\psi_\varepsilon(x, y) = \phi_\varepsilon(x) + \phi_\varepsilon(y), \tag{20a}$$

so that (19) hold when $\zeta_\delta$ is given by (7).

If $\phi_\varepsilon(x)$ is taken to be a function of $d_\Gamma(x)$, which is often the case in applications [26], then so is $|\nabla \phi_\varepsilon(x)|$ and we may let

$$\zeta_\varepsilon^b(d_\Gamma(x)) = |\nabla \phi_\varepsilon(x)|. \tag{20b}$$

The above discussion, in analogous fashion for (11), renders the nonlocal formulation for DDM: for $x \in \Omega$

$$-2 \int_\Omega \frac{u^{\delta,\varepsilon}(y) - u^{\delta,\varepsilon}(x)}{|y - x|^2} \psi_\varepsilon(x, y) \zeta_\delta(|x - y|)\, dy = \zeta_\varepsilon^b(d_\Gamma(x)) \tilde{g}(x, u^{\delta,\varepsilon}(x)). \tag{20c}$$

The term on the right hand side can be similarly replaced by a more general nonlocal formulation as discussed in Section 3.4. Alternatively, the term $\nabla \phi_\varepsilon$ can also be replaced by nonlocal weighted gradient operators presented in [13].

## 4. Mass conservation

Consider a special case of the diffusion system (3)

$$\begin{cases} u_t = \Delta u, & \Omega \times (0, T) \\ \dfrac{\partial u}{\partial n} = g, & \Gamma \times (0, T) \\ u(\cdot, 0) = u_0, & \Omega. \end{cases} \tag{21}$$

If we integrate the system above over $\Omega$, invoke the divergence theorem and the solvability condition (4b), then

$$\int_\Omega u(x,t)\,dx = \int_\Omega u_0(x)\,dx,$$

follows. If the $\Delta u$ is replaced by the integral operator of (6a), then solvability (6b) implies the same conclusion for the nonlocal analogue of (21).[1] In other words, the nonlocal analogue also conserves mass.

An important question, though, is whether the various source terms $\tilde{f}$ introduced in Section 3 are robust. For instance, for the terms given by a volume constraint, do we recover the same flux over $\Omega$ when scaling parameters decrease to zero? This is tantamount to the solvability of the steady state problem (6). A possible modification to (16a) is

$$\begin{cases} -\Delta u^\varepsilon(x) = \zeta_\varepsilon^b(d_\Gamma(x))\tilde{g}_1(x, u^\varepsilon(x)), & x \in \Omega, \\ \dfrac{\partial u^\varepsilon}{\partial n} = 0, & x \in \Gamma, \end{cases} \tag{22a}$$

where $\tilde{g}_1(x,u) = \tilde{g}(x,u) - c$ with the constant $c$ defined by

$$\begin{aligned} c &= \left(\int_\Omega \zeta_\varepsilon^b(d_\Gamma(x))dx\right)^{-1} \left(\int_\Omega \zeta_\varepsilon^b(d_\Gamma(x))\tilde{g}_1(x,u^\varepsilon)\,dx - \int_\Gamma g\,d\Gamma\right) \\ &= \left(\int_\Omega \zeta_\varepsilon^b(d_\Gamma(x))dx\right)^{-1} \int_\Omega \zeta_\varepsilon^b(d_\Gamma(x))\tilde{g}_1(x,u^\varepsilon)\,dx. \end{aligned} \tag{22b}$$

With such a modification, the problem (22a) is solvable, and moreover the constant $c \to 0$ as $\varepsilon \to 0$.

Similar modifications can be applied to more general forms of (22a) involving the nonlocal diffusion. For example, the modification to assume the total mass conservation for (14b) can be defined as:

$$\begin{aligned} &2\int_\Omega \frac{u(y)-u(x)}{|y-x|^2}\zeta_\delta(|x-y|)\,dz - \zeta_\varepsilon^b(d_\Gamma(x))\,c \\ &\quad = \zeta_\varepsilon^b(d_\Gamma(x))m_\mu(x)\int_\Omega K_\mu(|x-y|)\tilde{g}(y,u(y))\,dy, \qquad x \in \Omega \end{aligned}$$

where the constant $c$ is defined by

$$c := \left(\int_\Omega \zeta_\varepsilon^b(d_\Gamma(x))dx\right)^{-1} \int_\Omega\int_\Omega \zeta_\varepsilon^b(d_\Gamma(x))m_\mu(x)K_\mu(|x-y|)\tilde{g}(y,u(y))\,dy\,dx.$$

## 5. Examples

This section considers three examples. The first two and third examples are analytical and numerical, respectively. The purpose of the examples is to illustrate the nonlocal approximation of a classical diffusion problem with Neumann boundary conditions. In particular, we are interested in accessing the kernel functions and the possible order of approximations. The first example is for a simple one-dimensional two-point boundary value problem where analytical constructions can be explicitly given. The second problem describes a Robin type boundary condition for the diffusion problem in a two dimensional disc.

