ANALYSIS AND APPROXIMATION OF NONLOCAL DIFFUSION PROBLEMS WITH VOLUME CONSTRAINTS

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Abstract. We exploit a recently developed nonlocal vector calculus to provide a variational analysis for a general class of nonlocal diffusion problems given by a linear integral equation on bounded domains in $\mathbb{R}^d$. The ubiquity of the nonlocal operator is illustrated by a number of applications ranging from continuum mechanics to graph theory. These applications elucidate different interpretations of the operator and the governing equation. A probabilistic perspective explains that the nonlocal operator corresponds to the infinitesimal generator for a symmetric jump process. Sufficient conditions on the kernel of the operator and the notion of volume constraints lead to a well-posed problem. The volume constraints are a proxy for boundary conditions that may not be defined for the given kernel. In particular, we demonstrate for a general class of kernels that the nonlocal operator is a mapping between a constrained subspace of a fractional Sobolev subspace and its dual. We also demonstrate for some other kernels the operator's inverse does not smooth but does correspond to diffusion. The impact of our analyses is that both a continuum analysis and a numerical method for the modeling of anomalous diffusion on bounded domains in $\mathbb{R}^d$ are provided. The analytical framework also allows us to consider finite dimensional approximations using both discontinuous or continuous Galerkin methods that are conforming for the nonlocal diffusion equation; error and condition number estimates are derived. The nonlocal vector calculus enables striking analogies to be drawn with the problem of classical diffusion including a notion of nonlocal flux.

Key words. nonlocal diffusion, nonlocal operator, fractional Laplacian, fractional operator, fractional Sobolev spaces, vector calculus, anomalous diffusion, finite element methods, nonlocal heat conduction, peridynamics

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1. Introduction. Let $\Omega \in \mathbb{R}^d$ denote a bounded, open subset, let $u, b\colon \Omega \to \mathbb{R}$, and let $\mathcal{L}$ denote the linear integral operator

$$\mathcal{L}u(\mathbf{x}) := 2\int_{\Omega} \big(u(\mathbf{y}) - u(\mathbf{x})\big)\, \gamma(\mathbf{x},\mathbf{y})\, d\mathbf{y}, \qquad \mathbf{x} \in \widetilde{\Omega} \subseteq \Omega \subseteq \mathbb{R}^d, \tag{1.1}$$

where the volume of $\widetilde{\Omega}$ is non-zero and the kernel $\gamma(\mathbf{x},\mathbf{y})\colon \Omega\times\Omega \to \mathbb{R}$ denotes a non-negative symmetric mapping, e.g., $\gamma(\mathbf{x},\mathbf{y}) = \gamma(\mathbf{y},\mathbf{x})$. Consider the *nonlocal volume-constrained problem*

$$\begin{cases} -\mathcal{L}u = b & \text{on } \widetilde{\Omega} \subseteq \Omega \\ \ \ \mathcal{V}u = 0 & \text{on } \Omega \setminus \widetilde{\Omega}, \end{cases} \tag{1.2}$$

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where $\mathcal{V}$ denotes a linear operator of constraints acting on the volume $\Omega \setminus \widetilde{\Omega}$. The operator $\mathcal{L}$ defined in (1.1) is nonlocal because the value of $\mathcal{L}u$ at a point $\mathbf{x}$ requires information about u at points $\mathbf{y} \neq \mathbf{x}$; this should be contrasted to *local* operators, e.g., the value of $\nabla \cdot \nabla u$ at a point $\mathbf{x}$ requires information about u only at $\mathbf{x}$. The problem (1.2) is the spatial contribution for *nonlocal* diffusion and *nonlocal* wave equations; see Sections 6.1 and 3.2, respectively. Volume constraints arise naturally when considering specific examples of diffusion; e.g., when $\widetilde{\Omega} = \Omega$ the diffusion is restricted to only occur in Ω whereas when $\mathcal{V}u = u$ on some finite volume $\Omega \setminus \widetilde{\Omega}$, diffusion vanishes outside of $\widetilde{\Omega}$. The latter two cases are nonlocal analogues for pure Neumann and homogenous Dirichlet boundary conditions, respectively.

If $\gamma(\mathbf{x}, \mathbf{y}) = \frac{\partial^2}{\partial \mathbf{y}^2} \delta(\mathbf{x} - \mathbf{y})$, where δ denotes the Dirac delta measure, then $\mathcal{L} \equiv \Delta$ in the sense of distributions. Selecting other kernels and under an appropriate rescaling, the operator $\mathcal{L}$ approximates the classical Laplacian operator [4, 46] or, more generally, the operator $\nabla \cdot \mathbf{D} \nabla$, where $\mathbf{D}$ denotes a second-order tensor [32]. In Section 2, using a recently developed nonlocal vector calculus [25, 32], the operator $\mathcal{L}$ is recast as the composition of a nonlocal divergence and gradient operators. In Sections 5.1 and 5.2, the fractional Laplacian and a fractional derivative operator, respectively, are derived as instances of $\mathcal{L}$.

The operator $\mathcal{L}$ and its generalizations arise in many applications such as image analyses [19, 30, 31, 36], machine learning [42], nonlocal Dirichlet forms [5, § 3.6], kinetic equations, e.g., [12] and more recently [35], the modeling of phase transitions [15] and the survey [29] containing an excellent annotated reference section, the peridynamic model for mechanics [43], its one-dimensional variants [44, 45] for which $\mathcal{L}$ arises directly, and nonlocal heat conduction [16]. We discuss some of the above applications and related mathematical work in Section 3, leaving the topic of anomalous diffusion for Sections 5 and 6.

Section 7 contains the primary contribution of our paper; there, the well posedeness of volume-constrained problems is demonstrated by exploiting the nonlocal vector calculus reviewed in Section 2. The notion of volume-constrained problems enables us to formulate and solve diffusion problems in situations where boundary conditions do not exist, e.g., diffusive regimes where the Fourier symbol of the self-adjoint fractional operator is of positive order less than a half. Diffusion problems on these spaces, e.g., the volume-constrained problem (1.2), allow discontinuous functions as solutions, given appropriate conditions on the kernel γ. The well posedeness of the fractional Laplacian and a fractional derivative operators on bounded domains in $\mathbb{R}^d$ also follows readily. Section 8 briefly discusses other volume-constrained problems not already considered, well-posedeness for nonlocal evolution problems, and vanishing nonlocality. The latter aspect demonstrates that in the limit when the support of γ decreases, the classical, local, diffusive operator is recovered.

Our nonlocal vector calculus makes transparent the analogies we draw between the steady-state version of the nonlocal problem (1.2) and the second-order scalar elliptic boundary-value problem

$$\begin{cases} -\nabla \cdot \mathbf{D} \nabla u = b & \text{on } \Omega \\ \mathcal{B}u = 0 & \text{on } \partial\Omega, \end{cases} \tag{1.3}$$

where $\mathbf{D} : \mathbb{R} \to \mathbb{R}^{d \times d}$ is a tensor and $\mathcal{B}$ denotes a linear operator acting on the boundary $\partial\Omega$ of the volume Ω. Section 4 reviews classical diffusion and energy principles whereas Section 6 considers the nonlocal case. In particular, crucial to the study of nonlocal diffusion is the identification of the nonlocal flux provided in the latter section. Our analogies replace the boundary-constraint operator $\mathcal{B}$ with the volume-constraint operator $\mathcal{V}$.

Another contribution of our paper is the analyses of the convergence and error and condition number estimates of finite-dimensional discretizations of nonlocal volume-constrained problems; these analyses are given in Section 9 where the focus is on finite element methods. The finite element methods considered are conforming and, for appropriate kernels γ, allow for the use of piecewise polynomials of nonnegative degree that are not required to be continuous across element faces; discontinuous Galerkin methods (DGMs) are an example of such methods. This is in stark contrast to DGMs for the discretization of, e.g., (1.3) for which they are nonconforming; see, e.g., [6].

At first glance, the differences between the volume-constrained and boundary-value problems (1.2) and (1.3), respectively, are obvious. First, the former involves an integral operator whereas the latter involves a differential operator. Second, in (1.2), constraints are imposed on the solution over a nonzero *volume* $\Omega \setminus \widetilde{\Omega}$ that is not necessarily located near or at the boundary of $\widetilde{\Omega}$; on the other hand, in (1.3), constraints are imposed precisely at the bounding *surface* $\partial\Omega$. These distinctions are essential in characterizing the differences in the properties of two problems (1.2) and (1.3) and of their solutions.

Discussion of the need for imposing volume constraints for problems involving the nonlocal operator $\mathcal{L}$ requires us to discuss in more detail and with greater precision the differences between problems involving that operator and those involving second-order elliptic operators. First, we recall that if $u = 0$ on $\partial\Omega$ and if appropriate conditions on $\mathbf{D}$ are assumed, then, given data $b \in H^{-1}(\Omega)$, a weak formulation of the boundary-value problem (1.3) is well posed in $H_0^1(\Omega)$, i.e., we have that the solution $u \in H_0^1(\Omega)$. Alternately, we have that $\nabla \cdot \mathbf{D}\nabla$ is a bounded operator from $H_0^1(\Omega) \to H^{-1}(\Omega)$ having a bounded inverse.

In contrast, if $\mathcal{V}u = u$, e.g., $u = 0$ on $\Omega \setminus \widetilde{\Omega}$, then, for appropriate choices for the kernel γ, we demonstrate in this paper that a variational formulation of the volume-constrained problem (1.2) is well posed in the space $H_c^s(\Omega)$ with $0 < s < 1$, provided the given data b belongs to the dual space of $H_c^s(\Omega)$, where $H_c^s(\Omega)$ is the subspace of the fractional Sobolev space $H^s(\Omega)$ constrained to satisfy the volume constraint. We even demonstrate, for a particular choice of kernel, that the variational formulation is well posed in $L_c^2(\Omega)$, provided the given data b belongs to $L_c^2(\Omega)$ as well. Alternately, we have that $\mathcal{L}$ is a bounded operator from $H_c^s(\Omega)$ to its dual space or from $L_c^2(\Omega) \to L_c^2(\Omega)$, as the kernel warrants. In particular, the solution operator for (1.2) regularizes, i.e., smooths, the data b to a lesser extent compared to the solution operator for (1.3) and, under appropriate conditions on γ, the solution is no smoother than the data. The latter occurs, for example, when $\mathcal{L}$ is a Hilbert-Schmidt operator.

The fact that weak formulations of the volume-constrained problem (1.2) are well posed in subspaces of $H^s(\Omega)$ for $s \in [0, 1/2]$ deserves further comment. First, why is treating such a case important? The answer is that it is precisely these spaces that contain functions with jump discontinuities. Thus, if one wants to admit solutions that have jump discontinuities, one has to work with spaces such as $H^s(\Omega)$ for $s \in [0, 1/2]$. We next ask: could we instead impose a surface constraint, e.g., could we consider the problem

$$\begin{cases} -\mathcal{L}u = b & \text{on } \Omega \\ \quad u = 0 & \text{on } \partial\Omega. \end{cases}$$

We have that, for appropriate kernels, $\mathcal{L}u$ is well defined for $u \in H^s(\Omega)$ for $s \in [0,1)$. However, the restriction of a function $u \in H^s(\Omega)$ onto $\partial\Omega$ is not defined for $s \in [0,1/2]$, i.e., the trace of such u is not defined. This means that if $s \in [0,1/2]$, we cannot impose constraints on u restricted to $\partial\Omega$. However, a volume constraint where the operator $\mathcal{V}$ is the restriction operator on $\Omega \setminus \widetilde{\Omega}$ is well-defined for all $s \in [0,1)$ and beyond. Thus, we conclude that *for nonlocal operator equations posed on bounded domains, the application of volume constraints is necessitated for operators that are bounded acting on $H^s(\Omega)$ functions with $s \in [0,1/2]$*. For instance, the well-posedness of (1.3) when $\nabla \cdot \mathbf{D}\nabla$ is replaced by Δ^{2s} (the fractional Laplacian) is not discussed when $0 < s < 1/2$. More generally, well-posedness and a tractable numerical method for pseudo-differential, or fractional, self-adjoint differential operator on bounded domains when the degree of the (Fourier) symbol lies in $0 < s < 1/2$ are not available. In contrast, the notion of a volume-constrained, nonlocal, problem (1.2) allows $s \in [0,1)$. For example, this immediately removes the limitation encountered in [7, 28] to only consider a fractional dispersion equation and kernels γ, respectively, where the solutions are in $H^s_0(\Omega)$ for $1/2 < s < 1$, and to present a numerical method for the solution of the fractional Laplacian on bounded domains in lieu of the random walk approximation used in [47].

