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Analysis and Approximation of Nonlocal Diffusion Problems with Volume Constraints*

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

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

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1. Introduction.

It is well understood that Fick's first law, which is a constitutive relation for diffusive fluxes, is a questionable model for numerous phenomena; see [11, 44, 45] for discussions and numerous citations to the literature. Equivalently, whenever the associated underlying stochastic process is not given by Brownian motion, the diffusion is deemed anomalous. In particular, anomalous superdiffusion refers to situations that can be, at times, modeled using fractional spatial derivatives or fractional spatial differential operators [44]. In this paper, we consider an integro-differential equation model for anomalous superdiffusion that, among other desirable features, has the fractional Laplacian and fractional derivative models as special cases. To distinguish our model from existing models for superdiffusion and to highlight that it applies to a wider range of phenomena, we refer to our model as a *nonlocal* model for diffusion.

Let $\Omega \subset \mathbb{R}^n$ denote a bounded, open domain. For $u(\mathbf{x})\colon \Omega \to \mathbb{R}$, define the action of the linear operator $\mathcal{L}$ on the function $u(\mathbf{x})$ as

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

where the volume of Ω is nonzero and the kernel $\gamma(\mathbf{x},\mathbf{y})\colon \Omega \times \Omega \to \mathbb{R}$ denotes a nonnegative symmetric mapping, i.e., $\gamma(\mathbf{x},\mathbf{y}) = \gamma(\mathbf{y},\mathbf{x}) \geq 0$. The operator $\mathcal{L}$ is deemed *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 with *local* operators, e.g., the value of Δu at a point $\mathbf{x}$ requires information about u only at $\mathbf{x}$. We have that $\mathcal{L}u$ is the spatial contribution in *nonlocal diffusion* equations (see (1.2a), section 3.3, and also, e.g., [4]) and *nonlocal wave* equations (see section B.2). Section 5.3 briefly discusses nonlocal advection-diffusion problems.

For specific choices of the kernel γ and under an appropriate rescaling, the operator $\mathcal{L}$ is a generalization of the classical Laplacian operator [4, 51] or, more generally, the operator $\nabla\cdot(\mathbf{C}\cdot\nabla)$, where $\mathbf{C}$ denotes a second-order tensor [27, 35]. In section 3.2, using a recently developed nonlocal vector calculus [27, 35], the operator $\mathcal{L}$ is recast as the composition of nonlocal divergence and gradient operators in analogy to the composition $\nabla \cdot (\mathbf{C} \cdot \nabla)$ for second-order elliptic operators.

The operator $\mathcal{L}$ and its generalizations arise in many applications such as image analyses [19, 33, 34, 40], machine learning [47], nonlocal Dirichlet forms [5, sec. 3.6], kinetic equations [12, 39], phase transitions [15, 32], nonlocal heat conduction [16], and the peridynamic model for mechanics [48] and its one-dimensional variants [49, 50] for which $\mathcal{L}$ arises directly. We briefly discuss some of the above applications and related mathematical work in Appendix B. Moreover, in Appendix A, we discuss the close connections between our model and existing models for anomalous superdiffusion; in particular, we show that *the fractional Laplacian operator and a fractional derivative operator are special cases of the operator* $\mathcal{L}$.

Our interest in the operator $\mathcal{L}$ is due to its participation in the time-dependent *nonlocal volume-constrained diffusion problem*

$$\begin{cases} u_t - \mathcal{L}u = b & \text{on } \Omega,\ t > 0,\\ u(\mathbf{x},0) = u_0 & \text{on } \Omega \cup \Omega_{\mathcal{I}},\\ \mathcal{V}u = g & \text{on } \Omega_{\mathcal{I}},\ t > 0, \end{cases} \tag{1.2a}$$

for the function $u(\mathbf{x},t)$ and its steady-state counterpart

$$\begin{cases} -\mathcal{L}u = b & \text{on } \Omega,\\ \mathcal{V}u = g & \text{on } \Omega_{\mathcal{I}}, \end{cases} \tag{1.2b}$$

where $\mathcal{V}$ denotes a linear operator of constraints acting on a volume $\Omega_{\mathcal{I}}$ that is disjoint from Ω. Volume constraints are natural extensions, to the nonlocal case, of boundary conditions for differential equation problems. For example, if $\mathcal{V}$ is the identity operator, the last equation in (1.2a) or (1.2b) is a nonlocal "Dirichlet" volume constraint. Nonlocal versions of Neumann and Robin boundary conditions are also naturally defined; see section 4.1.

The nonlocal vector calculus of [27] makes transparent the analogies we draw between the nonlocal problems (1.2a) and (1.2b) and parabolic and elliptic boundary-value problems, respectively, involving second-order scalar elliptic operators. For example, we will draw several analogies between (1.2a) and the classical diffusion problem

$$\begin{cases} u_t - \nabla \cdot (\mathbf{C} \cdot \nabla u) = b & \text{on } \Omega, \\ u(\mathbf{x}, 0) = u_0 & \text{on } \Omega, \\ \mathcal{B}u = g & \text{on } \partial\Omega, \end{cases} \tag{1.3a}$$

as well as between (1.2b) and the (generalized) Poisson problem

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

where $\mathbf{C} : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ denotes a second-order tensor and $\mathcal{B}$ denotes a linear operator acting on the boundary $\partial\Omega$ of the volume Ω.

At first glance, the differences between the volume-constrained problems (1.2a) and (1.2b) and the boundary-value problems (1.3a) and (1.3b), respectively, are obvious. First, the former pair involves the integral operator $\mathcal{L}$, whereas the latter pair involves a second-order spatial differential operator. Second, in (1.2a) and (1.2b), constraints are imposed on the solution over a nonzero *volume* $\Omega_{\mathcal{I}}$ that is not necessarily located near or at the boundary of Ω; on the other hand, in (1.3a) and (1.3b), constraints are imposed precisely at the bounding *surface* $\partial\Omega$. These distinctions are essential in characterizing the differences in the properties of, e.g., problems (1.2b) and (1.3b) and their solutions. In section 1.1, we discuss why volume constraints are not only useful, but also necessary to treat certain classes of nonlocal problems having the form (1.2a) or (1.2b).

Section 2 reviews classical diffusion problems and, in particular, the notions of a local flux, local balance laws, local diffusion problems, and the well-posedness of steady-state local diffusion problems. This discussion serves to set up sections 3 and 4, in which analogous notions for nonlocal volume-constrained problems are considered. In section 3.1, the notion of a nonlocal flux is discussed. That discussion is crucial to section 3.3, in which nonlocal balance laws are posed from which nonlocal diffusion problems of the type (1.2a) are derived; the latter derivation depends on results from the nonlocal vector calculus of [27] that is briefly reviewed in section 3.2. The material in sections 2 and 3 renders transparent the correspondences between local and nonlocal diffusion problems, with a central correspondence between the boundary-constraint operator $\mathcal{B}$ in the local case and the volume-constraint operator $\mathcal{V}$ in the nonlocal case.

Section 4 contains the primary contribution of our paper; there, the well-posedness of steady-state volume-constrained diffusion problems of the type (1.2b) is demonstrated by exploiting the nonlocal vector calculus reviewed in section 3.2. The notion of volume-constrained problems enables us to formulate and solve diffusion problems in situations where boundary conditions are not well defined, e.g., diffusive regimes where the Fourier symbol of the self-adjoint diffusive operator is of nonnegative order less than or equal to 1/2. Such diffusion problems, e.g., the volume-constrained problem (1.2b), allow discontinuous functions as solutions, given appropriate conditions on the kernel γ. Also, because the fractional Laplacian operator and fractional derivative operators are special cases of the operator $\mathcal{L}$ (see section A), the well-posedness of volume-constrained problems on bounded domains in $\mathbb{R}^n$ posed in terms of these operators also readily follows, a previously unavailable result.

In section 5, the well-posedness of nonlocal evolution problems such as (1.2a) and a nonlocal wave equation are briefly discussed and a nonlocal model for advection-diffusion problems involving the operator $\mathcal{L}$ is presented. Also, a brief discussion of vanishing nonlocality is given that demonstrates that, in the limit when the support of the kernel γ decreases, the classical local diffusive operator is recovered. Another contribution of our paper is the analyses of the convergence and of error and condition number estimates for finite-dimensional discretizations of nonlocal volume-constrained problems; these analyses are given in section 6, 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 that are not required to be continuous across element faces, e.g., *discontinuous Galerkin methods are conforming* in those cases. This is in stark contrast to discontinuous Galerkin methods for the discretization of, e.g., (1.3b), for which they are nonconforming [6].

An inspiration for this paper is to extend results of [30, 51] and [4, Chaps. 1–3] to the volume-constrained problem (1.2b) on bounded domains. The well-posedness results derived in this paper extend the result established in [35] 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. In [4, Chap. 1] the well-posedness of the Cauchy problem for the nonlocal diffusion equation (1.2a) is considered, whereas [4, Chaps. 2–3] consider a special choice of volume constraints for the case of γ a radial function, i.e., $\gamma(\mathbf{x},\mathbf{y}) = \gamma(\mathbf{y}-\mathbf{x})$, with $\gamma(\mathbf{0}) > 0$ and $\int_{\mathbb{R}^n} \gamma(\mathbf{z})\,d\mathbf{z} = 1$. Such conditions on γ imply that $\mathcal{L}$ is a mapping from $L^2(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$; conditions such that inversions of $\mathcal{L}$ smooth the data are not considered.