[1] In the nonlocal case, the derivation leading to (6b) is an instance of a nonlocal divergence theorem; see [4] for details.

**Example 1.** Consider the one dimensional problem (4) on the unit interval with boundary conditions $u'(0) = g_0$, $u'(1) = g_1$, and the kernels $\zeta(r) = \frac{3}{2}r^2$, $\zeta^b(r) = 2$, and

$$\tilde{g}(x, u) = \begin{cases} -g_0, & x \in (0, 1/2) \\ g_1, & x \in [1/2, 1). \end{cases}$$

The negative sign on $g_0$ is expedient because the normal at $x = 0$ points in the direction of the negative $x$-axis.

Both formulations (11) and (14b) render the same steady-state problem since $\tilde{g}(y, u(y))$ is taken to be constant $-g_0$ and $g_1$, near $y = 0$ and $y = 1$. Taking the limit $\delta \to 0$ leads to the one-dimensional case of (16a) or

$$-\frac{du^\varepsilon(x)}{dx} = -\frac{2}{\varepsilon} g_0 \chi_{(0,\varepsilon/2)}(x) + \frac{2}{\varepsilon} g_1 \chi_{(1-\varepsilon/2,1)}(x) \quad x \in (0, 1).$$

To demonstrate the order of accuracy, we consider a special case of the corresponding steady state equations given by (4a) and (22a) or

$$-\frac{d^2u(x)}{dx^2} = 2 \quad \text{in } (0, 1), \qquad \frac{du(0)}{dx} = 1, \qquad \frac{du(1)}{dx} = -1,$$

and

$$-\frac{d^2u^\varepsilon(x)}{dx^2} = 2 - \frac{g_0}{\varepsilon}\chi_{(0,\varepsilon)}(x) - \frac{g_1}{\varepsilon}\chi_{(1-\varepsilon,1)}(x) \quad \text{in } (0, 1), \qquad \frac{du^\varepsilon(0)}{dx} = 0, \qquad \frac{du^\varepsilon(1)}{dx} = 0.$$

We pick the solutions of $u$ and $u^\varepsilon$ to match at $x = 1/2$. The analytic forms give us $u(x) = x - x^2$ for $x \in (0, 1)$ and $u^\varepsilon(x) = u(x)$ for $x \in (\varepsilon, 1 - \varepsilon)$ but

$$u^\varepsilon(x) = \frac{\varepsilon}{2} + \frac{x^2}{2\varepsilon} - x^2, \quad x \in (0, \varepsilon); \qquad u^\varepsilon(x) = u^\varepsilon(1 - x), \quad x \in (1 - \varepsilon, 1).$$

Thus, we have

$$\|u - u^\varepsilon\|_{L^\infty} = u^\varepsilon(0) - u(0) = u^\varepsilon(1) - u(1) = \frac{\varepsilon}{2}, \quad \text{and} \quad \|u - u^\varepsilon\|_{L^1} = \frac{\varepsilon^3}{3}.$$

That is, although the point-wise error order is only of first-order, the $L^1$ error is of cubic order. We do not expect convergence point-wise for the derivative but the asymptotic estimate

$$\left\| \frac{du}{dx} - \frac{du^\varepsilon}{dx} \right\|_{L^1} = \varepsilon,$$

does hold. For comparison, we consider the CSR-SPH approach, i.e., the choices of $\zeta^b$ and $\tilde{g}$ given by (16b), so that the above steady-state equation takes the form,

$$-\frac{d^2u^\varepsilon(x)}{dx^2} = 2 - 2g_0 W(x - 0) + 2g_1 W(x - 1), \quad \text{in } (0, 1), \qquad \frac{du^\varepsilon(0)}{dx} = 0, \qquad \frac{du^\varepsilon(1)}{dx} = 0.$$

To simplify analytical treatment we assume the Gaussian form of $W$, $W^\varepsilon(x) = \frac{1}{\sqrt{2\pi\varepsilon}} \exp\left(-\frac{x^2}{2\varepsilon^2}\right)$. We also assume that $W^\varepsilon(x > 3\varepsilon) = 0$. Then, as before, the analytic solution is $u^\varepsilon(x) = u(x)$ for $x \in (3\varepsilon, 1 - 3\varepsilon)$.