An inspiration for this paper is to extend results of [27, 46] and [4, Chapters 1-3] to the volume-constrained problem (1.2) on bounded domains. The well-posedness results derived in this paper extend the result established in [32] on a bounded domain for a class of kernels γ and volume constraint operators that lead to an operator $\mathcal{L}$ whose inversion does not regularize the data. This latter result was extended in [2] to another class of volume constraints. Chapter 1 of [4] considers the well posedness of the Cauchy problem for the nonlocal diffusion equation (1.1) whereas Chapters 2 and 3 consider a special choice of volume constraints for the case of $J \equiv \gamma$ a nonnegative radial function that satisfies $J(0) > 0$ and $\int_{\mathbb{R}^d} J = 1$. Such conditions on γ imply that $\mathcal{L}$ is a mapping from $L^2(\Omega)$ to $L^2(\Omega)$; conditions such that $\mathcal{L}$ smooths the data are not considered.

2. Nonlocal vector calculus.

In [25], a nonlocal vector calculus was developed; here, we briefly review those aspects of that calculus that will be useful in the sequel. The nonlocal vector calculus, a generalization of the conventional vector calculus to nonlocal operators, enables us to recast nonlocal diffusion problems in a manner analogous to classical diffusion. The clarity achieved benefits both the mathematical analyses and physical interpretations, as the remainder of our paper demonstrates.

Suppose we are given an open subset $\Omega \subset \mathbb{R}^d$ and the vector mappings

$$\mathbf{f}(\mathbf{x},\mathbf{y}),\ \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\colon \Omega\times\Omega \to \mathbb{R}^d,$$

where the components of $\boldsymbol{\alpha}$ are anti-symmetric. Then, for any $\widehat{\Omega} \subseteq \Omega$, define the *nonlocal divergence operator* $\mathcal{D}$ acting on $\mathbf{f}(\mathbf{x},\mathbf{y})$ as

$$\mathcal{D}(\mathbf{f})(\mathbf{x}) := \int_\Omega \big(\mathbf{f}(\mathbf{x},\mathbf{y}) + \mathbf{f}(\mathbf{y},\mathbf{x})\big)\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \quad \text{for } \mathbf{x} \in \widehat{\Omega} \subseteq \Omega \tag{2.1a}$$

and the operator $\mathcal{N}$ acting on $\mathbf{f}(\mathbf{x},\mathbf{y})$ as well as

$$\mathcal{N}(\mathbf{f})(\mathbf{x}) := -\int_\Omega \big(\mathbf{f}(\mathbf{x},\mathbf{y}) + \mathbf{f}(\mathbf{y},\mathbf{x})\big)\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega \setminus \widehat{\Omega}. \tag{2.1b}$$

We shall see later that the operator $\mathcal{N}$ is a nonlocal analog of the normal derivative operator at the boundary encountered in the classical differential vector calculus; just as the normal derivative operator is related to the diffusive flux at a boundary, we shall also see that $\mathcal{N}\mathbf{f}$ is related to a *nonlocal diffusive flux* from $\widehat{\Omega}$ to its complement $\Omega\setminus\widehat{\Omega}$. Note that $\mathcal{D}$ and $\mathcal{N}$ have similar definitions, with the only differences being the sign and the regions over which $\mathcal{D}\mathbf{f}$ and $\mathcal{N}\mathbf{f}$ are defined. Note also that the mapping $\mathbf{f}\mapsto\mathcal{D}(\mathbf{f})$ is scalar-valued in analogous fashion to the local differential divergence of a vector function.

With $\mathcal{D}$ and $\mathcal{N}$ defined as in (2.1a) and (2.1b), respectively, we have the *nonlocal Gauss' theorem*

$$\int_{\widehat{\Omega}}\mathcal{D}(\mathbf{f})\,d\mathbf{x}=\int_{\Omega\setminus\widehat{\Omega}}\mathcal{N}(\mathbf{f})\,d\mathbf{x}\quad\forall\,\widehat{\Omega}\subseteq\Omega. \tag{2.2}$$

Corresponding to $\mathcal{D}$, we have the adjoint operator $\mathcal{D}^*$ acting on a scalar function $u(\mathbf{x})$ given by

$$\mathcal{D}^*(u)(\mathbf{x},\mathbf{y})=-\big(u(\mathbf{y})-u(\mathbf{x})\big)\,\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\quad\text{for }\mathbf{y},\mathbf{x}\in\Omega. \tag{2.3}$$

Note that the mapping $u\mapsto\mathcal{D}^*(u)$ is vector-valued in analogous fashion to the local differential gradient of a scalar function $u(\mathbf{x})$. With $\mathcal{D}^*$ being the adjoint of the nonlocal divergence, we view $\mathcal{D}^*$ as (the negative of) a *nonlocal gradient*.

Let $u(\mathbf{x})$ and $v(\mathbf{x})$ denote scalar functions and let $\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})$ denote a symmetric, positive definite (in the matrix sense) "constitutive" second-order tensor $\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\colon\Omega\times\Omega\to\mathbb{R}^{d\times d}$ having elements that are symmetric in $\mathbf{x}$ and $\mathbf{y}$, i.e., $\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})=\boldsymbol{\Theta}(\mathbf{y},\mathbf{x})$. Then, it is a simple matter to show that the nonlocal divergence theorem (2.2) implies the *nonlocal Green's first identity*

$$-\int_{\widehat{\Omega}}v\mathcal{D}(\boldsymbol{\Theta}\mathcal{D}^*u)\,d\mathbf{x}+\int_{\Omega}\int_{\Omega}(\mathcal{D}^*v)\cdot(\boldsymbol{\Theta}\mathcal{D}^*u)\,d\mathbf{y}d\mathbf{x}=-\int_{\Omega\setminus\widehat{\Omega}}v\mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^*u)\,d\mathbf{x}. \tag{2.4}$$

From (2.1a) and (2.3), one easily deduces that

$$\mathcal{D}\big(\boldsymbol{\Theta}\,\mathcal{D}^*u\big)=-2\int_{\widehat{\Omega}}\big(u(\mathbf{y})-u(\mathbf{x})\big)\boldsymbol{\alpha}\cdot\boldsymbol{\Theta}\boldsymbol{\alpha}\,d\mathbf{x}$$

so that, comparing with (1.1), we have that

$$-\mathcal{L}u=\mathcal{D}\big(\boldsymbol{\Theta}\,\mathcal{D}^*u\big)\qquad\text{with}\qquad\gamma=\boldsymbol{\alpha}\cdot\boldsymbol{\Theta}\boldsymbol{\alpha}.$$

Thus we see that the operator $-\mathcal{L}$ is non-negative self-adjoint because $\mathcal{D}$ and $\mathcal{D}^*$ are adjoint operators; see [30, Proposition 2.1] and also [12, 25, 32]. Thus, using the nonlocal calculus introduced in [25], we have shown that the operator $\mathcal{L}$ is a composition of nonlocal divergence and gradient operators.

To partially justify calling $\mathcal{D}$ and $-\mathcal{D}^*$ the nonlocal divergence and nonlocal gradient, respectively, and $\mathcal{N}\mathbf{f}$ a nonlocal flux, consider the special case of $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})=-\frac{\partial}{\partial\mathbf{y}}\delta(\mathbf{y}-\mathbf{x})$, where δ denotes the Dirac delta measure. Then, a formal application of Propositions 4 and 5 in [25] yields that

$$\mathcal{D}(\mathbf{f})=\nabla\cdot\mathbf{f}(\mathbf{x},\mathbf{x})\qquad\text{and}\qquad-\int_{\Omega}\mathcal{D}^*(u)d\mathbf{y}=\nabla u(\mathbf{x}).$$

Moreover, comparing the classical Gauss' theorem for $\mathbf{f}(\mathbf{x},\mathbf{x})$ with the nonlocal Gauss' theorem (2.2) yields, in this special case, that

$$\int_{\Omega\setminus\widehat{\Omega}} \mathcal{N}(\mathbf{f})\,d\mathbf{x} = \int_{\partial\widehat{\Omega}} \mathbf{f}(\mathbf{x},\mathbf{x})\cdot\mathbf{n}\,dA.$$

For details concerning the nonlocal calculus, see [25], where one also finds further results for the nonlocal divergence operator $\mathcal{D}$, including a nonlocal Green's second identity as well as analogous results for nonlocal gradient and curl operators.

3. Applications of the nonlocal operator $\mathcal{L}$. We briefly describe four applications in which the operator $\mathcal{L}$ defined in (1.1) or a generalization to vector fields arise. The application to nonlocal diffusion is discussed in subsection 6.1.

3.1. Peridynamic model for solid mechanics. Silling [43] derived the linearized peridynamic balance of linear momentum

$$\mathbf{u}_{tt}(\mathbf{x},t) = \mathbf{\Lambda}\mathbf{u}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t) \qquad \mathbf{x}\in\mathbb{R}^d, t>0, \tag{3.1a}$$

where $\mathbf{u}:\Omega\times(0,T]\to\mathbb{R}^d$ and

$$\mathbf{\Lambda}\mathbf{u}(\mathbf{x},t) := \int_{\mathbb{R}^d} \frac{\big(\mathbf{y}-\mathbf{x}\big)\otimes\big(\mathbf{y}-\mathbf{x}\big)}{\sigma(|\mathbf{y}-\mathbf{x}|)}\big(\mathbf{u}(\mathbf{y},t)-\mathbf{u}(\mathbf{x},t)\big)\,d\mathbf{y}. \tag{3.1b}$$

The operators $\mathcal{L}$ and $\mathbf{\Lambda}$ coincide when $d=1$ and $\gamma(x,y)=(y-x)^2/2\sigma(|y-x|)$. In [46], results are provided about the well-posedness of both the balance law (3.1a) and the associated equilibrium equation $\mathbf{\Lambda}\mathbf{u}+\mathbf{b}=\mathbf{0}$. In [27], analyses are provided for model one- and two-dimensional volume-constrained problems on bounded domains that are evocative of boundary-value problems with Dirichlet and Neumann boundary conditions. The theory developed in [27, 46] relies upon the analytic properties of σ, showing how the data γ determines the regularity (or lack thereof) of the solution of the volume-constrained problems involving the operator $\mathcal{L}$.

3.2. Nonlocal wave equation. The operator $\mathcal{L}$ also arises in the nonlocal wave equation:

$$\begin{cases} u_{tt} + \mathcal{D}\big(\mathbf{\Theta}\,\mathcal{D}^* u\big) = 0\,, & \forall\,\mathbf{x}\in\widetilde{\Omega}\subseteq\Omega\,,\ t>0 \\ \mathcal{V}u = 0, & \forall\,\mathbf{x}\in\Omega\setminus\widetilde{\Omega}\,,\ t>0 \\ u(\mathbf{x},0) = u_0(\mathbf{x}), & \forall\,\mathbf{x}\in\widetilde{\Omega} \\ u_t(\mathbf{x},0) = v_0(\mathbf{x}) & \forall\,\mathbf{x}\in\widetilde{\Omega} \end{cases} \tag{3.2}$$

that can be viewed as a special case of the time-dependent peridynamic model. The one-dimensional free-space problem for the nonlocal wave equations was studied in [45]. Define the energy

$$\mathcal{E}(t) := \frac{1}{2}\int_\Omega \left(u_t^2 + \int_\Omega (\mathcal{D}^* u)\cdot(\mathbf{\Theta}\mathcal{D}^* u)\,d\mathbf{y}\right) d\mathbf{x}.$$

An application of the nonlocal Green's first identity (2.4) with $\widehat{\Omega}=\widetilde{\Omega}$ and the antisymmetry of the integrand of $\mathcal{D}\big(\mathbf{\Theta}\,\mathcal{D}^*(u)\big)$ grants that

$$\frac{d}{dt}\mathcal{E}(t) = \int_{\widetilde{\Omega}} \big(u_{tt} + \mathcal{D}(\mathbf{\Theta}\mathcal{D}^* u)\big)u_t\,d\mathbf{x} + \int_{\Omega\setminus\widetilde{\Omega}} \big(u_{tt} - \mathcal{N}(\mathbf{\Theta}\mathcal{D}^* u)\big)u_t\,d\mathbf{x}.$$

If the volume constraint $\mathcal{V}$ implies that the above integral is zero, e.g., $u = 0$ on $\Omega \setminus \widetilde{\Omega}$, then $\dot{\mathcal{E}}(t) = 0$ and the nonlocal wave equation conserves energy. This is an instance of the peridynamic balance of energy, e.g., [43, Sect.4].