1.1. The Need for Volume Constraints. Consideration 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 $\mathcal{L}$ and those involving second-order elliptic partial differential operators. First, we recall that if $u = 0$ on $\partial\Omega$, i.e., if in (1.3b) $g = 0$ and $\mathcal{B}$ is the identity operator, and if appropriate conditions on Ω and $\mathbf{C}$ are assumed, then, given data $b \in H^{-1}(\Omega)$, a weak formulation of the boundary-value problem (1.3b) is well posed in $H_0^1(\Omega)$, i.e., there exists a unique solution $u \in H_0^1(\Omega)$ and, moreover, that solution depends continuously on the data b. Alternatively, we have that $\nabla \cdot (\mathbf{C} \cdot \nabla)$ is a bounded operator from $H_0^1(\Omega) \to H^{-1}(\Omega)$ having a bounded inverse.

In contrast, if $g = 0$ and $\mathcal{V}$ is the identity operator in (1.2b), i.e., if $u = 0$ on $\Omega_{\mathcal{I}}$, then, for appropriate choices for the kernel γ, we demonstrate, in section 4, that a variational formulation of the volume-constrained problem (1.2b) is well posed in the space $H_c^s(\Omega \cup \Omega_{\mathcal{I}})$ for $0 < s < 1$, provided the given data b belongs to the dual space of $H_c^s(\Omega \cup \Omega_{\mathcal{I}})$, where $H_c^s(\Omega \cup \Omega_{\mathcal{I}})$ is the subspace of the fractional Sobolev space $H^s(\Omega \cup \Omega_{\mathcal{I}})$ constrained to satisfy the volume constraint $u = 0$ on $\Omega_{\mathcal{I}}$. We even demonstrate, for a particular class of kernels γ, that the variational formulation is well posed in $L_c^2(\Omega \cup \Omega_{\mathcal{I}})$, provided the given data b belongs to $L_c^2(\Omega \cup \Omega_{\mathcal{I}})$ as well.

Alternatively, we have that $\mathcal{L}$ is a bounded operator from $H^s_c(\Omega \cup \Omega_{\mathcal{I}})$ to its dual space or from $L^2_c(\Omega \cup \Omega_{\mathcal{I}}) \to L^2_c(\Omega \cup \Omega_{\mathcal{I}})$, as the kernel warrants, and that $\mathcal{L}$ has a bounded inverse. In particular, the solution operator for (1.2b) regularizes, i.e., smooths, the data b to a lesser extent compared to the solution operator for (1.3b) 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 (1.2b) are well posed in subspaces of $H^s(\Omega \cup \Omega_{\mathcal{I}})$ 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 $H^s(\Omega \cup \Omega_{\mathcal{I}})$ for $s \in [0, 1/2]$. We next ask whether we could instead impose a surface constraint, e.g., 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 $u \in H^s(\Omega \cup \Omega_{\mathcal{I}})$ for $s \in [0, 1)$. However, the restriction of a function $u \in H^s(\Omega \cup \Omega_{\mathcal{I}})$ onto $\partial(\Omega \cup \Omega_{\mathcal{I}})$ is not defined for $s \in [0, 1/2]$, i.e., the trace of such a u is not defined. This means that if $s \in [0, 1/2]$, we cannot impose constraints on u restricted to $\partial(\Omega \cup \Omega_{\mathcal{I}})$. However, a volume constraint for which the operator $\mathcal{V}$ is the restriction operator onto $\Omega_{\mathcal{I}}$ 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 necessary for operators that are bounded acting on $H^s(\Omega \cup \Omega_{\mathcal{I}})$ functions with $s \in [0, 1/2]$.*

For example, the well-posedness of (1.3b) when $\nabla \cdot \nabla$ is replaced by Δ^{2s} (the fractional Laplacian) is not discussed whenever $s \in [0, 1/2]$ because of the lack of well-defined traces of functions belonging to $H^s(\Omega)$. More generally, the well-posedness of and tractable numerical methods for pseudodifferential or fractional self-adjoint differential operators on bounded domains when the degree of the (Fourier) symbol lies in $s \in (0, 1/2]$ are not available. In contrast, the volume-constrained, nonlocal problem (1.2b) is, for appropriate kernels γ, well posed for $s \in [0, 1)$, and finite element discretizations are easily defined from the variational characterizations possible for such problems. Thus, we see that in such cases, volume constraints are expedient. As further examples, we note that the use of volume constraints for equations involving the operator $\mathcal{L}$ immediately removes the limitation encountered in [7, 31] to only consider a fractional dispersion equation and kernels γ, respectively, where the solutions are in $H^s_0(\Omega)$ for $s \in (1/2, 1)$, and to present a numerical method for the solution of the fractional Laplacian operator equations on bounded domains in lieu of the random walk approximation used in [52].

2. The Classical Local Differential Equation Setting for Diffusion.

We review well-known notions related to diffusion in the classical differential equation setting, starting with the notion of a local flux. This review serves as a template for the discussion of similar notions in sections 3 and 4 for nonlocal diffusion and also provides comparisons of and analogies between the local and nonlocal cases.

2.1. Local Fluxes.

Let $\Omega_1 \subset \mathbb{R}^n$ and $\Omega_2 \subset \mathbb{R}^n$ 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 sufficiently smooth[1] vector function $\mathbf{q}(\mathbf{x})$, the expression

$$\int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\, dA \tag{2.1}$$

represents the *classical local flux 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 $\mathbb{R}^n$; $\mathbf{q}\cdot\mathbf{n}_1$ is referred as the *flux density* along $\partial\Omega_{12}$. The flux, then, conveys a notion of direction out of and into a region and is a proxy for the *interaction* between Ω_1 and Ω_2. It is important to note 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 (2.1) is then deemed to be *local* because there is no interaction between Ω_1 and Ω_2 when separated by a finite distance. The classical flux satisfies the action-reaction principle

$$\int_{\partial\Omega_{12}} \mathbf{q}\cdot\mathbf{n}_1\, dA + \int_{\partial\Omega_{21}} \mathbf{q}\cdot\mathbf{n}_2\, dA = 0, \tag{2.2}$$

where, of course, $\partial\Omega_{12} = \partial\Omega_{21}$ and $\mathbf{n}_2 = -\mathbf{n}_1$ denotes the unit normal on $\partial\Omega_{12}$ 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.

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

$$\frac{d}{dt}\int_{\widetilde{\Omega}} u\, d\mathbf{x} = \int_{\widetilde{\Omega}} b\, d\mathbf{x} - \int_{\partial\widetilde{\Omega}} \mathbf{q}\cdot\mathbf{n}\, dA \qquad \forall\, \widetilde{\Omega}\subseteq\Omega,\ t>0, \tag{2.3}$$

where $\mathbf{n}$ denotes the unit normal on $\partial\widetilde{\Omega}$ pointing outwards from $\widetilde{\Omega}$, b denotes the source density for u in $\widetilde{\Omega}$, and $\mathbf{q}\cdot\mathbf{n}$ denotes the flux density along $\partial\widetilde{\Omega}$ corresponding to u. In words, (2.3) states that the temporal rate of change of the quantity $\int_{\widetilde{\Omega}} u(\mathbf{x},t)\, d\mathbf{x}$ is given by the amount of u created within $\widetilde{\Omega}$ by the source b minus the flux of u out of $\widetilde{\Omega}$ through its boundary $\partial\widetilde{\Omega}$. If $b=0$ in $\widetilde{\Omega}$ and $\mathbf{q}\cdot\mathbf{n}=0$ on $\partial\widetilde{\Omega}$, then $\int_{\widetilde{\Omega}} u(\mathbf{x},t)\, d\mathbf{x} = \int_{\widetilde{\Omega}} u(\mathbf{x},0)\, d\mathbf{x}$; i.e., if there are no sources of u within $\widetilde{\Omega}$ and there is no flux of u out of $\widetilde{\Omega}$, then $\int_{\widetilde{\Omega}} u(\mathbf{x},t)\, d\mathbf{x}$, the quantity of u in $\widetilde{\Omega}$, is conserved.

Applying the Gauss theorem, we have from (2.3) that

$$\frac{d}{dt}\int_{\widetilde{\Omega}} u\, d\mathbf{x} = \int_{\widetilde{\Omega}} b\, d\mathbf{x} - \int_{\widetilde{\Omega}} \nabla\cdot\mathbf{q}\, d\mathbf{x} \qquad \forall\, \widetilde{\Omega}\subseteq\Omega,\ t>0. \tag{2.4}$$

Because $\widetilde{\Omega}\subseteq\Omega$ is arbitrary, (2.4) leads to the field equation

$$u_t + \nabla\cdot\mathbf{q} = b \qquad \forall\, \mathbf{x}\in\Omega,\ t>0. \tag{2.5}$$

Classical diffusion arises when the relation between $\mathbf{q}$ and u is given by Fick's first law $\mathbf{q} = -\mathbf{C}\cdot\nabla u$, where $\mathbf{C}(\mathbf{x})$ denotes a symmetric, positive definite second-order tensor. Substitution into (2.5) yields the *classical diffusion equation*

$$u_t - \nabla\cdot(\mathbf{C}\cdot\nabla u) = b \qquad \forall\, \mathbf{x}\in\Omega,\ t>0. \tag{2.6a}$$

[1]The components of $\mathbf{q}$ belonging to $H^1(\Omega)$ is sufficient, but one can have even weaker spaces.