For $x < 3\varepsilon$

$$-\frac{du^\varepsilon(x)}{dx} = 2x - 2\sqrt{\varepsilon}\,\mathrm{Erf}\left(\frac{x}{2\varepsilon}\right) \approx 2x - \frac{x}{\sqrt{\pi\varepsilon}}$$

and

$$u^\varepsilon(x) \approx -x^2 + \frac{x^2}{2\sqrt{\pi\varepsilon}} + 3\varepsilon - \frac{9}{2\sqrt{\pi}}\varepsilon^{\frac{3}{2}},$$

so that $\|u - u^\varepsilon\|_{L^\infty} = O(\varepsilon)$ results.

In order to achieve higher order accuracy, let us consider (20c). We take $\delta \to 0$ as in the above for simple illustration that corresponds to (17). Let $\phi_\varepsilon(x) = \min\{x/\varepsilon, (1-x)/\varepsilon, 1\}$. We solve

$$-\frac{d}{dx}\left(\phi_\varepsilon(x)\frac{du^\varepsilon(x)}{dx}\right) = 2 - \left|\frac{d\phi_\varepsilon(x)}{dx}\right|,$$

without the need to impose any boundary condition (due to the degeneracy of the coefficients at the boundary). Over the interval $(0, \varepsilon)$, the preceding equation simplifies to

$$-x\frac{du^\varepsilon(x)}{dx} = (2\varepsilon - 1)x.$$

A particular solution is given by $u^\varepsilon(x) = (1-2\varepsilon)x + \varepsilon^2$ in $(0, \varepsilon)$, $u^\varepsilon(x) = x - x^2$ in $(\varepsilon, 1/2)$, and symmetric with respect to $1/2$. The approximation matches with the solution $u(x)$ exactly away from the $\varepsilon$ boundary layer. Moreover, the asymptotic estimates

$$\|u - u^\varepsilon\|_{L^\infty} = O(\varepsilon^2) \quad \text{and} \quad \left\|\frac{du}{dx} - \frac{du^\varepsilon}{dx}\right\|_{L^\infty} = O(\varepsilon),$$

are satisfied leading to a higher order point wise convergence rate than the previously discussed formulations.

**Example 2.** Consider the steady-state problem (4) on the unit disc with the choice of flux $g = -u$, and kernels $\zeta(r) = \frac{6}{\pi}r(1-r)$ and $\zeta^b(r)$ for $r \in (0, 1)$. This leads to the steady-state problem

$$\frac{12}{\pi\delta^3}\int_{\Omega\cap B(x,\delta)} \frac{u^{\delta,\varepsilon}(y) - u^{\delta,\varepsilon}(x)}{|y-x|}\left(1 - \frac{|x-y|}{\delta}\right)dy = \frac{2}{\varepsilon^2}u^{\delta,\varepsilon}(x)\max\{\varepsilon - 1 + |x|, 0\} \quad x \in \Omega.$$

This avoids the discontinuous $\zeta^b$ used in the earlier example, and is also an example where the geometry of the boundary is simple so that the Jacobian $|J(r, p)|$ of the coordinate transformation is $1 - r = |x|$ for $0 < |x| < 1$.

**Example 3.** We now consider the numerical solution of

$$\begin{cases} u_t = \dfrac{\partial u^2}{\partial x^2} + r, & \text{in } (0,1) \times (0,T) \\ \dfrac{\partial u}{\partial x} = g, & \text{on } (x=0) \times (0,T) \\ \dfrac{\partial u}{\partial x} = -g, & \text{on } (x=1) \times (0,T) \\ u = \tilde{u}(0.5), & \text{on } (0,1) \times (t=0). \end{cases} \tag{23}$$

with $r = 2g = 0.8$ and $\tilde{u}(x) = gx - \frac{r}{2}x^2$ satisfying the steady-state formulation. We first compute the solution using the SPH discretization (8a) on a uniform mesh of points over $(-\varepsilon, 1+\varepsilon)$ with the relations (7) and the fourth-order weighting function

$$W^\varepsilon(r) = \frac{81}{359\pi\varepsilon}\begin{cases} \left(3 - \dfrac{3r}{\varepsilon}\right)^5 - 6\left(2 - \dfrac{3r}{\varepsilon}\right)^5 + 15\left(1 - \dfrac{3r}{\varepsilon}\right)^5, & 0 \le r < \dfrac{1}{3}\varepsilon \\ \left(3 - \dfrac{3r}{\varepsilon}\right)^5 - 6\left(2 - \dfrac{3r}{\varepsilon}\right)^5, & \dfrac{1}{3}\varepsilon \le r < \dfrac{2}{3}\varepsilon \\ \left(3 - \dfrac{3r}{\varepsilon}\right)^5, & \dfrac{2}{3}h \le r < \varepsilon \\ 0, & r > \varepsilon \end{cases}$$

given in [1]. The discrete source term in the SPH discretizations (8a) is given by $2gW^\varepsilon(1-x_i) + 2gW^\varepsilon(x_i)$.