3.3. Graph Laplacian. The paper [37] introduces a precise notion of the limit of a sequence of dense finite graphs.[1] The limit is a symmetric measurable function $W : [0,1] \times [0,1] \mapsto [0,1]$ and represents the continuum analog of an adjacency matrix for a simple unweighted graph. When $W \equiv \gamma$ and $(0,1) \equiv \Omega$, the operator $\mathcal{L}$ represents the continuum analog of the graph Laplacian for a simple unweighted graph. This allows consideration of many properties of a graph associated with its Laplacian matrix to be independent of the size of the graph size or its connectivity. This includes a continuum analog of diffusion on a graph, where $\widetilde{\Omega} = \Omega$ then corresponds to diffusion restricted to occurring on the limit of a sequence of dense finite graphs; in effect, the continuum analog of the graph Laplacian assumes the volume constraint $\int_{\mathbb{R}\setminus[0,1]}(u(y) - u(x))W(x,y)\,dy = 0$. See also [23] for a discussion and applications of finite graphs with boundary conditions.

We also remark that a discrete vector calculus has precedence in the graph theory and machine learning literature; see, e.g., [24, Sect. 3] and [10, 34, 33] for some recent work and citations to the literature. Our nonlocal vector calculus, then, is a generalization of a discrete vector calculus to a graph with an uncountable number of vertices. The remarkable result [37] then suggests that a continuum analogue of a discrete vector calculus and its analysis and applications is of interest. This topic is the subject of work that will be reported elsewhere.

3.4. Probabilistic interpretation. The operator $\mathcal{L}$ is also the infinitesimal generator for a symmetric jump process[2] and has been the subject of much recent activity. For instance, Harnack inequalities, heat kernel estimates, and Hölder continuity for $\mathcal{L}$ are the subjects of [13, 14]; the Dirichlet fractional Laplacian and Cauchy martingale problems for $\mathcal{L}$ are studied in [22] and [1], respectively. The stochastic interpretation associated with volume constraints is that the sample path for a symmetric jump process exhibits discontinuous behavior and so “jumps ” to a point in the exterior of a bounded domain; this exterior region, or volume, constrains the sample path. For instance, a statistic of interest is the exit time for a process to exit a domain; see, e.g., [20] for further discussion. Our results complement these probabilistic analyses and provides a variational approach useful for numerical simulations.

4. Fluxes, diffusion, and energy principles in the classical local setting. Let $\Omega \subseteq \mathbb{R}^d$ denote an open region and let $\Omega_1 \subset \Omega$ and $\Omega_2 \subset \Omega$ denote two disjoint open regions. If Ω_1 and Ω_2 have a nonempty common boundary $\partial\Omega_{12} := \overline{\Omega}_1 \cap \overline{\Omega}_2$, then, for a vector-valued function $\mathbf{q}$, referred as the *flux density*, the expression

$$\int_{\partial\Omega_{12}} \mathbf{q} \cdot \mathbf{n}_1 \, dA \tag{4.1}$$

represents the *classical, local flux* of $\mathbf{q}$ out of Ω_1 into Ω_2, where $\mathbf{n}_1$ denotes the unit normal on $\partial\Omega_{12}$ pointing outward from Ω_1 and dA denotes a surface measure in $\mathbb{R}^d$. The flux, then, conveys a notion of direction out of and into a region and is a proxy

[1] A graph with n vertices is dense if the number of edges normalized by the number of vertices is proportional to n.

[2] The infinitesimal generator corresponds to the operator $\mathcal{L}$ with a singular kernel; see **Case 1** in Section 7.2.

for an *interaction* between Ω_1 and Ω_2. It is important to note for later reference that the flux from Ω_1 into Ω_2 occurs across their common boundary and that if the two disjoint regions have no common boundary, then the flux from one to the other is zero. The classical flux (4.1) is then deemed local since there is no interaction between Ω_1 and Ω_2 when separated by a finite distance.

The classical flux satisfies action-reaction:[3]

$$\int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\, dA + \int_{\partial\Omega_{21}} \mathbf{q}\cdot\mathbf{n}_2\, dA = \int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\, dA - \int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\, dA = 0, \tag{4.2}$$

where, of course, $\partial\Omega_{12} = \partial\Omega_{21}$ and $\mathbf{n}_2 = -\mathbf{n}_1$ denotes the unit normal on $\partial\Omega_{21}$ pointing outward from Ω_2. In words, the flux $\int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\, dA$ from Ω_1 into Ω_2 across their common boundary $\partial\Omega_{12}$ is equal and opposite to the flux $\int_{\partial\Omega_{21}} \mathbf{q}\cdot\mathbf{n}_2\, dA$ from Ω_2 into Ω_1 across that same surface.

4.1. Local diffusion. Let Ω denote a bounded, open set in $\mathbb{R}^d$. Then, classical balance laws have the form

$$\frac{d}{dt}\int_{\widehat\Omega} u(\mathbf{x},t)\, dx = \int_{\widehat\Omega} b\, d\mathbf{x} - \int_{\partial\widehat\Omega} \mathbf{q}\cdot\mathbf{n}\, dA \qquad \forall\, \widehat\Omega \subseteq \Omega, \tag{4.3}$$

where $\mathbf{n}$ denotes the unit normal on $\partial\widehat\Omega$ pointing outwards from $\widehat\Omega$, b denotes the source density for u in $\widehat\Omega$, and $\mathbf{q}$ now denotes the flux density along $\partial\widehat\Omega$ corresponding to u. In words, (4.3) states that the temporal rate of change of the quantity $\int_{\widehat\Omega} u(\mathbf{x},t)\, dx$ is given by the amount of u created within $\widehat\Omega$ by the source b minus the flux of u out of $\widehat\Omega$ through its boundary $\partial\widehat\Omega$.

The classical diffusion flux for a quantity u arises when the flux density $\mathbf{q} \equiv -\mathbf{D}\nabla u$, where $\mathbf{D}$ denotes a symmetric, positive definite second-order tensor. Substitution into (4.3) yields that

$$\frac{d}{dt}\int_{\widehat\Omega} u(\mathbf{x},t)\, dx = \int_{\widehat\Omega} b\, d\mathbf{x} + \int_{\partial\widehat\Omega} (\mathbf{D}\nabla u)\cdot\mathbf{n}\, dA \qquad \forall\, \widehat\Omega \subseteq \Omega, \tag{4.4}$$

If $b \equiv 0$ in $\widehat\Omega$ and $(\mathbf{D}\nabla u)\cdot\mathbf{n} \equiv 0$ on $\partial\widehat\Omega$, then $\int_\Omega u(\mathbf{x},t)\, dx = \int_\Omega u(\mathbf{x},0)\, dx$, that is, $\int_{\widehat\Omega} u(\mathbf{x},t)$ is conserved in $\widehat\Omega$.

Because $\widehat\Omega \subseteq \Omega$ is arbitrary, the balance law (4.4) implies, using Gauss' theorem, the *classical diffusion equation*

$$u_t - \nabla\cdot(\mathbf{D}\nabla u) = b \qquad \forall\, \mathbf{x}\in\Omega\,,\ t>0. \tag{4.5a}$$

It is well known that (4.5a) does not uniquely determine u so that one must also require u to satisfy an initial condition

$$u(\mathbf{x},0) = u_0(\mathbf{x}) \qquad \forall\, \mathbf{x}\in\Omega \tag{4.5b}$$

and a boundary condition

$$\mathcal{B}u = g \qquad \forall\, \mathbf{x}\in\partial\Omega\,,\ t>0, \tag{4.5c}$$

where $\mathcal{B}$ denotes an operator acting on functions defined on $\partial\Omega$. Common choices include $\mathcal{B}v = v$, $\mathcal{B}v = (\mathbf{D}\nabla v)\cdot\mathbf{n}$, or $\mathcal{B}v = (\mathbf{D}\nabla v)\cdot\mathbf{n} + \varphi v$ (with $\varphi(\mathbf{x},t)\geq 0$), for v in

[3]One example is in mechanics where Newton's third law, i.e., the force exerted upon on object is equal and opposite to the force exerted by the object, is an action-reaction archtype.

appropriate spaces, applied on all of $\partial\Omega$, giving the classical Dirichlet, Neumann, and Robin problems, respectively. One can also have cases of mixed boundary conditions for which two or more of these choices are applied on disjoint, covering parts of $\partial\Omega$. In (4.5a)–(4.5c), $b(\mathbf{x},t):\Omega\times(0,T)\to\mathbb{R}$, $u_0(\mathbf{x}):\Omega\to\mathbb{R}$, and $g(\mathbf{x},t):\partial\Omega\times(0,T)\to\mathbb{R}$ are given functions. The balance law (4.4) models diffusion because if $b=0$ and $g=0$ and for any of the choices for $\mathcal{B}$, we have that $\frac{d}{dt}\int_\Omega u^2\,dx = -2\int_\Omega(\mathbf{D}\nabla u)\cdot\nabla u\,dx<0$ for u not a constant function.

4.2. Steady-state local diffusion. Steady-state diffusion occurs when $u_t=0$ in (4.5a) or, equivalently, $\frac{d}{dt}\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx = 0$ all $\widehat{\Omega}\subseteq\Omega$. We then have that the initial-boundary value problem (4.5a)–(4.5c) reduces to the elliptic boundary-value problem (1.3), where, of course, now b and g do not depend on t.

The variational analysis for steady-state diffusion starts by considering the solution of

$$\min_{u\in H^1(\Omega)}\frac{1}{2}\int_\Omega \mathbf{D}\nabla u\cdot\nabla u\,d\mathbf{x}+\frac{1}{2}\int_{\partial\Omega_r}\varphi u^2\,dA-\int_\Omega ub\,d\mathbf{x}-\int_{\partial\Omega_n\cap\partial\Omega_r} ug_2\,dA \qquad \text{subject to}\quad u=g_1\quad\text{on}\quad \partial\Omega_d, \tag{4.6}$$

where $\partial\Omega_d$, $\partial\Omega_n$, and $\partial\Omega_r$ are the disjoint parts of the boundary $\partial\Omega$ on which Dirichlet, Neumann, and Robin boundary conditions are applied, respectively. For economy of exposition, we will consider only the "pure" Dirichlet and Neumann problems, that is, $\partial\Omega_r$ is empty and either $\partial\Omega_n$ or $\partial\Omega_d$ are empty as well, respectively. The cases of Robin and mixed boundary condition can be treated in a similar manner. Again for economy of exposition, we only consider the homogeneous boundary condition cases.