It is well known that (2.6a) does not uniquely determine u, so that one must also require u to satisfy an initial condition

$$u(\mathbf{x},0) = u_0(\mathbf{x}) \qquad \forall\, \mathbf{x} \in \Omega \tag{2.6b}$$

and a boundary condition

$$\mathcal{B}u = g \qquad \forall\, \mathbf{x} \in \partial\Omega,\ t > 0, \tag{2.6c}$$

where $\mathcal{B}$ denotes an operator acting on functions defined on $\partial\Omega$. Common choices include $\mathcal{B}u = u$, $\mathcal{B}u = (\mathbf{C}\cdot\nabla u)\cdot\mathbf{n}$, or $\mathcal{B}u = (\mathbf{C}\cdot\nabla u)\cdot\mathbf{n} + \varphi u$ (with $\varphi(\mathbf{x},t) \geq 0$) for u belonging to appropriate spaces, applied on all of $\partial\Omega$, giving the classical Dirichlet, Neumann, and Robin problems, respectively. One can also have mixed boundary conditions for which two or more of these choices are applied on disjoint, covering parts of $\partial\Omega$. In (2.6), $b(\mathbf{x},t) : \Omega \times (0,T) \to \mathbb{R}$, $u_0(\mathbf{x}) : \Omega \to \mathbb{R}$, and $g(\mathbf{x},t) : \partial\Omega \times (0,T) \to \mathbb{R}$ are given functions. The system (2.6) characterizes diffusion because if $b = 0$ and $g = 0$ and for the choices for $\mathcal{B}$, we have that, using Green's first identity,

$$\frac{1}{2}\frac{d}{dt}\int_\Omega u^2\,dx + \int_\Omega \nabla u\cdot(\mathbf{C}\cdot\nabla u)\,dx \leq 0,$$

so that the rate of decay of $\|u\|_{L^2(\Omega)}$ depends upon spatial variations. For Dirichlet or Neumann boundary conditions, this relation holds as an equality.

2.3. Steady-State Local Diffusion with Boundary Constraints. Steady-state diffusion occurs when $u_t = 0$ in (2.6a). We then have that the initial boundary-value problem (2.6) reduces to the elliptic boundary-value problem (1.3b), where, of course, b and g now do not depend on t.

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

$$\begin{aligned} &\text{minimize}\left\{\frac{1}{2}\int_\Omega \nabla u\cdot(\mathbf{C}\cdot\nabla u)\,d\mathbf{x} + \frac{1}{2}\int_{\partial\Omega_r}\varphi u^2\,dA - \int_\Omega ub\,d\mathbf{x} - \int_{\partial\Omega_n} ug_n\,dA\right. \\ &\qquad\qquad \left. - \int_{\partial\Omega_r} ug_r\,dA\right\} \qquad \text{subject to} \quad u = g_d \quad \text{on} \quad \partial\Omega_d \\ &\qquad\qquad\qquad\qquad\qquad \text{and, if } \partial\Omega = \partial\Omega_n, \quad \int_\Omega u\,d\mathbf{x} = c_n, \end{aligned} \tag{2.7}$$

where $\partial\Omega_d$, $\partial\Omega_n$, and $\partial\Omega_r$ are the disjoint, covering parts of the boundary $\partial\Omega$ on which Dirichlet, Neumann, and Robin boundary conditions are applied, respectively; $\varphi > 0$, b, g_d, g_n, and g_r denote given functions, and c_n is a given constant. The Euler–Lagrange equations corresponding to the minimization problem (2.7) lead to the boundary-value problem

$$-\nabla\cdot(\mathbf{C}\cdot\nabla u) = b \qquad \text{in } \Omega, \tag{2.8a}$$

$$(\mathbf{C}\cdot\nabla u)\cdot\mathbf{n} = g_n \qquad \text{on } \partial\Omega_n, \tag{2.8b}$$

$$(\mathbf{C}\cdot\nabla u)\cdot\mathbf{n} + \varphi u = g_r \qquad \text{on } \partial\Omega_r, \tag{2.8c}$$

$$u = g_d \qquad \text{on } \partial\Omega_d, \tag{2.8d}$$

$$\int_{\partial\Omega} u\,dA = c_n \qquad \text{if } \partial\Omega = \partial\Omega_n, \tag{2.8e}$$

where, if $\partial\Omega = \partial\Omega_n$, the data b and g_n are required to satisfy the compatibility condition

$$\int_\Omega b\,d\mathbf{x} + \int_{\partial\Omega} g_n\,dA = 0. \tag{2.9}$$

Note that (2.8d) and (2.8e) are *essential* boundary conditions that must be imposed on candidate solutions of the minimization problem (2.7), whereas (2.8b) and (2.8c) are *natural* boundary conditions that need not be explicitly imposed on candidate solutions. Note also that in the case $\partial\Omega = \partial\Omega_n$, (2.9) is necessary to show the existence of a solution of (2.8), whereas (2.8e) is sufficient to ensure that that solution is unique.

The above formal procedures are made precise and well-posedness results are obtained for (2.8) by choosing appropriate function spaces for the data and solution, then defining the symmetric bilinear form $a(u,v) := \int_\Omega \nabla v\cdot(\mathbf{C}\cdot\nabla u)\,d\mathbf{x} + \int_{\partial\Omega_r}\varphi uv\,dA$ and the linear functional $l(v) := \int_\Omega vb\,d\mathbf{x} + \int_{\partial\Omega_n} vg_n\,dA + \int_{\partial\Omega_r} vg_r\,dA$, 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 (2.8), hold true; see, e.g., [18]. For example, if $\partial\Omega = \partial\Omega_d$ and $g_d = 0$, i.e., for the homogeneous Dirichlet problem, we have that $u \in H^1_0(\Omega)$ and $b \in H^{-1}(\Omega)$, whereas if $\partial\Omega = \partial\Omega_n$, $g_n = 0$, and $c_n = 0$, i.e., for the homogeneous Neumann problem, we have that $u \in H^1_c(\Omega) := \{v \in H^1(\Omega)\ :\ \int_\Omega v\,d\mathbf{x} = 0\}$ and $b \in (H^1_c(\Omega))^*$, where the latter space denotes the dual of $H^1_c(\Omega)$.

3. Nonlocal Fluxes, a Nonlocal Vector Calculus, and Nonlocal Diffusion. In this section and in section 4, we parallel, for the nonlocal case, the presentation given in section 2 for the local diffusion case; in particular, sections 3.1 and 3.3 mimic sections 2.1 and 2.2, respectively, whereas section 4 mimics section 2.3. Recall that, in sections 2.2 and 2.3, elements of classical vector calculus for differential operators were invoked; analogously, in sections 3.3 and 4, elements of a vector calculus for nonlocal operators are invoked. Thus, the nonlocal vector calculus, which is a generalization of classical vector calculus to nonlocal operators, enables us to study nonlocal diffusion problems in a manner analogous to how classical diffusion is studied. Because the nonlocal calculus may not be familiar to the reader, we provide in section 3.2 a brief review of the nonlocal vector calculus developed in [27].

The clarity achieved through the use of the nonlocal vector calculus to enable a development of nonlocal diffusion that mimics in every way that of local diffusion benefits both mathematical analyses and physical interpretations, as is demonstrated in the remainder of the paper.

3.1. Nonlocal Fluxes. The key to understanding (1.2a) as a model for nonlocal diffusion is the identification of a nonlocal flux. This enables us to state a nonlocal balance law that postulates that the rate of change of an extensive quantity over some region is equal to the production of that quantity in that region minus the flux of the same quantity out of that region. Here, we review the discussion about nonlocal fluxes given in [27], where a detailed discussion is provided. In the discussion, $\psi(\mathbf{x},\mathbf{y})$ may be a scalar or vector or tensor function. For the sake of brevity, in this subsection and in section 3.2, we suppress explicit reference to the time dependence of variables.