We also compute the solution for the nonlocal analogue using a finite volume discretization of the DDM scheme (20) by setting $\phi_\varepsilon(x) = \min\{x/\varepsilon, (1-x)/\varepsilon, 1\}$, $\psi_\varepsilon(x, y) = \phi_\varepsilon(x) + \phi_\varepsilon(y)$, and $\zeta_\delta(r) = -rW_r^\varepsilon(r)$ with $\delta = \varepsilon$.

Fig. 1 shows the $L_1$ errors between the analytical ($\tilde{u}$), DDM method (non-local) and SPH steady state solutions as a function of $\varepsilon/L$ for $\alpha = \Delta x/\varepsilon = 0.25$ and 0.125, where $L = 1$ is the size of the domain. Our results show that the dependence of $L_1$ on $\varepsilon$ is not affected by $\Delta x$ as long as $\alpha \le 0.125$. Moreover, the experiments also show that the

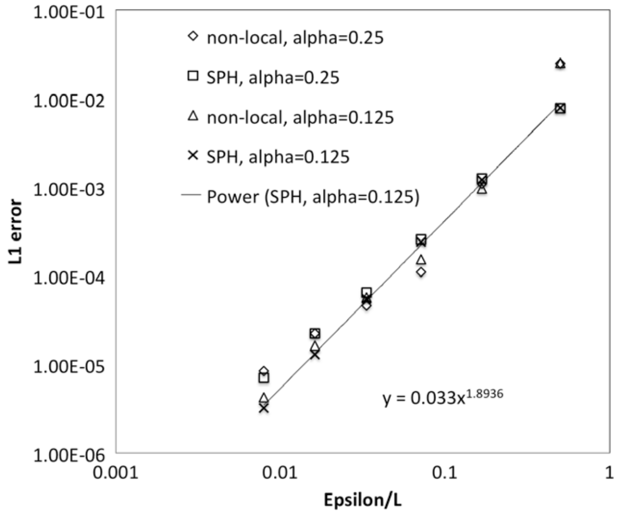


Fig. 1. $L_1$ error between analytical and non-local and SPH steady state solutions versus $\varepsilon/L$ for $\alpha = \Delta x/\varepsilon = 0.25$ and $0.125$, where $L = 1$ is the size of the domain. The solid line is the best power law fit to the $L_1$ difference between SPH and analytical solutions with $\alpha = 0.125$.

$L_1$ errors are approximately on the order of $O(\varepsilon^2)$. There are obviously a number of contributing factors that lead to such an order of convergence, for example, type of discretization, the choices of scaling parameters $\delta$ and $\varepsilon$, and the particle spacing $\Delta x$.

## 6. Conclusion

Smoothed Particle Hydrodynamics is a numerical method for discretizing PDES and its approximation to the classical diffusion problem provides a convenient setting in which to understand the SPH method. There have been many studies of SPH over the years, yet a systematic and rigorous mathematical framework is still lacking. We demonstrate in this work that a suitable "volume-constrained" problem with the integral operator may serve as a conduit between the boundary value problem involving the inhomogeneous diffusion operator and its SPH approximations. This leads to a new mathematical framework based on the recently developed theory for volume-constrained nonlocal diffusion problems and their numerical approximations. The new approach allows us to both distinguish and relate two key limiting processes, namely, the use of an integral operator with a kernel function with a diminishing support to approximate the differential operator and the use of a numerical quadrature with a diminishing mesh size to approximate the integral operator. The new approach also enables the construction of a better-behaved SPH discretization scheme given that the volume constrained continuum problem is well-posed. The modified SPH discretization can therefore be shown to converge to the solution of the volume constrained problem as the number of particles increase. Then by letting the support of the nonlocal kernel decrease to zero, the solution of the volume-constrained problem approximates that of a boundary value problem. It is this two-step process of discretizing the integral operator and letting both the number of points increase and the support of nonlocal kernel decrease that proves critical in understanding carefully the underlying approximations.

We note that in the discrete setting, the roles played by the scaling parameters (measuring nonlocality) and the particle spacing (determining quadrature accuracy) can become important to the convergence and accuracy. In practice, and in particular for SPH, it has also been the case that these parameters are taken to be proportional to each other, leading to a complex issue of analyzing the numerical convergence. Some related discussions have been made in [12]. By establishing the connections, this work points out the possibility that we can borrow similar ideas to gain a better understanding on similar numerical analysis issues that are important to SPH.

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