For the Dirichlet problem, define the constrained subspace $H_c^1(\Omega):=H_0^1(\Omega)$. We then have that, for $b\in H^{-1}(\Omega)$, solutions $u\in H_0^1(\Omega)$ of the minimization problem (4.6) equivalently satisfy the Euler-Lagrange equations

$$\int_\Omega \mathbf{D}\nabla v\cdot\nabla u\,d\mathbf{x}=\int_\Omega vb\,d\mathbf{x}\qquad\forall\, v\in H_0^1(\Omega). \tag{4.7}$$

On the other hand, for the Neumann problem, that is, for $(\mathbf{D}\nabla u)\cdot\mathbf{n}=0$ on $\partial\Omega$, we now define the constrained subspace $H_c^1(\Omega):=\{u\in H^1(\Omega)\mid \int_\Omega u\,d\mathbf{x}=0\}$. We then have that, for $b\in(H_c^1(\Omega))'$ such that $\int_\Omega b\,d\mathbf{x}=0$, where $(H_c^1(\Omega))'$ denotes the dual space of $H_c^1(\Omega)$, solutions $u\in H_c^1(\Omega)$ of the minimization problem (4.6) equivalently satisfy the Euler-Lagrange equation

$$\int_\Omega \mathbf{D}\nabla v\cdot\nabla u\,d\mathbf{x}=\int_\Omega vb\,d\mathbf{x}\qquad\forall\, v\in H_c^1(\Omega). \tag{4.8}$$

The above formal procedures are made precise by defining the symmetric bilinear form $a(u,v):=\int_\Omega \mathbf{D}\nabla v\cdot\nabla u\,d\mathbf{x}$ and the linear functional $l(v):=\int_\Omega vb\,d\mathbf{x}$ and then invoking the Lax-Milgram theorem. Necessary hypotheses are that the bilinear form is continuous and coercive and the linear functional is continuous which, for both (4.7) and (4.8), hold true; see, e.g., [18].

For sufficiently smooth u, (4.7) is equivalent to the second-order elliptic boundary value problem

$$\begin{cases} -\nabla\cdot(\mathbf{D}\nabla u)=b & \text{in }\Omega\\ u=0 & \text{on }\partial\Omega.\end{cases} \tag{4.9}$$

This is easily seen by using the classical Green's first identity and recalling that $v = 0$ on $\partial\Omega$. Likewise, (4.8) is equivalent to the second-order elliptic boundary value problem

$$\begin{cases} -\nabla\cdot(\mathbf{D}\nabla u) = b & \text{in } \Omega \\ \displaystyle\int_\Omega u = 0 & \\ (\mathbf{D}\nabla u)\cdot\mathbf{n} = 0 & \text{on } \partial\Omega. \end{cases} \tag{4.10}$$

Note that the second equations in both (4.9) and (4.10) are *essential* constraints, i.e., they must be imposed on candidate minimizers of the problem (4.6). On the other hand, the third equation in (4.10), i.e., the Neumann boundary condition, is a *natural* constraint and does no have to be imposed on candidate minimizers.

5. Anomalous diffusion. The diffusion modeled by the balance law (4.4) is deemed classical. The surface integral $\int_{\partial\widehat{\Omega}} \mathbf{D}\nabla u\cdot\mathbf{n}\,dA$ represents the diffusive flux into $\widehat{\Omega}$ and is a statement of Fick's first law. However, it is well understood that Fick's first law which is a constitutive relation for the balance of diffusion, is a questionable model for numerous phenomena; see [11, 40] for discussions and numerous citations to the literature. Equivalently, when the associated stochastic process is not given by Brownian motion, then the diffusion is deemed anomalous.

In this section, we discuss two approaches for the modeling of anomalous diffusion that replace $\nabla\cdot(\mathbf{D}\nabla u)$ with the fractional Laplacian or a fractional derivative operator. Then, in Section 6, we explain how, compared to problems involving fractional Laplacian or fractional derivative operators, a nonlocal volume-constrained problem leads to the expedient modeling of a broader range of anomalous diffusion over general domains in $\mathbb{R}^d$. In particular, we demonstrate that instances of the integral operator $\mathcal{L}$ include both the fractional Laplacian and fractional derivative operators. However, as we will demonstrate, the notion of volume constraints and the nonlocal vector calculus enable us to discuss well posedeness over bounded domains in $\mathbb{R}^d$ for a more general class of diffusion problems.

5.1. Fractional Laplacian. The fractional Laplacian is the pseudo-differential operator with Fourier symbol $\mathcal{F}$ satisfying

$$\mathcal{F}\big((-\Delta)^s u\big)(\xi) = |\xi|^{2s}\hat{u}(\xi), \qquad 0 < s \le 1,$$

where $\hat{u}$ denotes the Fourier transform of u. Suppose that $u \in L^2(\mathbb{R}^d)$ and that $\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}(u(\mathbf{x}) - u(\mathbf{y}))^2|\mathbf{y}-\mathbf{x}|^{-(d+2s)}d\mathbf{y}\,d\mathbf{x} < \infty$; the vector space of such functions defines the fractional Sobolev space $H^s(\mathbb{R}^d)$ when $0 < s < 1$. The Fourier transform can be used to show that an equivalent characterization of the fractional Laplacian is given by

$$(-\Delta)^s u = C_{d,s}\int_{\mathbb{R}^d}\frac{u(\mathbf{x}) - u(\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^{d+2s}}\,d\mathbf{y}, \qquad 0 < s < 1,$$

for some normalizing constant $C_{d,s}$. When $\widetilde{\Omega} \equiv \mathbb{R}^d$ and $\gamma(\mathbf{x},\mathbf{y}) \equiv |\mathbf{y}-\mathbf{x}|^{-(d+2s)}$, then

$$\mathcal{L} = -\big(-\Delta\big)^s, \qquad 0 < s < 1,$$

thus establishing that, when $\widetilde{\Omega} = \Omega = \mathbb{R}^d$, *the fractional Laplacian is the special case of the operator* $\mathcal{L}$ for the choice of $\gamma(\mathbf{x},\mathbf{y})$ proportional to $1/|\mathbf{y}-\mathbf{x}|^{d+2s}$.

A standard definition for the fractional Laplacian on a bounded domain Ω is

$$\int_{\Omega} \frac{u(\mathbf{x}) - u(\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^{d+2s}}\, d\mathbf{y}, \qquad 0 < s < 1.$$

However, in order for the constrained minimization problem

$$\min_{u \in H^s(\Omega)} \int_{\Omega}\int_{\Omega} \frac{\big(u(\mathbf{x}) - u(\mathbf{y})\big)^2}{|\mathbf{y}-\mathbf{x}|^{d+2s}}\, d\mathbf{y}\, d\mathbf{x} - \int_{\Omega} ub\, d\mathbf{x} \quad \text{subject to} \quad u = 0 \quad \text{on } \partial\Omega \tag{5.1}$$

to be well-posed, the condition $1/2 < s < 1$ is required. On the other hand, as we will demonstrate, replacing the above boundary constraint with the volume constraint

$$u = 0 \quad \text{on } \Omega \setminus \widetilde{\Omega} \tag{5.2}$$

delivers a well-posed minimization problem for $0 < s < 1$ for $\Omega \setminus \widetilde{\Omega}$ of nonzero volume. This in turn demonstrates that the volume-constrained problem (1.2) is a well-posed reformulation of the fractional Laplacian operator on bounded domains for $0 < s < 1$.

5.2. Fractional derivatives. The authors of [39] propose the free-space fractional dispersion equation

$$\begin{cases} u_t(\mathbf{x}, t) = c\nabla_M^{2s} u(\mathbf{x}, t) & \mathbf{x} \in \mathbb{R}^d, t > 0 \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}) & \mathbf{x} \in \mathbb{R}^d, \end{cases} \tag{5.3}$$

where $0 < s \le 1$ and the Fourier symbol of ∇_M^{2s} is given by

$$\mathcal{F}\big(\nabla_M^{2s} u(\mathbf{x})\big) := \hat{u}(\xi) \int_{\|\theta\|=1} \big(i\xi \cdot \theta\big)^{2s} M(d\theta),$$

$M(d\theta)$ denotes an arbitrary probability measure on the unit sphere, and $\hat{u}$ denotes the Fourier transform of u. The operator ∇_M^{2s} is a generalization of the fractional Laplacian; the latter operator is recovered when the measure $M(d\theta)$ is the uniform measure over the unit sphere. The paper [38] introduces a fractional divergence enabling the consideration of a fractional flux.

In the special case when $M(d\theta)$ corresponds to a symmetric measure $\omega(d\theta)$, i.e., $\omega(d\theta) = \omega(-d\theta)$, then the Fourier symbol of ∇_ω^{2s} is given by

$$\mathcal{F}\big(\nabla_\omega^{2s} u(\mathbf{x})\big) := \hat{u}(\xi) \cos \pi s \int_{\|\theta\|=1} |\xi \cdot \theta|^{2s}\, \omega(d\theta);$$

see [39, Eq.(8)]. The inverse Fourier transform may then be used to determine a kernel γ so that when $\widetilde{\Omega} \equiv \mathbb{R}^d$,

$$\mathcal{L} = C_{d,s,\omega} \nabla_\omega^{2s} \qquad 0 < s \le 1$$

for a constant $C_{d,s,\omega}$. In words, the fractional derivative operator ∇_ω^{2s} and the nonlocal operator $\mathcal{L}$ are equivalent on bounded domains, e.g., $\widetilde{\Omega} = \Omega = \mathbb{R}^d$.

A limitation of both the fractional Laplacian and derivative based approaches for the modeling of anomalous diffusion occurs on general bounded domains on $\mathbb{R}^d$ when the field u is constrained, e.g., boundary conditions when $1/2 < s < 1$. This limitation is apparent when considering a numerical method for fractional partial differential; see [41] for recent work including many references to the literature. In an impressive attempt to improve numerical methods for fractional differential equations, the authors of [28] consider an equivalent reformulation of the fractional dispersion equation (5.3) on bounded domains on $\mathbb{R}^d$ including a systematic numerical method. The authors define a fractional derivative function space and demonstrate equivalence with the fractional Sobolev space $H^s(\Omega)$ for $s > 0$ excluding integer multiples of $1/2$. However, the authors replace the volume constraint $\mathcal{V}$ of (1.2) with the boundary constraint $\mathcal{B}u = u$ and thus can only discuss the well-posedness over $H^s_0(\Omega)$ for $1/2 < s < 1$. Hence, a restricted notion of steady-state diffusion is addressed; see [28, Theorem 6.1]. In contrast, the volume-constrained problem (1.2) is a well-posed reformulation of the fractional derivative operator on bounded domains for $0 < s < 1$ includes, as will be demonstrated, a conforming finite element method.

6. Nonlocal fluxes and diffusion. The key to understanding (1.1) as a model for nonlocal diffusion is the identification of a nonlocal flux. This enables us to postulate a nonlocal balance law that describes nonlocal diffusion as an instance of an abstract balance law that postulates that the rate of change of an extensive quantity over some region is equal to production of that quantity in that region minus the flux of the same quantity out of that region.