For any point $\mathbf{x} \in \mathbb{R}^n$, we identify

$$\int_{\widetilde{\Omega}} \psi(\mathbf{x},\mathbf{y})\,d\mathbf{y} \qquad \forall\,\widetilde{\Omega} \subseteq \mathbb{R}^n \tag{3.1}$$

as the *nonlocal flux density* at $\mathbf{x}$ into $\widetilde{\Omega}$. We have that the following three statements are equivalent:

(3.2a) • $\psi(\mathbf{x},\mathbf{y})$ *is an antisymmetric function*, i.e., $\psi(\mathbf{x},\mathbf{y}) = -\psi(\mathbf{y},\mathbf{x})$;

(3.2b) • there are *no self-interactions,* i.e., $\int_{\widetilde{\Omega}}\int_{\widetilde{\Omega}} \psi(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} = 0 \quad \forall\, \widetilde{\Omega} \subseteq \mathbb{R}^n$;

• for two regions $\Omega_1, \Omega_2 \subset \mathbb{R}^n$, both having nonzero volume, we have the *nonlocal action-reaction principle*

$$\int_{\Omega_1}\int_{\Omega_2} \psi(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} + \int_{\Omega_2}\int_{\Omega_1} \psi(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} = 0 \qquad \forall\, \Omega_1, \Omega_2 \subset \mathbb{R}^n. \tag{3.2c}$$

With (3.1) denoting a nonlocal flux density, for any two open regions $\Omega_1 \subseteq \mathbb{R}^n$ and $\Omega_2 \subseteq \mathbb{R}^n$, both having nonzero volume, we identify

$$\int_{\Omega_1}\int_{\Omega_2} \psi(\mathbf{x},\mathbf{y})\, d\mathbf{y} d\mathbf{x} \tag{3.3}$$

as a scalar *interaction* or *nonlocal flux from* Ω_1 *into* Ω_2. Because we require no self-interactions, i.e., that the flux from a region into itself vanishes so that (3.2b) holds whenever $\Omega_1 = \Omega_2$, we have that $\psi : (\Omega_1 \cup \Omega_2) \times (\Omega_1 \cup \Omega_2) \to \mathbb{R}$ is an *antisymmetric* function. By (3.1), $\int_{\Omega_2} \psi(\mathbf{x},\mathbf{y})\, d\mathbf{y}$ is the *nonlocal flux density* at a point $\mathbf{x} \in \Omega_1$ into the region Ω_2. As is the case for the local flux density $\mathbf{q} \cdot \mathbf{n}_1$, the nonlocal flux density $\int_{\Omega_2} \psi(\mathbf{x},\mathbf{y})\, d\mathbf{y}$ is related to an intensive variable through a constitutive relation; see section 3.3.

Based on the above discussion, we see that (3.2c) is the nonlocal analogue of (2.2). In other words, (3.2c) states that the flux (or interaction) from Ω_1 into Ω_2 is equal and opposite to the flux (or interaction) from Ω_2 into Ω_1. The flux is *nonlocal* because, by (3.2c), *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 local interactions for which we have seen that the interaction between Ω_1 and Ω_2 vanishes if their closures have empty intersection, i.e., if they have no common boundary.

3.2. Elements of a Nonlocal Vector Calculus. In [27], a nonlocal vector calculus is developed; here, we briefly review the aspects of that calculus that are useful in what follows.

Given the vector mappings $\boldsymbol{\nu}(\mathbf{x},\mathbf{y}), \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$ with $\boldsymbol{\alpha}$ antisymmetric, i.e., $\boldsymbol{\alpha}(\mathbf{y},\mathbf{x}) = -\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})$, the action of the *nonlocal divergence operator* $\mathcal{D}$ on $\boldsymbol{\nu}$ is defined in [27] as[2]

$$\mathcal{D}\big(\boldsymbol{\nu}\big)(\mathbf{x}) := \int_{\mathbb{R}^n} \big(\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x})\big) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \qquad \text{for } \mathbf{x} \in \mathbb{R}^n, \tag{3.4}$$

where $\mathcal{D}(\boldsymbol{\nu})\colon \mathbb{R}^n \to \mathbb{R}$. The nonlocal divergence operator $\mathcal{D}$ is motivated by equating $\psi(\mathbf{x},\mathbf{y})$ introduced in section 3.1 with the integrand of (3.4); for a full justification of this choice, see [27]. Here we just mention that this choice results from an application of the Schwarz kernel theorem after making the natural assumptions that the nonlocal divergence operator should be a linear operator and that the integral of the nonlocal divergence of a vector over any domain should equal the flux out of that domain; the latter assumption is motivated by the fact that the classical differential divergence operator may be so defined.

[2]In [27], a more general expression for the nonlocal divergence operator is derived; however, the specialized definition (3.4) suffices for the treatment of nonlocal diffusion given in this paper.

Given the mapping $u(\mathbf{x})\colon \mathbb{R}^n \to \mathbb{R}$, the *adjoint operator* $\mathcal{D}^*$ *corresponding to* $\mathcal{D}$ is the operator whose action on u is given by

$$\mathcal{D}^*\big(u\big)(\mathbf{x},\mathbf{y}) = -\big(u(\mathbf{y}) - u(\mathbf{x})\big)\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) \qquad \text{for } \mathbf{x},\mathbf{y} \in \mathbb{R}^n, \tag{3.5}$$

where $\mathcal{D}^*(u)\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$. With $\mathcal{D}^*$ denoting the adjoint of the nonlocal divergence operator, we view $-\mathcal{D}^*$ as a *nonlocal gradient*. The mapping $\mathcal{D}(\boldsymbol{\nu})$ is scalar-valued in analogous fashion to the local differential divergence of a vector function and the mapping $\mathcal{D}^*(u)$ is vector-valued in analogous fashion to the local differential gradient of a scalar function $u(\mathbf{x})$.

From (3.4) and (3.5), one easily deduces that if $\boldsymbol{\Theta}(\mathbf{x},\mathbf{y}) = \boldsymbol{\Theta}(\mathbf{y},\mathbf{x})$ denotes a second-order tensor satisfying $\boldsymbol{\Theta} = \boldsymbol{\Theta}^T$, then

$$\mathcal{D}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^*u\big)(\mathbf{x}) = -2\int_{\mathbb{R}^n} \big(u(\mathbf{y}) - u(\mathbf{x})\big)\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\cdot\big(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\big)\,d\mathbf{y} \quad \text{for } \mathbf{x} \in \mathbb{R}^n,$$

where $\mathcal{D}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^*u\big)\colon \mathbb{R}^n \to \mathbb{R}$. Comparing with (1.1), we have that

$$\mathcal{L}u = -\mathcal{D}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^*u\big) \qquad \text{with} \qquad \gamma = \boldsymbol{\alpha}\cdot(\boldsymbol{\Theta}\cdot\boldsymbol{\alpha}). \tag{3.6}$$

Thus, the operator $\mathcal{L}$ is a composition of nonlocal divergence and gradient operators so that if $\boldsymbol{\Theta}$ is the identity tensor, $\mathcal{L}$ can be interpreted as a nonlocal Laplacian operator. Because $\mathcal{D}$ and $\mathcal{D}^*$ are adjoint operators, if $\boldsymbol{\Theta}$ is also positive definite, the operator $-\mathcal{L}$ is nonnegative; see [33, Proposition 2.1] and also [12, 27, 35] for discussion when $\boldsymbol{\Theta}$ is the unit tensor.

Given an open subset $\Omega \subset \mathbb{R}^n$, the corresponding *interaction domain* is defined as

$$\Omega_{\mathcal{I}} := \{\mathbf{y} \in \mathbb{R}^n \setminus \Omega \quad \text{such that} \quad \boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) \neq \mathbf{0} \quad \text{for some } \mathbf{x} \in \Omega\}, \tag{3.7}$$

so that $\Omega_{\mathcal{I}}$ consists of those points outside of Ω that interact with points in Ω. Note that the situation $\Omega_{\mathcal{I}} = \mathbb{R}^n \setminus \Omega$ is allowable, as is $\Omega = \mathbb{R}^n$, in which case $\Omega_{\mathcal{I}} = \emptyset$. Then, corresponding to the divergence operator $\mathcal{D}\big(\boldsymbol{\nu}\big)\colon \mathbb{R}^n \to \mathbb{R}$ defined in (3.4), we define the action of the nonlocal *interaction operator* $\mathcal{N}(\boldsymbol{\nu})\colon \mathbb{R}^n \to \mathbb{R}$ on $\boldsymbol{\nu}$ by

$$\mathcal{N}\big(\boldsymbol{\nu}\big)(\mathbf{x}) := -\int_{\Omega\cup\Omega_{\mathcal{I}}} \big(\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x})\big)\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega_{\mathcal{I}}. \tag{3.8}$$

In [27], based on a discussion along the lines of that in section 3.1, it is shown that $\int_{\Omega_{\mathcal{I}}} \mathcal{N}(\boldsymbol{\nu})\,d\mathbf{x}$ can be viewed as a nonlocal flux out of Ω into $\Omega_{\mathcal{I}}$. The main difference between the local and nonlocal cases is that, in the former case, the flux out of a domain Ω is given by the *boundary* integral $\int_{\partial\Omega} \mathbf{q}\cdot\mathbf{n}\,dA$, whereas, in the nonlocal case, that flux is given by the *volume* integral $\int_{\Omega_{\mathcal{I}}} \mathcal{N}(\boldsymbol{\nu})\,d\mathbf{x}$.