For two disjoint open regions $\Omega_1, \Omega_2 \subset \mathbb{R}^d$, both having nonzero volume, we identify

$$\int_{\Omega_1}\int_{\Omega_2} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} \tag{6.1}$$

as the interaction, or *nonlocal flux* from Ω_1 into Ω_2, where $f : (\Omega_1 \cup \Omega_2)\times(\Omega_1\cup\Omega_2) \to \mathbb{R}$ denotes an anti-symmetric function, e.g., $f(\mathbf{x},\mathbf{y}) = -f(\mathbf{y},\mathbf{x})$ for all $\mathbf{x},\mathbf{y} \in \Omega_1 \cup \Omega_2$. The antisymmetry of $f(\mathbf{x},\mathbf{y})$ is equivalent to the nonlocal action-reaction principle

$$\int_{\Omega_1}\int_{\Omega_2} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} + \int_{\Omega_2}\int_{\Omega_1} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} = 0 \qquad \forall\,\Omega_1,\Omega_2 \subset \Omega; \tag{6.2}$$

(6.2) is the nonlocal analogue of (4.2). In words, (6.2) states that the interaction of Ω_1 upon Ω_2 is equal and opposite to the interaction of Ω_2 upon Ω_1. The interaction is *nonlocal* because, by (6.2), *the interaction may be nonzero even when the closures of* Ω_1 *and* Ω_2 *have an empty intersection.* This is in stark contrast to classical local interactions for which we have seen that the interaction between Ω_1 and Ω_2 vanishes if their closures have empty intersection. Note that, because of the antisymmetry of $f(\mathbf{x},\mathbf{y})$, we have the useful relation that

$$\int_{\Omega_1}\int_{\Omega_2} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} = \int_{\Omega_1}\int_{\Omega_1\cap\Omega_2} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x}. \tag{6.3}$$

6.1. Nonlocal diffusion. Let Ω denote a bounded, open set in $\mathbb{R}^d$. Nonlocal balance laws are stated as

$$\frac{d}{dt}\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx = \int_{\widehat{\Omega}} b\,d\mathbf{x} - \int_{\widehat{\Omega}}\int_{\Omega\setminus\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} \qquad \forall\,\widehat{\Omega} \subseteq \widetilde{\Omega}, \tag{6.4}$$

where b denotes the source density for u in $\widehat{\Omega}$ and $\int_{\Omega\setminus\widehat{\Omega}} f\,d\mathbf{x}$ denotes the flux density corresponding to u. In words, the temporal rate of change of the quantity $\int_{\widehat{\Omega}} u(\mathbf{x},t)\,dx$

is given by the amount of u created within $\widehat{\Omega} \subset \Omega$ by the source b minus the nonlocal flux of u out of $\widehat{\Omega}$ into $\Omega \setminus \widehat{\Omega}$.

Nonlocal diffusion flux arises when, in analogy to local diffusion,[4]

$$\begin{aligned}\int_{\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{x} &= \int_{\widehat{\Omega}} \big(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) + \boldsymbol{\Theta}(\mathbf{y},\mathbf{x})\mathcal{D}^*(u)(\mathbf{y},\mathbf{x})\big)\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,d\mathbf{x} \\ &= 2\int_{\widehat{\Omega}} \boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\mathcal{D}^*(u)(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,d\mathbf{x},\end{aligned} \tag{6.5}$$

where $\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})$ denotes a symmetric, positive definite (in the matrix sense) second-order tensor having elements that are symmetric functions of $\mathbf{x}$ and $\mathbf{y}$. Successively using (6.2), (6.3), (6.5), and (2.1b) leads to the identity

$$\begin{aligned}-\int_{\widehat{\Omega}}\int_{\Omega\setminus\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} &= \int_{\Omega\setminus\widehat{\Omega}}\int_{\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} \\ &= \int_{\Omega\setminus\widehat{\Omega}}\int_{\widehat{\Omega}} f(\mathbf{x},\mathbf{y})\,d\mathbf{y}\,d\mathbf{x} \\ &= 2\int_{\Omega\setminus\widehat{\Omega}}\int_{\Omega} (\boldsymbol{\Theta}\mathcal{D}^* u)\cdot\boldsymbol{\alpha}\,d\mathbf{y}\,d\mathbf{x} \\ &= -\int_{\Omega\setminus\widehat{\Omega}} \mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^* u)\,d\mathbf{x}.\end{aligned}$$

Once again, the operator $\mathcal{N}$ plays a role in the definition of the nonlocal diffusion flux. Substitution of this result into (6.4) leads to the balance law governing nonlocal diffusion:

$$\frac{d}{dt}\int_{\widehat{\Omega}} u(\mathbf{x},t)\,d\mathbf{x} = \int_{\widehat{\Omega}} b\,d\mathbf{x} - \int_{\Omega\setminus\widehat{\Omega}} \mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^* u)\,d\mathbf{x} \qquad \forall\,\widehat{\Omega}\subseteq\Omega. \tag{6.6}$$

If $b \equiv 0$ in $\widehat{\Omega} \equiv \Omega$ and $\mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^* u) \equiv 0$ on $\Omega \setminus \widehat{\Omega}$, then $\int_\Omega u(\mathbf{x},t)\,d\mathbf{x} = \int_\Omega u(\mathbf{x},0)\,d\mathbf{x}$, that is, $\int_{\widehat{\Omega}} u(\mathbf{x},t)\,d\mathbf{x}$ is conserved in $\widehat{\Omega}$.

Let $\widetilde{\Omega}$ denote a given subset of Ω. Because $\widehat{\Omega} \subseteq \widetilde{\Omega} \subset \Omega$ can be chosen arbitrarily, the balance law (6.6) implies, using the nonlocal Gauss' theorem (2.2), the *nonlocal diffusion equation*

$$u_t + \mathcal{D}\big(\boldsymbol{\Theta}\,\mathcal{D}^* u\big) = b \qquad \forall\,\mathbf{x}\in\widetilde{\Omega}\subset\Omega\,,\ t>0. \tag{6.7}$$

To (6.7), we append the initial condition (4.5a) and a volume constraint

$$\mathcal{V}u = g \qquad \text{on } \Omega\setminus\widetilde{\Omega}, \tag{6.8}$$

where examples of the operator $\mathcal{V}$ are given in Section 7.

The balance law (6.6) represents diffusion because if $b = 0$ and $g = 0$, then

$$\frac{d}{dt}\int_\Omega u^2(\mathbf{x},t)\,dx = -2\int_\Omega\int_\Omega \mathcal{D}^* u\,\cdot\,\big(\boldsymbol{\Theta}\,\mathcal{D}^* u\big)\,d\mathbf{y}\,d\mathbf{x} < 0$$

if u is not a constant function. This relationship is derived by multiplying (6.7) by u, integrating the result over $\widetilde{\Omega}$, and using the nonlocal Green's first identity (2.4) with $\widehat{\Omega} = \widetilde{\Omega}$.

[4] Recall that $\mathcal{D}^*$, being the adjoint of the nonlocal divergence, represents the negative of a nonlocal gradient. This accounts for the absence of the minus sign when compared to the local relation $\mathbf{q} = -\mathbf{D}\nabla u$.

7. Steady-state nonlocal volume-constrained diffusion problems. In this section, as we did in Section 4.2 for classical local diffusion, we study the steady-state nonlocal diffusion problem. For simplicity of exposition, we only treat homogeneous volume constraints.

7.1. Nonlocal variational problems with volume constraints. Given an open region $\Omega \subset \mathbb{R}^d$, let $\widetilde{\Omega} \subset \Omega$ and define the energy functional

$$E(u) = E_f(u) + E_b(u), \tag{7.1}$$

where, with $\gamma = \boldsymbol{\alpha} \cdot \boldsymbol{\Theta}\boldsymbol{\alpha}$,

$$\begin{cases} E_f(u) := \dfrac{1}{2}\displaystyle\int_\Omega\int_\Omega \mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) \cdot \boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\, \mathcal{D}^*(u)(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\ \qquad\quad = \dfrac{1}{2}\displaystyle\int_\Omega\int_\Omega \big(u(\mathbf{y}) - u(\mathbf{x})\big)^2 \gamma(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\ E_b(u) := -\displaystyle\int_{\widetilde{\Omega}} b(\mathbf{x})u(\mathbf{x})\, d\mathbf{x}. \end{cases}$$

Consider the constrained minimization problem

$$\min E(u) \quad \text{subject to} \quad E_c(u) = 0, \tag{7.2}$$

where $E_c(u)$ denotes a constraint functional. Proceeding formally, the first-order necessary conditions corresponding to the minimization problem (7.2) are given by

$$\int_\Omega\int_\Omega \mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) \cdot \boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\, \mathcal{D}^*(v)(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} = \int_{\widetilde{\Omega}} b(\mathbf{x})v(\mathbf{x})\, d\mathbf{x}, \tag{7.3}$$

where the test functions $v(\mathbf{x})$ satisfy the constraint $E_c(v) = 0$.

For example, first let

$$E_c(u) = E_c^d(u) := \int_{\Omega\setminus\widetilde{\Omega}} u^2\, d\mathbf{x}. \tag{7.4a}$$

Note that $E_c^d(u) = 0$ implies that $u(\mathbf{x}) = 0$ a.e. in $\Omega \setminus \widetilde{\Omega}$. Then, using the nonlocal Green's first identity (2.4), we obtain, using $E_c^d(v) = 0$, that

$$\int_{\widetilde{\Omega}} v\mathcal{D}(\boldsymbol{\Theta}\mathcal{D}^*u)\, d\mathbf{x} + \int_{\Omega\setminus\widetilde{\Omega}} v\mathcal{N}(\boldsymbol{\Theta}\mathcal{D}^*u)\, d\mathbf{x} = \int_{\widetilde{\Omega}} bv\, d\mathbf{x} \qquad \text{for } \mathbf{x} \in \widetilde{\Omega}.$$

Because $v(\mathbf{x}) = 0$ a.e. in $\Omega \setminus \widetilde{\Omega}$ but is otherwise arbitrary in $\widetilde{\Omega}$, we obtain, for the constraint (7.4a), that solutions of the minimization problem (7.2) satisfy

$$\begin{cases} -\mathcal{L}(u) = \mathcal{D}\big(\boldsymbol{\Theta}\mathcal{D}^*u\big) = b & \text{on } \widetilde{\Omega} \\ \qquad\qquad\qquad\quad\; u = 0 & \text{on } \Omega \setminus \widetilde{\Omega}. \end{cases} \tag{7.4b}$$

On the other hand, if

$$E_c(u) = E_c^n(u) := \Big(\int_\Omega u\, d\mathbf{x}\Big)^2 \tag{7.5a}$$

and if we assume that

$$\int_{\Omega} b \, d\mathbf{x} = 0, \tag{7.5b}$$

then, proceeding as we did for (7.4a), we obtain that solutions of the minimization problem (7.2) satisfy[5]

$$\begin{cases} -\mathcal{L}(u) = \mathcal{D}\big(\mathbf{\Theta}\mathcal{D}^* u\big) = b & \text{on } \widetilde{\Omega} \\ \mathcal{N}\big(\mathbf{\Theta}\mathcal{D}^* u\big) = 0 & \text{on } \Omega \setminus \widetilde{\Omega} \\ \displaystyle\int_{\Omega} u \, d\mathbf{x} = 0. \end{cases} \tag{7.5c}$$

The two choices discussed for the constraint operator $E_c(u)$ in the variational principle (7.2), or, equivalently, the second equation in the nonlocal volume-constrained problem (7.4b) and the third equation in (7.5c), are essential to the variational principle (7.2), i.e., they must be imposed on candidate minimizers. The second equation in (7.5c), however, is natural to the variational principle (7.2), i.e., it does not have to be imposed on candidate minimizers. Also, note that the constraints $E_c^d(\cdot)$ and $E_c^n(\cdot)$ are quite different; the former constraint involves the selection of a subdomain $\widetilde{\Omega} \subset \Omega$ and the *square of the integral* of u over the complement of this subdomain whereas the latter constraint does not require the selection of a subdomain and involves the *square of the integral* of u over the domain Ω. This leads to distinct forms for the constraints appearing in the nonlocal volume-constrained problems (7.4b) and (7.5c); the former constraint holds pointwise almost everywhere in the subdomain $\widetilde{\Omega}$ whereas the latter is a single integral constraint. With some justification and in analogy with Neumann boundary-value problems for elliptic partial differential equations, one can view (7.5c) as a nonlocal "Neumann" volume-constrained problem.[6] On the other hand, again with justification, one can view the second equation in (7.4b) as a nonlocal "Dirichlet" constraint. See [25] for a related discussion.

In general, we assume that $E_c(\cdot)$ denotes a bounded, quadratic functional on a suitable Hilbert space, e.g., if that space is $L^2(\Omega)$, we have

$$E_c(u) \le \widehat{c}\, \|u\|^2_{L^2(\Omega)} \qquad \forall\, u \in L^2(\Omega). \tag{7.6}$$

Moreover, we assume that the intersection of the set of constant-valued functions with the set of functions satisfying $E_c(u) = 0$ is $u \equiv 0$. Clearly, $E_c(u)$ as defined in both (7.4a) and (7.5a) satisfy these assumptions.

7.2. The kernel. We assume that the domain Ω is bounded with piecewise smooth boundary and satisfies the interior cone condition. For simplicity, we also assume that both $\widetilde{\Omega}$ and $\Omega \setminus \widetilde{\Omega}$ have the same properties. The smoothing effected by the inversion of $\mathcal{L} = -\mathcal{D}\big(\mathbf{\Theta}\,\mathcal{D}^*(\cdot)\big)$ depends upon the regularity associated with $\gamma = \boldsymbol{\alpha} \cdot \mathbf{\Theta}\boldsymbol{\alpha}$.

[5] Equation (7.5b) is a compatibility condition needed to ensure the existence of solutions of the nonlocal problem (7.5c) whereas the third equation in (7.5c) is a constraint that ensures the uniqueness of that solution.

[6] Equivalently, the contraint $\int_{\mathbb{R}^d \setminus \Omega} \big(u(\mathbf{y}) - u(\mathbf{x})\big)\gamma(\mathbf{x},\mathbf{y})\, d\mathbf{y} = 0$ is prescribed for the problem $\int_{\mathbb{R}^d} \big(u(\mathbf{y}) - u(\mathbf{x})\big)\gamma(\mathbf{x},\mathbf{y})\, d\mathbf{y} = b, \quad \mathbf{x} \in \Omega$. This is the approach taken in [4, Chapter 3].

Given positive constants γ_0 and ε, we first assume that γ satisfies

$$\gamma(\mathbf{x},\mathbf{y}) \geq 0 \quad \forall\, \mathbf{y} \in B_\varepsilon^{\mathbf{x}} \tag{7.7a}$$

$$\gamma(\mathbf{x},\mathbf{y}) = 0 \quad \forall\, \mathbf{y} \in \Omega \setminus B_\varepsilon^{\mathbf{x}}, \tag{7.7b}$$

where $B_\varepsilon^{\mathbf{x}} := \{\mathbf{y} \in \Omega \colon |\mathbf{y}-\mathbf{x}| \leq \varepsilon\}$. Obviously, (7.7) imply that although interactions are nonlocal, the are limited to a ball of radius ε. Also, recall that γ is symmetric, e.g., $\gamma(\mathbf{x},\mathbf{y}) = \gamma(\mathbf{y},\mathbf{x})$. In addition, we consider the following two special cases.
Case 1. There exist positive constants $s \in (0,1)$, γ_*, and γ^* such that

$$\frac{\gamma_*}{|\mathbf{y}-\mathbf{x}|^{d+2s}} \leq \gamma(\mathbf{x},\mathbf{y}) \leq \frac{\gamma^*}{|\mathbf{y}-\mathbf{x}|^{d+2s}} \qquad \text{for } |\mathbf{y}-\mathbf{x}| \leq \varepsilon. \tag{7.8}$$

Case 2. There exist positive constants γ_1 and γ_2 such that

$$\gamma_1 \leq \int_{\Omega \cap B_\varepsilon^{\mathbf{x}}} \gamma(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \forall\, \mathbf{x} \in \widetilde{\Omega} \subseteq \Omega \tag{7.9a}$$

$$\int_\Omega \gamma^2(\mathbf{x},\mathbf{y})\, d\mathbf{y} \leq \gamma_2^2 \quad \forall\, \mathbf{x} \in \widetilde{\Omega} \subseteq \Omega. \tag{7.9b}$$

We remark that a complete classification of kernels is not our goal; rather, we treat a sufficiently broad class, as given by the above two cases, that are of substantial mathematical and practical interest.

7.3. Equivalence of spaces. We define the energy norm, nonlocal energy space, and nonlocal volume-constrained energy space by

$$|||u||| := \big(E_f(u)\big)^{1/2} \tag{7.10a}$$

$$V(\Omega) = \big\{u \in L^2(\Omega) \;:\; |||u||| < \infty\big\} \tag{7.10b}$$

$$V_c(\Omega) = \{u \in V(\Omega) \;:\; E_c(u) = 0\}\,, \tag{7.10c}$$

respectively. We also define $|||u|||_{V_c^*(\Omega)}$ to be the norm for the dual space $V_c^*(\Omega)$ of $V_c(\Omega)$ with respect to the standard $L^2(\Omega)$ duality pairing.

We now proceed to show that for **Case 1**, the nonlocal energy space $V(\Omega)$ is equivalent to the fractional-order Sobolev space $H^s(\Omega)$ whereas for **Case 2**, the nonlocal energy space is equivalent to $L^2(\Omega)$. The equivalence of the nonlocal energy space with a fractional Sobolev space or with $L^2(\Omega)$ implies that the quotient space $V_c(\Omega)$ is a Hilbert space equipped with the norm $(E_f(u))^{1/2}$. As a result, the nonlocal volume-constrained problems (7.4b) and (7.5c) are well posed; see Section 7.4.

For $s \in (0,1)$, the standard fractional-order Sobolev space is defined as

$$H^s(\Omega) := \big\{u \in L^2(\Omega) : \|u\|_{L^2(\Omega)} + |u|_{H^s(\Omega)} < \infty\big\}\,,$$

where

$$|u|^2_{H^s(\Omega)} := \int_\Omega \int_\Omega \frac{\big(u(\mathbf{y}) - u(\mathbf{x})\big)^2}{|\mathbf{y}-\mathbf{x}|^{d+2s}}\, d\mathbf{y} d\mathbf{x}.$$

Moreover, define the subspace

$$H_c^s(\Omega) := \{u \in H^s(\Omega) \;:\; E_c(u) = 0\}$$

and recall that $|\cdot|_{H^s(\Omega)}$ is an equivalent norm on the quotient space $H_c^s(\Omega)$. Similarly, we define the subspace

$$L_c^2(\Omega) := \big\{u \in L^2(\Omega) \;:\; E_c(u) = 0\big\}\,.$$

7.3.1. Case 1. The following two lemmas will be used to demonstrate that, for this case, the spaces $V_c(\Omega)$ and $H^s_c(\Omega)$ are continuously embedded within each other.

LEMMA 7.1. *Let the function* γ *satisfy* (7.7) *and the lower bound of* (7.8). *Then,*

$$|u|^2_{H^s(\Omega)} \leq \gamma_*^{-1}|||u|||^2 + 4|\Omega|\varepsilon^{-(d+2s)}\|u\|^2_{L^2(\Omega)}.$$

Proof. We have

$$\begin{aligned}|u|^2_{H^s} &= \int_\Omega\int_{B_\varepsilon(\mathbf{x})\cap\Omega}\frac{\big(u(\mathbf{y})-u(\mathbf{x})\big)^2}{|\mathbf{y}-\mathbf{x}|^{d+2s}}\,d\mathbf{y}d\mathbf{x} + \int_\Omega\int_{\Omega\setminus B_\varepsilon(\mathbf{x})}\frac{\big(u(\mathbf{y})-u(\mathbf{x})\big)^2}{|\mathbf{y}-\mathbf{x}|^{d+2s}}\,d\mathbf{y}d\mathbf{x}\\ &\leq \gamma_*^{-1}|||u|||^2 + 2\varepsilon^{-(d+2s)}\int_\Omega\int_\Omega\big(u^2(\mathbf{x})+u^2(\mathbf{y})\big)\,d\mathbf{y}d\mathbf{x}\\ &= \gamma_*^{-1}|||u|||^2 + 4|\Omega|\varepsilon^{-(d+2s)}\|u\|^2_{L^2(\Omega)}.\end{aligned}$$

□

LEMMA 7.2. *Let the function* γ *satisfy* (7.7) *and the upper bound of* (7.8). *Then,*

$$|||u|||^2 \leq \gamma^*|u|^2_{H^s(\Omega)}.$$

Proof. The result directly follows from

$$\int_\Omega\int_\Omega \mathcal{D}^*u\,\cdot\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\mathcal{D}^*u\,d\mathbf{y}\,d\mathbf{x} \leq \gamma^*\int_\Omega\int_\Omega\frac{\big(u(\mathbf{y})-u(\mathbf{x})\big)^2}{|\mathbf{y}-\mathbf{x}|^{d+2s}}\,d\mathbf{y}d\mathbf{x}.$$

□

The following is the first of two nonlocal Poincaré-type inequalities presented in this paper. The inequality established in the next result depends crucially upon the compact embedding of the fractional space $H^s(\Omega)$ into $L^2(\Omega)$.

LEMMA 7.3. (Nonlocal Poincaré inequality I) *Let the function* γ *satisfy* (7.7) *and* (7.8). *Then, there exists a positive constant* C *such that*

$$\|u\|^2_{L^2(\Omega)} \leq C|||u|||^2 \qquad \forall\, u\in V_c(\Omega). \tag{7.11}$$

Proof. We exploit the standard technique for establishing a Poincaré type inequality by implying a contradiction. Assume there exists a sequence $\{u_k\in V_c(\Omega)\}$ where $\|u_k\|^2_{L^2(\Omega)}=1$ for all k such that $1>k|||u_k|||$. By Lemma 7.1, we have

$$\|u_k\|_{H^s(\Omega)} < 4|\Omega|\varepsilon^{-(d+2s)}+1$$

for sufficiently large k. Because the embedding $H^s(\Omega)\hookrightarrow L^2(\Omega)$ is compact and $H^s(\Omega)$ is a Hilbert space, there exists a subsequence $\{u_{k_j}\}$ of $\{u_k\}$ and an element $\tilde{u}\in H^s(\Omega)$ such that $u_{k_j}\to\tilde{u}$ strongly in $L^2(\Omega)$ so that

$$\|\tilde{u}\|_{L^2(\Omega)} = 1. \tag{7.12}$$

By Lemma 7.2, we have, for any $v\in H^s(\Omega)$, that v also belongs to $V(\Omega)$. By the dominated convergence theorem

$$\lim_{k_j\to\infty}|||u_{k_j}||| = |||\tilde{u}||| = 0$$

since $1 > k|||u_k|||$. The definition of $|||\cdot|||$ implies that $\tilde{u}$ is a constant. Moreover

$$E_c(\tilde{u}) = \lim_{k_j\to\infty} E_c(u_{k_j}) = 0$$

so that $\tilde{u} = 0$. However, this contradicts (7.12) so that the conclusion (7.11) now follows. □

Lemmas 7.1–7.3 lead to the following result.

THEOREM 7.4. *If the function* γ *satisfies* (7.7) *and* (7.8), *then*

$$C_*\|u\|_{H^s} \le |||u||| \le C^*\|u\|_{H^s} \quad \forall\, u \in V_c(\Omega),$$

where C_* *is a positive constants satisfying* $C_*^{-2} = \max\left(\gamma_*^{-1}, C(1+4|\Omega|\varepsilon^{-(d+2s)})\right)$ *and* $C^* = \gamma^*$.

Proof. Lemmas 7.1 and 7.3 grant that

$$\|u\|_{H^s}^2 \le \gamma_*^{-1}|||u|||^2 + \left(1+4|\Omega|\varepsilon^{-(d+2s)}\right)\|u\|_{L^2(\Omega)}^2 \le C_*^{-1}\,|||u|||^2.$$

In a similar fashion, Lemmas 7.2 and 7.3 lead to

$$|||u||| \le \gamma^*|u|_{H^s(\Omega)}^2 \le \gamma^*\left(|u|_{H^s(\Omega)}^2 + \|u\|_{L^2(\Omega)}^2\right) = C^*\|u\|_{H^s}.$$

□

We then immediately obtain the following equivalence result between constrained energy spaces and constrained Sobolev spaces.

COROLLARY 7.5. *If the function* γ *satisfies* (7.7) *and* (7.8), *then we have the equivalence of the constrained spaces* $H_c^s(\Omega)$ *and* $V_c(\Omega)$.

This theorem and corollary explain that, if the function γ satisfies the two conditions (7.7) and (7.8), then $V(\Omega)$ and its constrained subspace $V_c(\Omega)$ are compactly embedded in $L^2(\Omega)$ and $L_c^2(\Omega)$, respectively.