With $\mathcal{D}$ and $\mathcal{N}$ defined as in (3.4) and (3.8), respectively, we have the *nonlocal Gauss theorem*

$$\int_{\Omega} \mathcal{D}(\boldsymbol{\nu})\,d\mathbf{x} = \int_{\Omega_{\mathcal{I}}} \mathcal{N}(\boldsymbol{\nu})\,d\mathbf{x}. \tag{3.9}$$

Next, let $u(\mathbf{x})$ and $v(\mathbf{x})$ denote scalar functions. Then it is a simple matter to show that the nonlocal divergence theorem (3.9) implies the generalized *nonlocal Green's first identity*

$$\int_{\Omega} v\mathcal{D}(\boldsymbol{\Theta}\cdot\mathcal{D}^*u)\,d\mathbf{x} - \int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}} (\mathcal{D}^*v)\cdot(\boldsymbol{\Theta}\cdot\mathcal{D}^*u)\,d\mathbf{y}d\mathbf{x} = \int_{\Omega_{\mathcal{I}}} v\mathcal{N}(\boldsymbol{\Theta}\cdot\mathcal{D}^*u)\,d\mathbf{x}. \tag{3.10}$$

For details concerning the nonlocal calculus, see [27], which also contains 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. In addition, in [27], further connections are made between the nonlocal operators and the corresponding local operators. For example, it is shown there that for the special kernel $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) = -\nabla_{\mathbf{y}}\delta(\mathbf{y}-\mathbf{x})$, where $\delta(\cdot)$ denotes the Dirac delta measure and $\nabla_{\mathbf{y}}$ denotes the differential gradient with respect to $\mathbf{y}$, one has that

$$\mathcal{D}(\boldsymbol{\nu}) = \nabla\cdot(\boldsymbol{\nu}(\mathbf{x},\mathbf{x})) = \nabla\cdot\big(\boldsymbol{\nu}(\mathbf{x},\mathbf{y})\big|_{\mathbf{y}=\mathbf{x}}\big), \qquad \int_{\mathbb{R}^n}\mathcal{D}^*(u)\,d\mathbf{y} = -\nabla u(\mathbf{x}),$$

and

$$\int_{\Omega_{\mathcal{I}}} v\mathcal{N}(\boldsymbol{\nu})\,d\mathbf{x} = \int_{\partial\Omega} v(\mathbf{x})\boldsymbol{\nu}(\mathbf{x},\mathbf{x})\cdot\mathbf{n}\,dA \qquad \forall\, v\in C_0^\infty(\mathbb{R}^n).$$

3.3. Nonlocal Diffusion. Let Ω denote a bounded, open set in $\mathbb{R}^n$. Nonlocal balance laws have the form

$$\frac{d}{dt}\int_{\widetilde{\Omega}} u\,dx = \int_{\widetilde{\Omega}} b\,d\mathbf{x} - \int_{\widetilde{\Omega}_{\mathcal{I}}}\mathcal{N}(\boldsymbol{\nu})\,d\mathbf{x} \qquad \forall\,\widetilde{\Omega}\subseteq\Omega,\ t>0, \tag{3.11}$$

where $b(\mathbf{x},t)$ denotes the source density for u in Ω and $\widetilde{\Omega}_{\mathcal{I}}\subseteq\Omega_{\mathcal{I}}$ denotes the interaction region corresponding to $\widetilde{\Omega}$. In words, (3.11) states that the temporal rate of change of the quantity $\int_{\widetilde{\Omega}} u(\mathbf{x},t)\,d\mathbf{x}$ is given by the amount of u created within $\widetilde{\Omega}\subseteq\Omega$ by the source b minus the nonlocal flux of u out of $\widetilde{\Omega}$ into $\widetilde{\Omega}_{\mathcal{I}}$. If $b\equiv 0$ and $\mathcal{N}(\boldsymbol{\nu})\equiv 0$ in $\widetilde{\Omega}_{\mathcal{I}}$, then $\int_{\widetilde{\Omega}} u(\mathbf{x},t)\,d\mathbf{x} = \int_{\widetilde{\Omega}} u(\mathbf{x},0)\,d\mathbf{x}$; i.e., just as in the local case, if there are no sources of u within $\widetilde{\Omega}$ and there is no flux of u out of $\widetilde{\Omega}$, then $\int_{\widetilde{\Omega}} u(\mathbf{x},t)$, the quantity of u in $\widetilde{\Omega}$, is conserved.

Applying the nonlocal Gauss theorem[3] (3.9) to the last term in (3.11) results in

$$\frac{d}{dt}\int_{\widetilde{\Omega}} u\,d\mathbf{x} = \int_{\widetilde{\Omega}} b\,d\mathbf{x} - \int_{\widetilde{\Omega}}\mathcal{D}(\boldsymbol{\nu})\,d\mathbf{x} \qquad \forall\,\widetilde{\Omega}\subseteq\Omega,\ t>0. \tag{3.12}$$

Because $\widetilde{\Omega}\subseteq\Omega$ can be chosen arbitrarily, the balance law (3.12) implies the nonlocal field equation

$$u_t + \mathcal{D}(\boldsymbol{\nu}) = b \qquad \forall\,\mathbf{x}\in\Omega,\ t>0. \tag{3.13}$$

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

$$\boldsymbol{\nu} = \boldsymbol{\Theta}\cdot(\mathcal{D}^* u), \tag{3.14}$$

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 $\mathbf{y}$. The relation (3.14) represents a nonlocal Fick's first law. Substitution of (3.14) into (3.13) leads to the *nonlocal diffusion equation*

$$u_t + \mathcal{D}(\boldsymbol{\Theta}\cdot\mathcal{D}^* u) = b \qquad \forall\,\mathbf{x}\in\Omega,\ t>0. \tag{3.15a}$$

[3]Recall that it is exactly at the analogous point in section 2.2, i.e., at (2.4), that we invoked the classical Gauss theorem.

[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 $\mathbf{q} = -\mathbf{C}\cdot\nabla u$.

We append the initial condition

$$u(\mathbf{x},0) = u_0(\mathbf{x}) \qquad \forall\, \mathbf{x} \in \Omega \tag{3.15b}$$

and the *volume* constraint

$$\mathcal{V}u = g \qquad \forall\, \mathbf{x} \in \Omega_{\mathcal{I}},\ t > 0, \tag{3.15c}$$

to (3.13). Examples of the operator $\mathcal{V}$ are given in section 4. The system (3.15) is the nonlocal analogue of the local differential system (2.6). From (3.6), we see that (3.15) is exactly the problem (1.2a) so that the latter is indeed a nonlocal diffusion problem. The system (3.15) represents diffusion because if $b = 0$ and $g = 0$, then, for the volume constraints considered in this paper,

$$\frac{1}{2}\frac{d}{dt}\int_{\Omega} u^2\, d\mathbf{x} + \int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}} \mathcal{D}^* u \cdot \big(\boldsymbol{\Theta}\cdot\mathcal{D}^* u\big)\, d\mathbf{y}\, d\mathbf{x} = 0.$$

This relationship is derived by multiplying (3.13) by u, integrating the result over Ω, and using the nonlocal Green's first identity (3.10). In analogy to local diffusion as explained at the end of section 2.2, the rate of decay of $\|u\|_{L^2(\Omega)}$ also depends upon spatial variations.

4. Steady-State Nonlocal Volume-Constrained Diffusion Problems.

As in section 2.3 for classical local diffusion, in this section we study the steady-state nonlocal diffusion problem. In section 4.1, we discuss general problems involving mixed inhomogeneous "Dirichlet," "Neumann," and "Robin"-type *volume constraints*; the correspondences between the discussions of local and nonlocal steady-state diffusion found in sections 2.3 and 4.1, respectively, are transparent. In sections 4.2–4.4, in which the well-posedness of nonlocal volume-constrained problems is considered, we specialize to homogeneous "Dirichlet" and "Neumann"-type problems.

4.1. Nonlocal Variational Problems and Volume-Constrained Problems.

Given an open region $\Omega \subset \mathbb{R}^n$ and the corresponding interaction domain $\Omega_{\mathcal{I}}$ as defined in (3.7), let $\Omega_{\mathcal{I}} = \Omega_{\mathcal{I}d} \cup \Omega_{\mathcal{I}n} \cup \Omega_{\mathcal{I}r}$ with $\Omega_{\mathcal{I}d}$, $\Omega_{\mathcal{I}n}$, and $\Omega_{\mathcal{I}r}$ mutually disjoint and with at most two empty. We then define the energy functional

$$\begin{aligned}
E(u; b, g_n, g_r) := {} & \frac{1}{2}\int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}} \mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) \cdot \big(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\cdot\mathcal{D}^*(u)(\mathbf{x},\mathbf{y})\big)\, d\mathbf{y}\, d\mathbf{x} \\
& + \frac{1}{2}\int_{\Omega_{\mathcal{I}r}} \varphi(\mathbf{x}) u^2(\mathbf{x})\, d\mathbf{x} \\
& - \int_{\Omega} b(\mathbf{x})u(\mathbf{x})\, d\mathbf{x} - \int_{\Omega_{\mathcal{I}n}} g_n(\mathbf{x})u(\mathbf{x})\, d\mathbf{x} - \int_{\Omega_{\mathcal{I}r}} g_r(\mathbf{x})u(\mathbf{x})\, d\mathbf{x} \\
= {} & \frac{1}{2}\int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}} \big(u(\mathbf{y})-u(\mathbf{x})\big)^2 \gamma(\mathbf{x},\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} + \frac{1}{2}\int_{\Omega_{\mathcal{I}r}} \varphi(\mathbf{x}) u^2(\mathbf{x})\, d\mathbf{x} \\
& - \int_{\Omega} b(\mathbf{x})u(\mathbf{x})\, d\mathbf{x} - \int_{\Omega_{\mathcal{I}n}} g_n(\mathbf{x})u(\mathbf{x})\, d\mathbf{x} - \int_{\Omega_{\mathcal{I}r}} g_r(\mathbf{x})u(\mathbf{x})\, d\mathbf{x},
\end{aligned}$$

where $\varphi(\mathbf{x}) > 0$, $b(\mathbf{x})$, $g_n(\mathbf{x})$, and $g_r(\mathbf{x})$ are given functions defined on $\Omega_{\mathcal{I}r}$, Ω, $\Omega_{\mathcal{I}n}$, and $\Omega_{\mathcal{I}r}$, respectively, and $\gamma(\mathbf{x},\mathbf{y}) = \boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) \cdot \big(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\big)$. Consider the constrained minimization problem

$$\min E(u; b, g_n, g_r) \quad \text{subject to} \quad E_c(u; g) = 0, \tag{4.1}$$

where $E_c(u;g)$ denotes a constraint functional. For example, let

$$E_c(u;g) = E_c^d(u;g_d) := \int_{\Omega_{\mathcal{I}d}} (u-g_d)^2\,d\mathbf{x} \qquad \text{if } \Omega_{\mathcal{I}d} \neq \emptyset, \tag{4.2}$$

where $g_d(\mathbf{x})$ is a given function defined on $\Omega_{\mathcal{I}d}$. Note that $E_c^d(u;g_d) = 0$ implies that $u(\mathbf{x}) = g_d(\mathbf{x})$ a.e. in $\Omega_{\mathcal{I}d}$, i.e., we have a "Dirichlet"-type condition applied over the interaction domain $\Omega_{\mathcal{I}d} \subseteq \Omega_{\mathcal{I}}$ having positive measure. On the other hand, if $\Omega_{\mathcal{I}d} \cup \Omega_{\mathcal{I}r} = \emptyset$, let

$$E_c(u;g) = E_c^n(u;c_n) := \Big(c_n - \int_{\Omega\cup\Omega_{\mathcal{I}}} u\,d\mathbf{x}\Big)^2 \qquad \text{when } \Omega_{\mathcal{I}n} = \Omega_{\mathcal{I}} \tag{4.3}$$

for a given constant c_n, so that $E_c^n(u;c_n) = 0$ implies that $\int_{\Omega\cup\Omega_{\mathcal{I}}} u\,d\mathbf{x} = c_n$. Proceeding formally with the use of standard techniques from the calculus of variations, we obtain the first-order necessary conditions corresponding to the minimization problem (4.1) given by

$$\begin{aligned} &\int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}} \mathcal{D}^*(u)(\mathbf{x},\mathbf{y}) \cdot \big(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\cdot\mathcal{D}^*(v)(\mathbf{x},\mathbf{y})\big)\,d\mathbf{y}\,d\mathbf{x} \\ &\qquad\qquad + \int_{\Omega_{\mathcal{I}r}} \varphi(\mathbf{x})u(\mathbf{x})v(\mathbf{x})\,d\mathbf{x} \\ &\qquad = \int_\Omega b(\mathbf{x})v(\mathbf{x})\,d\mathbf{x} + \int_{\Omega_{\mathcal{I}n}} g_n(\mathbf{x})v(\mathbf{x})\,d\mathbf{x} + \int_{\Omega_{\mathcal{I}r}} g_r(\mathbf{x})v(\mathbf{x})\,d\mathbf{x}, \end{aligned} \tag{4.4}$$

where test functions $v(\mathbf{x})$ satisfy the constraint $E_c(v;0) = 0$, e.g., for the case $E_c^d(v;0) = 0$, we have that $v = 0$ a.e. in $\Omega_{\mathcal{I}d}$. Note that if $\Omega_{\mathcal{I}} = \Omega_{\mathcal{I}n}$, i.e., if $\Omega_{\mathcal{I}d} \cup \Omega_{\mathcal{I}r} = \emptyset$, then by setting $v(\mathbf{x}) = 1$ in (4.4) we conclude that the data b and g_n are required to satisfy the compatibility condition

$$\int_\Omega b\,d\mathbf{x} + \int_{\Omega_{\mathcal{I}}} g_n\,d\mathbf{x} = 0 \qquad \text{when } \Omega_{\mathcal{I}} = \Omega_{\mathcal{I}n}. \tag{4.5}$$

By applying the nonlocal Green's first identity (3.10) to (4.4), we obtain, because $v(\mathbf{x}) = 0$ a.e. in $\Omega_{\mathcal{I}d}$,

$$\begin{aligned} \int_\Omega v\mathcal{D}(\boldsymbol{\Theta}\cdot\mathcal{D}^*u)\,d\mathbf{x} + \int_{\Omega_{\mathcal{I}r}} \varphi uv\,d\mathbf{x} - \int_{\Omega_{\mathcal{I}n}\cup\Omega_{\mathcal{I}r}} v\mathcal{N}(\boldsymbol{\Theta}\cdot\mathcal{D}^*u)\,d\mathbf{x} \\ = \int_\Omega bv\,d\mathbf{x} + \int_{\Omega_{\mathcal{I}n}} g_n v\,d\mathbf{x} + \int_{\Omega_{\mathcal{I}r}} g_r v\,d\mathbf{x}. \end{aligned}$$

Because $v(\mathbf{x})$ is arbitrary in $\Omega \cup \Omega_{\mathcal{I}n} \cup \Omega_{\mathcal{I}r}$, we then obtain that solutions of the minimization problem (4.1) satisfy[5]

$$-\mathcal{L}(u) = \mathcal{D}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^*u\big) = b \qquad \text{on } \Omega, \tag{4.6a}$$

$$-\mathcal{N}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^*u\big) = g_n \qquad \text{on } \Omega_{\mathcal{I}n}, \tag{4.6b}$$

$$-\mathcal{N}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^*u\big) + \varphi u = g_r \qquad \text{on } \Omega_{\mathcal{I}r}, \tag{4.6c}$$

$$u = g_d \qquad \text{on } \Omega_{\mathcal{I}d}, \tag{4.6d}$$

$$\int_{\Omega\cup\Omega_{\mathcal{I}}} u\,d\mathbf{x} = c_n \qquad \text{if } \Omega_{\mathcal{I}} = \Omega_{\mathcal{I}n}. \tag{4.6e}$$

[5]The correspondence between (2.8) and (4.6) is obvious. We only point out that the apparent sign differences between (2.8a)–(2.8c) and (4.6a)–(4.6c), respectively, result because $\mathcal{D}^*$ denotes the negative of a nonlocal gradient operator.

Because we have associated $\mathcal{N}(\cdot)$ with the nonlocal flux out of Ω into $\Omega_{\mathcal{I}}$, we refer to (4.6b) and (4.6c) as nonlocal "Neumann" and nonlocal "Robin" volume constraints, whereas, of course, (4.6d) is a nonlocal "Dirichlet" volume constraint. Thus, if $\Omega_{\mathcal{I}} = \Omega_{\mathcal{I}d}$, we have the nonlocal "Dirichlet" problem (4.6a) and (4.6d). If $\Omega_{\mathcal{I}} = \Omega_{\mathcal{I}r}$, we have the nonlocal "Robin" problem (4.6a) and (4.6c). If $\Omega_{\mathcal{I}} = \Omega_{\mathcal{I}n}$, we have the nonlocal "Neumann" problem (4.6a), (4.6b), and (4.6e);[6] in this case, the compatibility condition (4.5) on the data is needed to ensure the existence of a solution, whereas (4.6e) is a constraint that ensures the uniqueness of that solution. See [27] for a related discussion.

The two choices (4.2) and (4.3) for the constraint operator $E_c(u; g)$ in the variational principle (4.1), or, equivalently, (4.6d) and (4.6e) in the nonlocal volume-constrained problem (4.6), respectively, are *essential* to the variational principle (4.1), i.e., they must be imposed on candidate minimizers. On the other hand, (4.6b) and (4.6c) are *natural* to the variational principle (4.1), i.e., they do not have to be imposed on candidate minimizers. Also, note that the constraints $E_c^d(\cdot;\cdot)$ and $E_c^n(\cdot;\cdot)$ are quite different; $E_c^d(u; 0)$ involves the interaction domain $\Omega_{\mathcal{I}}$ and *the integral of the square of* u over that domain, whereas $E_c^n(u; 0)$ involves the *square of the integral of* u over the domain $\Omega \cup \Omega_{\mathcal{I}}$. This leads to distinct forms for the constraints appearing in the nonlocal volume-constrained problem (4.6); the constraint (4.6d) holds pointwise almost everywhere in the subdomain $\Omega_{\mathcal{I}d}$, whereas (4.6e) is a single integral constraint.