We note that the space equivalence holds with no restrictions on the exponent $s \in (0,1)$ because of our consideration of volume constraints in lieu of constraints on the boundary of the domain (or some other lower dimensional manifold). This is an important point, particularly, for $s \le 1/2$. Indeed, for $s \le 1/2$, there is no well-defined trace space in the standard manner for functions in the Sobolev space $H^s(\Omega)$ which is why conventional boundary value problems have not been discussed for such cases in the literature. The volume-constrained problem (1.2), however, is well-posed for any $s \in (0,1)$, as will be demonstrated in Section 7.4.

7.3.2. Case 2. We now demonstrate that, in this case, the constrained space $V_c(\Omega) = L_c^2(\Omega)$. We choose to work with the more stringent conditions (7.9) rather than other more general assumptions. This allows us to apply well-known results about integral operators. The reader is referred [2, 4] for the case where γ is radial and only $L^1(\Omega)$ integrable.

We state the analogue of Lemma 7.2 that can be established through direct calculation; see, e.g., [32, 46] for details.

LEMMA 7.6. *If the function* γ *satisfies* (7.7) *and* (7.9), *then*

$$|||u||| \le C_2\|u\|_{L^2(\Omega)} \quad \forall\, u \in V_c(\Omega)$$

for some positive constant C_2.

Next, we present a second Poincaré inequality that relies, in contrast to the hypotheses of Lemma 7.3, on the compactness of a Hilbert-Schmidt kernel; see, e.g., [8, Chap. 12].

LEMMA 7.7. (Nonlocal Poincaré inequality II) *If the function* γ *satisfies* (7.7) *and* (7.9)*, then*

$$C_1\|u\|_{L^2(\Omega)} \leq |||u||| \quad \forall\, u \in V_c(\Omega)$$

for some positive constant C_1.

Proof. Because

$$-\frac{1}{2}\mathcal{L}u(\mathbf{x}) = \int_\Omega u(\mathbf{y})\,\gamma(\mathbf{x},\mathbf{y})\,d\mathbf{y} - u(\mathbf{x})\int_\Omega \gamma(\mathbf{x},\mathbf{y})\,d\mathbf{y},$$

we see that the hypothesis on the function γ imply that the nonlocal diffusion operator $-\mathcal{L} = \mathcal{D}\big(\boldsymbol{\Theta}\,\mathcal{D}^*\big)$ is a self-adjoint operator on $L^2_c(\Omega)$. As established at the end of Section 2, $-\mathcal{L}$ is a non-negative operator. Moreover, by the properties of Hilbert-Schmidt integral operators, we find that $-\mathcal{L}$ is also a compact perturbation of a scalar multiple of the identity operator and is, in fact, uniformly bounded both above and below by positive constant multiples of the identity operator. Furthermore, the kernel of $-\mathcal{L}$ in $L^2_c(\Omega)$ contains only the zero element. Therefore,

$$\lambda_1 := \inf_{u\in L^2(\Omega)} \frac{|||u|||^2}{||u||^2_{L^2(\Omega)}} > 0,$$

e.g., the smallest eigenvalue of $-\mathcal{L}$ is strictly positive, and therefore we have

$$\sqrt{\lambda_1}\,\|u\|_{L^2(\Omega)} \leq |||u||| \quad \forall\, u \in L^2_c(\Omega).$$

Thus, the conclusion of this lemma holds with $C_1 = \sqrt{\lambda_1}$. ☐

The following result is an immediate consequence of Lemmas 7.6 and 7.7.

COROLLARY 7.8. *If the function* γ *satisfies the conditions* (7.7) *and* (7.9)*, then* $V_c(\Omega) = L^2_c(\Omega)$.

7.4. Well-posedness of nonlocal volume-constrained problems. Subsection 7.3.1–7.3.2 established that the nonlocal energy space $V_c(\Omega)$ is equivalent to $H^s_c(\Omega)$ or $L^2_c(\Omega)$ depending upon whether **Case 1** or **Case 2**, respectively, are assumed. The following result demonstrates that minimization problem (7.2) has a unique minimizer given general constraint functional (7.6).

THEOREM 7.9. *The nonlocal variational problem of minimizing* $E(u) = E_f(u) + E_b(u)$ *over* $V_c(\Omega)$ *has a unique solution* u *for any* $b \in V^*_c(\Omega)$*. Moreover, the Euler-Lagrange equation is given by* (7.4b) *for* $E_c = E^d_c$ *and* (7.5c) *for* $E_c = E^n_c$*. Furthermore, there exists a constant* $C > 0$*, independent of* b*, such that*

$$|||u||| \leq C\|b\|_{V^*_c(\Omega)}. \tag{7.13}$$

Proof. The theorem is established via a direct application of the Lax-Milgram theorem; see, e.g., [8, Section 3.6]. ☐

In Section 7.3, we established that the nonlocal constrained energy space $V_c(\Omega)$ is equivalent to $H^s_c(\Omega)$ or $L^2_c(\Omega)$ for **Case 1** and **Case 2**, respectively. Thus, for problems for which the function γ satisfies the assumptions of **Case 1** or **Case 2**, respectively, the estimate (7.13) implies that

$$\|u\|_{H^s(\Omega)} \le C\|b\|_{H^{-s}(\Omega)}, \quad 0 < s < 1, \quad \text{or} \tag{7.14a}$$

$$\|u\|_{L^2(\Omega)} \le C\|b\|_{L^2(\Omega)}, \tag{7.14b}$$

hold, respectively. These should be contrasted with the analogous result for (1.3), i.e., for classical boundary-value problems for elliptic partial differential equations, for which we have

$$\|u\|_{H^1(\Omega)} \le C\|b\|_{H^{-1}(\Omega)}. \tag{7.14c}$$

The inequalities (7.14a)–(7.14b) explain that a gain of regularity of $2s$ and 0, respectively, occurs for **Case 1** or **Case 2**, respectively. In contrast, the inequality (7.14c) results in a gain of regularity of 2. In other words, the solutions of the nonlocal volume-constrained problems have no more than $2s$ more derivatives than the data b whereas the boundary-value problem (1.3) has two more derivatives. These regularity conditions are analogous to those established in [46] for restricted classes of one- and two-dimensional peridynamic models with constraints suggestive of nonlocal volume-constrained conditions.

8. Additional comments about nonlocal volume-constrained problems.

In this section, we briefly discuss other volume-constrained problems not already considered, well-posedeness for nonlocal evolution problems and vanishing nonlocality.

8.1. Other volume-constrained problems.

We briefly describe how other volume-constrained problems can be handled in the variational setting.

The essential volume constraint $v = 0$ in (7.4b) is replaced by the essential inhomogeneous volume constraint $u = g$ by simply setting $E_c(u) = \int_{\Omega\setminus\widetilde{\Omega}} (u-g)^2\, d\mathbf{x}$. On the other hand, the natural volume constraint $\mathcal{N}\big(\mathbf{\Theta}\mathcal{D}^* u\big) = 0$ in (7.5c) is replaced by the natural inhomogeneous volume constraint $\mathcal{N}\big(\mathbf{\Theta}\mathcal{D}^* u\big) = g$ by adding the energy contribution $E_g(u) = -\int_{\Omega\setminus\widetilde{\Omega}} ug\, d\mathbf{x}$ to the energy functional $E(u)$. In this case, the compatibility condition (7.5b) is replaced by $\int_{\widetilde{\Omega}} b\, d\mathbf{x} + \int_{\Omega\setminus\widetilde{\Omega}} g\, d\mathbf{x} = 0$.

More generally, mixed "Dirichlet"-"Neumann" nonlocal constrained-value problems are defined by splitting $\Omega \setminus \widetilde{\Omega}$ into two measurable, disjoint, subregions Ω_d and Ω_n and then setting $E_c(u) = \int_{\Omega_d} (u - g_d)^2\, d\mathbf{x}$ and adding the contribution $E_g(u) = -\int_{\Omega_n} ug_n\, d\mathbf{x}$ to the energy functional $E(u)$. No compatibility condition on the data is needed. The resulting volume-constrained problem is given by

$$\begin{cases} \mathcal{D}\big(\mathbf{\Theta}\mathcal{D}^* u\big) = b & \text{on } \widetilde{\Omega} \\ \qquad\qquad u = g_d & \text{on } \Omega_d = \Omega \setminus (\widetilde{\Omega} \cup \Omega_n) \\ \mathcal{N}\big(\mathbf{\Theta}\mathcal{D}^* u\big) = g_n & \text{on } \Omega_n = \Omega \setminus (\widetilde{\Omega} \cup \Omega_d). \end{cases}$$

The second equation is an essential volume constraint whereas the third equation is natural.

Finally, we consider the case of a "Robin" volume constraint that is treated by adding the term $E_r(u) = \frac{1}{2}\int_{\Omega\setminus\widetilde{\Omega}} \varphi u^2\, d\mathbf{x}$ for $\varphi(\mathbf{x}) \ge 0$ to $E_f(u)$ and the term $E_g(u) = -\int_{\Omega\setminus\widetilde{\Omega}} ug\, d\mathbf{x}$ to the energy functional $E(u)$. No compatibility condition on the data is needed. The resulting volume-constrained problem is given by

$$\begin{cases} \mathcal{D}\big(\boldsymbol{\Theta}\mathcal{D}^*u\big) = b & \text{on } \widetilde{\Omega} \\ \mathcal{N}\big(\boldsymbol{\Theta}\mathcal{D}^*u\big) + \varphi u = g & \text{on } \Omega\setminus\widetilde{\Omega}. \end{cases}$$

The second equation is a natural volume constraint. Well-posedness results for these volume-constrained problems are entirely similar to those in Section 7 and Section 9 and can be obtained using techniques similar to those used in those sections.

8.2. Well-posedness for nonlocal evolution equations. Using the results on the nonlocal operators and the variational problems established in this paper, we may use standard techniques to establish the well-posedness for nonlocal evolution equations such as the nonlocal diffusion (6.7) and the nonlocal wave (3.2) equations, respectively . As an illustration, we consider the special case for which the constrained energy space $V_c(\Omega)$ associated with the functional (7.4a) is established to be a Hilbert space with its dual space $V_c^*(\Omega)$ and that the operator $\mathcal{D}\big(\boldsymbol{\Theta}\,\mathcal{D}^*\big)$ is bounded and coercive in $V_c(\Omega)$. For that case, we have the following result.

THEOREM 8.1. *The initial and volume-constrained problem* (6.7) *along with* (6.7) *and* (6.8) *has a unique solution* $u \in C(0,T;V_c(\Omega)) \cap H^1(0,T;V_c^*(\Omega))$ *provided that* $b \in L^2(0,T;V_c^*(\Omega))$ *and* $u_0 \in V_c(\Omega)$. *Moreover, the initial and volume constrained problem* (3.2) *has a unique solution* $u \in L^2(0,T;V_c(\Omega)) \cap L^2(0,T;L^2(\Omega)) \cap H^1(0,T;V_c^*(\Omega))$ *provided that* $b \in L^2(0,T;V_c^*(\Omega))$ *with* $u_0 \in V_c(\Omega)$ *and* $u_1 \in L^2(\Omega)$.

These results are consequences of standard semi-group theory or Galerkin type arguments. We refer to [46] for more detailed proofs of these results in a special case for which the techniques used are directly generalizable to the problems considered here.

8.3. Vanishing nonlocality. In [25], the local limit of the operator $\mathcal{D}(\boldsymbol{\Theta}\mathcal{D}^*)$ was examined and we demonstrated that the free-space operator, e.g., $\mathcal{L}$ where $\widetilde{\Omega} = \mathbb{R}^d$, converges to $-\nabla\cdot(D\nabla)$ as $\varepsilon \to 0$ under suitable conditions on the kernel function. More recently, in [4, 26], for kernel functions of radial type $\gamma(\mathbf{x},\mathbf{y}) = \tilde{\gamma}(|\mathbf{x}-\mathbf{y}|)$ with $\tilde{\gamma}$ an element of L^1, the local limit of the nonlocal diffusion equation has been studied. Further, in the paper [26] finite element solutions for nonlocal diffusion and the peridynamic model are also investigated.