Equations (4.2) and (4.3) may not be the only choices for $E_c(u; g)$. Here, in general, we only assume that $E_c(\cdot; 0)$ denotes a bounded, quadratic functional on a Hilbert space which is defined in section 4.3.

In what follows, for the sake of brevity, we at times confine the discussion to the homogeneous nonlocal "Dirichlet" problem

$$\mathcal{D}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^* u\big) = b \quad \text{on } \Omega, \tag{4.7a}$$

$$u = 0 \quad \text{on } \Omega_{\mathcal{I}} \tag{4.7b}$$

and the homogeneous nonlocal "Neumann" problem

$$\mathcal{D}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^* u\big) = b \quad \text{on } \Omega, \tag{4.8a}$$

$$\mathcal{N}\big(\boldsymbol{\Theta}\cdot\mathcal{D}^* u\big) = 0 \quad \text{on } \Omega_{\mathcal{I}}, \tag{4.8b}$$

$$\int_{\Omega\cup\Omega_{\mathcal{I}}} u\, d\mathbf{x} = 0. \tag{4.8c}$$

4.2. 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 $\Omega_{\mathcal{I}}$ and $\Omega \cup \Omega_{\mathcal{I}}$ have the same properties.

Given positive constants γ_0 and ε, we first assume that the symmetric kernel γ satisfies, for all $\mathbf{x} \in \Omega \cup \Omega_{\mathcal{I}}$,

$$\gamma(\mathbf{x}, \mathbf{y}) \geq 0 \quad \forall\, \mathbf{y} \in B_\varepsilon(\mathbf{x}) \quad \text{with} \quad \gamma(\mathbf{x}, \mathbf{y}) \geq \gamma_0 > 0 \quad \forall\, \mathbf{y} \in B_{\varepsilon/2}(\mathbf{x}), \tag{4.9a}$$

$$\gamma(\mathbf{x}, \mathbf{y}) = 0 \quad \forall\, \mathbf{y} \in (\Omega \cup \Omega_{\mathcal{I}}) \setminus B_\varepsilon(\mathbf{x}), \tag{4.9b}$$

where $B_\varepsilon(\mathbf{x}) := \{\mathbf{y} \in \Omega \cup \Omega_{\mathcal{I}} \colon |\mathbf{y} - \mathbf{x}| \leq \varepsilon\}$. Obviously, (4.9) implies that although interactions are nonlocal, they are limited to a ball of radius ε.

[6] This is equivalent to the approach taken in [4, Chap. 3], where the constraint $\int_{\mathbb{R}^n\setminus\Omega}\big(u(\mathbf{y}) - u(\mathbf{x})\big)\gamma(\mathbf{x}, \mathbf{y})\, d\mathbf{y} = 0$ is prescribed for the problem $\int_{\mathbb{R}^n}\big(u(\mathbf{y}) - u(\mathbf{x})\big)\gamma(\mathbf{x}, \mathbf{y})\, d\mathbf{y} = b$ for $\mathbf{x} \in \Omega$.

The smoothing effected by the inversion of $-\mathcal{L} = \mathcal{D}\big(\boldsymbol{\Theta}\,\mathcal{D}^*(\cdot)\big)$ depends upon the regularity associated with $\gamma = \boldsymbol{\alpha}\cdot(\boldsymbol{\Theta}\cdot\boldsymbol{\alpha})$. We consider the following two special cases.

Case 1. There exist $s \in (0,1)$ and positive constants γ_* and γ^* such that, for all $\mathbf{x} \in \Omega$,

$$\frac{\gamma_*}{|\mathbf{y}-\mathbf{x}|^{n+2s}} \le \gamma(\mathbf{x},\mathbf{y}) \le \frac{\gamma^*}{|\mathbf{y}-\mathbf{x}|^{n+2s}} \qquad \text{for } \mathbf{y} \in B_\varepsilon(\mathbf{x}). \tag{4.10}$$

An example for this case is given by the kernel in (A.2) or, more generally, by

$$\gamma(\mathbf{x},\mathbf{y}) = \frac{\sigma(\mathbf{x},\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^{n+2s}} \tag{4.11}$$

with $\sigma(\mathbf{x},\mathbf{y})$ bounded from above and below by positive constants; in particular, if σ is not a radial function, i.e., if $\sigma(\mathbf{x},\mathbf{y}) \ne \sigma(|\mathbf{x}-\mathbf{y}|)$, then (4.11) can account for inhomogeneous media properties.

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

$$\gamma_1 \le \int_{(\Omega\cup\Omega_{\mathcal{I}})\cap B_\varepsilon^{\mathbf{x}}} \gamma(\mathbf{x},\mathbf{y})\,d\mathbf{y} \qquad \forall\, \mathbf{x} \in \Omega, \tag{4.12a}$$

$$\int_{\Omega\cup\Omega_{\mathcal{I}}} \gamma^2(\mathbf{x},\mathbf{y})\,d\mathbf{y} \le \gamma_2^2 \qquad \forall\, \mathbf{x} \in \Omega. \tag{4.12b}$$

Examples for this case are provided by the kernels used in [2, 3, 4].

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

4.3. Equivalence of Spaces. For the sake of brevity, in the remainder of this section we consider only the homogeneous nonlocal "Dirichlet" and "Neumann" problems (4.7) and (4.8), respectively.

We define the nonlocal energy norm, nonlocal energy space, and nonlocal volume-constrained energy space by

$$\begin{aligned} |||u||| &:= \big(E(u;0,0,0)\big)^{1/2} \\ &= \left(\frac{1}{2}\int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}} \mathcal{D}^*(u)(\mathbf{x},\mathbf{y})\cdot\big(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\cdot\mathcal{D}^*(u)(\mathbf{x},\mathbf{y})\big)\,d\mathbf{y}\,d\mathbf{x}\right)^{1/2}, \end{aligned} \tag{4.13a}$$

$$V(\Omega\cup\Omega_{\mathcal{I}}) := \big\{u \in L^2(\Omega\cup\Omega_{\mathcal{I}}) \;:\; |||u||| < \infty\big\}, \tag{4.13b}$$

$$V_c(\Omega\cup\Omega_{\mathcal{I}}) := \{u \in V(\Omega\cup\Omega_{\mathcal{I}}) \;:\; E_c(u;0) = 0\}, \tag{4.13c}$$

respectively, where the constraint equation $E_c(u;0)=0$ is given by (4.7b) and (4.8c) for the nonlocal "Dirichlet" and "Neumann" problems, respectively, and where we have used the fact that $\Omega_{\mathcal{I}r} = \emptyset$ for both (4.7) and (4.8). We also define $|||u|||_{V_c^*(\Omega\cup\Omega_{\mathcal{I}})}$ to be the norm for the dual space $V_c^*(\Omega\cup\Omega_{\mathcal{I}})$ of $V_c(\Omega\cup\Omega_{\mathcal{I}})$ with respect to the standard $L^2(\Omega\cup\Omega_{\mathcal{I}})$ duality pairing.

The precise assumptions made about the constraint functional are that $E_c(\cdot;0)$ is a bounded, quadratic functional on $V(\Omega\cup\Omega_{\mathcal{I}})\cap L^2(\Omega\cup\Omega_{\mathcal{I}})$, that for some constant $\widehat{c}$

$$E_c(u;0) \le \widehat{c}\,\big(|||u|||^2 + \|u\|^2_{L^2(\Omega\cup\Omega_{\mathcal{I}})}\big) \qquad \forall\, u \in V(\Omega\cup\Omega_{\mathcal{I}}). \tag{4.14}$$

Moreover, we assume that the intersection of the set of constant-valued functions with the set of functions satisfying $E_c(u;0)=0$ is $u\equiv 0$. Clearly, $E_c(u;g)$ as defined by either (4.2) or (4.3) satisfies these assumptions.

We now proceed to show that for Case 1, the nonlocal energy space $V(\Omega\cup\Omega_{\mathcal{I}})$ is equivalent to the fractional-order Sobolev space $H^s(\Omega\cup\Omega_{\mathcal{I}})$, whereas for Case 2, the nonlocal energy space is equivalent to $L^2(\Omega\cup\Omega_{\mathcal{I}})$. These equivalences imply that the quotient space $V_c(\Omega\cup\Omega_{\mathcal{I}})$ is a Hilbert space equipped with the norm $|||u|||$. As a result, the nonlocal volume-constrained problems (4.7) and (4.8) are well posed; see section 4.4.