As an example of a local limit, let $\widetilde{\Omega}$ be a bounded domain independent of ε and $\mathbf{D} := \lim_{\varepsilon\to 0}\mathbf{D}_\varepsilon$, where

$$(\mathbf{D}_\varepsilon)_{ij} = \int_{B_\varepsilon(0)} \tilde{\gamma}(|\mathbf{z}|)\, z_i z_j\, d\mathbf{z} \qquad \text{for} \qquad i,\, j = 1,\, 2, \ldots, d;$$

then, a particular consequence of the results in [26] is

$$\lim_{\varepsilon\to 0}\int_\Omega\int_\Omega \mathcal{D}^*u\cdot\big(\boldsymbol{\Theta}\,\mathcal{D}^*v\big)\,d\mathbf{y}\,d\mathbf{x} = \int_\Omega \nabla u\,\cdot\big(\mathbf{D}\,\nabla v\big)\,d\mathbf{x} \tag{8.1}$$

for any given $u, v \in H^1(\Omega)$ with support in $\widetilde{\Omega}$. A more general form of the above limit was given in [26] for piecewise smooth functions with respect to a triangulation of the domain which was used to examine the limiting properties of finite element approximations and the corresponding error estimators. By setting $u = v$, we see from (8.1) that

$$\lim_{\varepsilon\to 0}\int_\Omega\int_\Omega \mathcal{D}^*u\cdot\big(\boldsymbol{\Theta}\,\mathcal{D}^*u\big)\,d\mathbf{y}\,d\mathbf{x} = \int_\Omega \nabla u\cdot\big(\mathbf{D}\,\nabla u\big)\,d\mathbf{x}.$$

This establishes the relationship between the nonlocal norms and the standard local Sobolev space norms in the local limit. Moreover, it has been also shown in [46] that, albeit for a special nonlocal boundary conditions, the solutions of nonlocal diffusion equation converge to the solution of the local diffusion equation in suitable spaces in such a limit. This relies on a key estimate showing that when $\mathbf{D}$ is positive definite, the smallest eigenvalue of the nonlocal diffusion operator $\mathcal{D}(\boldsymbol{\Theta}\mathcal{D}^*)$ remains larger than a positive constant uniformly in ε as $\varepsilon \to 0$. In the context of peridynamic models, this is equivalent to the assumption that the materials have well-defined elastic moduli [46]. When such a property holds for more general volume-constrained problems considered here, we may also see that the solutions u_ε of (7.3) converge, at least weakly in $L^2(\Omega)$ to the unique solution u of the equation (4.8) in the local limit. By passing to the limit in the respective weak forms, we recover stronger convergence results, in particular, for b bounded in $L^2(\Omega)$, we get

$$\lim_{\varepsilon\to 0}\int_\Omega\int_\Omega \mathcal{D}^* u_\varepsilon \cdot \big(\boldsymbol{\Theta}\mathcal{D}^* u_\varepsilon\big)\, d\mathbf{y}\, d\mathbf{x} = \int_\Omega \nabla u \cdot \big(\mathbf{D}\,\nabla u\big)\, d\mathbf{x}\,.$$

One may draw analogy of the above results with other existing studies on the characterization of Sobolev spaces and their norms, for instance, using the characterization established in [17], it was shown in [7] that

$$\lim_{n\to\infty}\int_\Omega\int_\Omega \frac{\big(u(\mathbf{x})-u(\mathbf{y})\big)^2}{|\mathbf{y}-\mathbf{x}|^2}\rho_n(|y-x|)\, d\mathbf{y}\, d\mathbf{x} \propto |u|_{H^1(\Omega)}$$

for a sequence of radial mollifiers $\{\rho_n\}$. In particular, the authors of [7] demonstrate that the norm induced by $\int_\Omega\int_\Omega \frac{(u(\mathbf{x})-u(\mathbf{y}))^2}{|\mathbf{y}-\mathbf{x}|^2}\rho_n(|y-x|)\, d\mathbf{y}\, d\mathbf{x}$ is equivalent to $|u|_{H_0^s\Omega}$ for $1/2 < s < 1$. We note that our results cover wider classes of Sobolev spaces and kernel functions.

9. Finite-dimensional approximations. Given the variational formulation (7.2) of the nonlocal volume-constrained problem (1.2), one may naturally consider its finite dimensional approximations within the variational framework. Here, we establish *a priori* error and condition number estimates for finite-dimensional approximations of the nonlocal volume-constrained problem (1.2) under both **Case 1** and **Case 2**. These results are analogous to those established in [46] for a restricted class of one- and two-dimensional volume-constrained problems associated with linear peridynamic models.

Let $\{V_c^n\}$ denote a sequence of finite-dimensional subspaces of $V_c(\Omega)$ and assume that, as $n\to\infty$, $\{V_c^n\}$ is dense in $V_c(\Omega)$, i.e., for any $v\in V_c(\Omega)$, there exists a sequence $\{v_n \in V_c^n\}$ such that

$$|||v - v_n||| \to 0 \quad \text{as} \quad n\to\infty\,. \tag{9.1}$$

Throughout the remainder of this section, we let u denote the solution of the variational problem. We seek the Ritz-Galerkin approximation $u_n \in V_c^n$ to the nonlocal variational problem posed on V_c^n that fall within the class of "internal" (see [9, p. 86]) or "conforming" approximations, i.e., we seek u_n that minimizes $E(\cdot)$ over $V_c^n \subset V_c(\Omega)$.

9.1. Convergence and error estimates. We first state an abstract convergence result which gives the best approximation property of the finite dimensional

Ritz-Galerkin solution.

THEOREM 9.1. *If the function γ satisfies* (7.7) *and either* (7.8) *or* (7.9)*, then, for any $b \in V_c^*(\Omega)$, we have*

$$|||u - u_n||| \leq \min_{v_n \in V_c^n} |||u - v_n||| \to 0 \quad \text{as} \;\; n \to \infty \,. \tag{9.2}$$

Proof. Standard variational argument shows that the Ritz-Galerkin approximation is the best approximation to u in V_c^n with respect to the energy norm. This, together with (9.1), gives the result of the theorem. ∎

We now consider a more concrete example of finite dimensional approximations. Let us focus on, in particular, finite element approximations for the case that both Ω and $\widetilde{\Omega}$ are polyhedral domains. For a given triangulation of Ω that simultaneously triangulates $\widetilde{\Omega}$, we let V_c^n consist of those functions in $V_c(\Omega)$ that are piecewise polynomials of degree no more than m defined with respect to the triangulation. We assume that the triangulation is shape-regular and quasiuniform [18] as the mesh parameter, the diameter of the largest element, $h \to 0$, i.e., as n, the dimension of the space V_c^n, goes to ∞. Note that generally n is of order h^d for small h. If the exact solution u is sufficiently smooth, we have the following result.

THEOREM 9.2. *Let m be a non-negative integer and $0 < s < 1$.*
Case 1. *Suppose that $u \in V_c(\Omega) \cap H^{m+t}(\Omega)$ where $0 \leq r \leq s$ and $s \leq t \leq 1$. Then, there exists a constant C such that for sufficiently small h,*

$$\|u - u_n\|_{H^r(\Omega)} \leq C h^{m+t-r} \|u\|_{H^{m+t}(\Omega)}. \tag{9.3a}$$

Case 2. *Suppose that $u \in V_c(\Omega) \cap H^{m+t}(\Omega)$ where $0 \leq t \leq 1$. Then, there exists a constant C such that for sufficiently small h,*

$$\|u - u_n\|_{L^2(\Omega)} \leq C h^{m+s} \|u\|_{H^{m+s}(\Omega)}. \tag{9.3b}$$

Proof. The proof follows similar derivations as that given in [46] for a linear peridynamic model. We thus only outline the main ingredients. By Theorem 9.1 and the norm equivalence established in earlier sections, the error estimate (9.3a) for the case $r = s$ and the estimate (9.3b) follow from standard approximation properties in Sobolev spaces [18] of integer order. The estimate for $r = 0$ can then be obtained via a standard duality argument as that for the conforming (internal) finite element approximations of second-order elliptic equations [9, 18]. One may then use interpolation theory for the more general case of (9.3a) for $r \in (0, s)$. ∎

In particular, if $m = 1$, then a second-order convergence with respect to the $L^2(\Omega)$ norm can be expected for linear elements by setting $r = 0$, $t = 1$ in **Case 1** and $t = 1$ in **Case 2**.

It is important to note that for **Case 1** for $s < 1/2$ and for **Case 2**, *discontinuous* (across element boundaries) finite element spaces are conforming. This should be contrasted with discontinuous Galrekin methods for second-order elliptic partial differential equations which are nonconforming and thus require special handling, e.g., penalty terms, at element boundaries. For nonlocal volume-constrained problems, no such special handling is needed if $s < q/2$.

9.2. Condition numbers. For the finite element approximations of the nonlocal operator $\mathcal{L}$ using basis functions $\{\phi_i\}_{i=1}^n$, let us consider the nonlocal stiffness matrix $\mathbf{K} = (k_{ij})_{n\times n}$, where the entries $\{k_{ij}\}$ are defined by

$$k_{ij} = -(\mathcal{L}(\phi_i), \phi_j) \quad \text{for } i, j = 1, \ldots, n.$$

The condition number of the stiffness matrix is an indicator for both the sensitive dependence of the discrete solution on the data and the performance of iterative solvers such as the conjugate-gradient method. Our condition number estimates allow the development of preconditioners for nonlocal problems and extend the existing results in [3] to the case when $\mathcal{L}$ smooths the data.

The choice of particular basis function can affect the order of condition numbers. We consider the case where the conventional nodal finite element basis $\{\phi_i\}_{i=1}^n$ is used [18], so that under the shape-regular and quasi-uniform mesh assumptions, there exist positive constants c_1 and c_2 such that, for h small,

$$c_1 h^d \sum_{i=1}^n u_i^2 \le \| \sum_{i=1}^n u_i \phi_i \|^2_{L^2(\Omega)} \le c_2 h^d \sum_{i=1}^n u_i^2$$

holds for any $u_h = \sum_{i=1}^n u_i \phi \in V_c^n(\Omega)$.

Then, we have the following condition number estimates.

THEOREM 9.3. *For the nonlocal stiffness matrix* $\mathbf{K}$*, we have, for h small,*
a) if γ satisfies (7.7) *and* (7.8)*, then for some generic constant $c > 0$,*

$$\mathrm{cond}(\mathbf{K}) \le ch^{-2s}; \tag{9.4}$$

b) if γ satisfies (7.7) *and* (7.9)*, then for some generic constant $c > 0$,*

$$\mathrm{cond}(\mathbf{K}) \le c. \tag{9.5}$$

Proof. The proof again follows the same line of derivations as that given in [46] for a linear nonlocal peridynamic model. The main ingredients are the norm equivalence as established in earlier sections and the inverse inequality of the type:

$$\|u^h\|^2_{H^s(\Omega)} \le ch^{-2s} \|u^h\|^2_{L^2(\Omega)}$$

for any finite element function

$$u_h = \sum_{i=1}^n u_i \phi \in V_c^n(\Omega)$$

with the conventional Sobolev space norms [18]. ▯

These results are again consistent with the ones given in [46] for special boundary conditions corresponding to special peridynamic nonlocal models. We again note that if $s \in (0, 1/2)$, the error and condition number estimates also hold for discontinuous Galerkin approximations, because in this case all the piecewise polynomial spaces with respect to the triangulation, globally continuous or not, are conforming elements for the internal discretization of the nonlocal problem; see [21, 46]. Moreover, note that for the **Case 1** with $s \in (0, 1)$, the condition number grows slower, as $h \to 0$, than that for elliptic partial differential equations for which the condition number grows with h^{-2}.

Interestingly, in relation to the discussion given earlier, the finite-dimensional stiffness matrices may also be related to graph Laplacians. We note that whereas in some cases the condition number may grow with the system size, in other cases, it may be uniformly bounded. Such results shed light on why for some graph or discrete Laplacians it remains challenging to find effective solvers and preconditioners while some other cases, fast iterative solvers are more readily available given the independence of the condition number on the system size.

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