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

$$H^s(\Omega\cup\Omega_{\mathcal{I}}) := \left\{u\in L^2(\Omega\cup\Omega_{\mathcal{I}}) : \|u\|_{L^2(\Omega\cup\Omega_{\mathcal{I}})} + |u|_{H^s(\Omega\cup\Omega_{\mathcal{I}})} < \infty\right\}, \tag{4.15}$$

where

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

Moreover, define the subspaces

$$H^s_c(\Omega\cup\Omega_{\mathcal{I}}) := \{u\in H^s(\Omega\cup\Omega_{\mathcal{I}}) \ : \ E_c(u;0)=0\} \tag{4.16}$$

and

$$L^2_c(\Omega\cup\Omega_{\mathcal{I}}) := \left\{u\in L^2(\Omega\cup\Omega_{\mathcal{I}}) \ : \ E_c(u;0)=0\right\}. \tag{4.17}$$

4.3.1. Case 1. The following two lemmas are used to demonstrate that, for this case, the spaces $V_c(\Omega\cup\Omega_{\mathcal{I}})$ and $H^s_c(\Omega\cup\Omega_{\mathcal{I}})$ are continuously embedded within each other.

LEMMA 4.1. *Let the function* γ *satisfy* (4.9) *and the lower bound of* (4.10). *Then*

$$|u|^2_{H^s(\Omega\cup\Omega_{\mathcal{I}})} \le \gamma_*^{-1}|||u|||^2 + 4|\Omega\cup\Omega_{\mathcal{I}}|\varepsilon^{-(n+2s)}\|u\|^2_{L^2(\Omega\cup\Omega_{\mathcal{I}})}.$$

Proof. We have

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

LEMMA 4.2. *Let the function* γ *satisfy* (4.9) *and the upper bound of* (4.10). *Then*

$$|||u|||^2 \le \gamma^*|u|^2_{H^s(\Omega\cup\Omega_{\mathcal{I}})}.$$

Proof. The result follows directly from

$$\int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}} \mathcal{D}^*u\cdot\big(\boldsymbol{\Theta}(\mathbf{x},\mathbf{y})\cdot\mathcal{D}^*u\big)\, d\mathbf{y}\, d\mathbf{x} \le \gamma^*\int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}} \frac{\big(u(\mathbf{y})-u(\mathbf{x})\big)^2}{|\mathbf{y}-\mathbf{x}|^{n+2s}}\, d\mathbf{y} d\mathbf{x}. \qquad \square$$

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 $H^s(\Omega \cup \Omega_{\mathcal{I}})$ into $L^2(\Omega \cup \Omega_{\mathcal{I}})$.

LEMMA 4.3 (nonlocal Poincaré inequality I). *Let the function γ satisfy* (4.9) *and* (4.10). *Then there exists a positive constant C such that*

$$\|u\|^2_{L^2(\Omega\cup\Omega_{\mathcal{I}})} \le C|||u|||^2 \qquad \forall\, u \in V_c(\Omega \cup \Omega_{\mathcal{I}}). \tag{4.18}$$

Proof. We exploit the standard technique for establishing a Poincaré-type inequality by implying a contradiction. Assume there exists a sequence $\{u_k \in V_c(\Omega \cup \Omega_{\mathcal{I}})\}$ where $\|u_k\|^2_{L^2(\Omega\cup\Omega_{\mathcal{I}})} = 1$ for all k such that $1 > k\,|||u_k|||$. By Lemma 4.1, we have

$$\|u_k\|^2_{H^s(\Omega\cup\Omega_{\mathcal{I}})} < 4|\Omega \cup \Omega_{\mathcal{I}}|\varepsilon^{-(n+2s)} + 1$$

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

$$\|\widetilde{u}\|_{L^2(\Omega\cup\Omega_{\mathcal{I}})} = 1. \tag{4.19}$$

By Lemma 4.2, we have that, for any $v \in H^s(\Omega \cup \Omega_{\mathcal{I}})$, v also belongs to $V(\Omega \cup \Omega_{\mathcal{I}})$. By Fatou's lemma on the convergence of integrals of function sequences that are convergent almost everywhere,

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

because $1 > k\,|||u_k|||$. The definition of $|||\cdot|||$ implies that $\widetilde{u}$ is a constant. Moreover, we have the convergence of u_{k_j} to $\widetilde{u}$ with respect to the norm $\big(|||u|||^2 + \|u\|^2_{L^2(\Omega\cup\Omega_{\mathcal{I}})}\big)^{1/2}$ and, by the continuity assumption on E_c, we obtain that

$$E_c(\widetilde{u}; 0) = \lim_{k_j\to\infty} E_c(u_{k_j}; 0) = 0,$$

so that $\widetilde{u} = 0$. However, this contradicts (4.19), so that the conclusion (4.18) now follows. ∎

Lemmas 4.1–4.3 lead to the following result.

THEOREM 4.4. *If the function γ satisfies* (4.9) *and* (4.10), *then*

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

where C_* is a positive constant satisfying $C_*^{-2} = \max\big(\gamma_*^{-1}, C(1+4|\Omega \cup \Omega_{\mathcal{I}}|\varepsilon^{-(n+2s)})\big)$ and $C^* = \gamma^*$.

Proof. Lemmas 4.1 and 4.3 imply that

$$\|u\|^2_{H^s(\Omega\cup\Omega_{\mathcal{I}})} \le \gamma_*^{-1}|||u|||^2 + \big(1 + 4|\Omega \cup \Omega_{\mathcal{I}}|\varepsilon^{-(n+2s)}\big)\|u\|^2_{L^2(\Omega\cup\Omega_{\mathcal{I}})} \le C_*^{-1}\,|||u|||^2.$$

In a similar fashion, Lemmas 4.2 and 4.3 lead to

$$|||u||| \le \gamma^*|u|^2_{H^s(\Omega\cup\Omega_{\mathcal{I}})} \le \gamma^*\big(|u|^2_{H^s(\Omega\cup\Omega_{\mathcal{I}})} + \|u\|^2_{L^2(\Omega\cup\Omega_{\mathcal{I}})}\big) = C^*\|u\|_{H^s(\Omega\cup\Omega_{\mathcal{I}})}. \qquad ∎$$

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

COROLLARY 4.5. *If the function γ satisfies* (4.9) *and* (4.10), *we then have the equivalence of the constrained spaces $H^s_c(\Omega \cup \Omega_{\mathcal{I}})$ and $V_c(\Omega \cup \Omega_{\mathcal{I}})$.*

This theorem and corollary explain that if the function γ satisfies (4.9) and (4.10), then $V(\Omega \cup \Omega_{\mathcal{I}})$ and its constrained subspace $V_c(\Omega \cup \Omega_{\mathcal{I}})$ are compactly embedded in $L^2(\Omega \cup \Omega_{\mathcal{I}})$ and $L^2_c(\Omega \cup \Omega_{\mathcal{I}})$, respectively.

We note that the equivalence of spaces 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 in the literature for such cases. The volume-constrained problem (1.2b), however, is well posed for any $s \in (0,1)$, as is demonstrated in section 4.4.

4.3.2. Case 2. We now demonstrate that, in this case, the constrained space $V_c(\Omega \cup \Omega_{\mathcal{I}}) = L^2_c(\Omega \cup \Omega_{\mathcal{I}})$. We choose to work with the more stringent conditions given in (4.12) rather than other more general assumptions. This allows us to apply well-known results about integral operators. See [2, 4] for the case in which γ is radial and only $L^1(\Omega \cup \Omega_{\mathcal{I}})$ integrable.

We state the analogue of Lemma 4.2 that can be established through direct calculation; see, e.g., [35, 51] for details.

LEMMA 4.6. *If the function γ satisfies* (4.9) *and* (4.12)*, then*

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

for some positive constant C_2.

Next, we present a second nonlocal Poincaré inequality that relies, in contrast to the hypotheses of Lemma 4.3, on the compactness of a Hilbert–Schmidt kernel; see, e.g., [8, Chap. 12].

LEMMA 4.7 (nonlocal Poincaré inequality II). *If the function γ satisfies* (4.9) *and* (4.12)*, then*

$$C_1 \|u\|_{L^2(\Omega \cup \Omega_{\mathcal{I}})} \le |||u||| \quad \forall\, u \in V_c(\Omega \cup \Omega_{\mathcal{I}})$$

for some positive constant C_1.

Proof. Because

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

we see that the hypotheses on the function γ imply that the nonlocal diffusion operator $-\mathcal{L} = \mathcal{D}(\boldsymbol{\Theta}\, \mathcal{D}^*)$ is a self-adjoint operator on $L^2_c(\Omega \cup \Omega_{\mathcal{I}})$. As established at the end of section 3.2, $-\mathcal{L}$ is a nonnegative 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 $L^2_c(\Omega \cup \Omega_{\mathcal{I}})$ contains only the zero element. Therefore,

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

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

$$\sqrt{\lambda_1}\, \|u\|_{L^2(\Omega \cup \Omega_{\mathcal{I}})} \le |||u||| \quad \forall\, u \in L^2_c(\Omega \cup \Omega_{\mathcal{I}}).$$

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

The following result is an immediate consequence of Lemmas 4.6 and 4.7.

COROLLARY 4.8. *If the function γ satisfies* (4.9) *and* (4.12)*, then $V_c(\Omega \cup \Omega_{\mathcal{I}})$ is equivalent to $L^2_c(\Omega \cup \Omega_{\mathcal{I}})$.*

4.4. Well-Posedness of Nonlocal Volume-Constrained Problems. Sections 4.3.1 and 4.3.2 established that the nonlocal constrained energy space $V_c(\Omega \cup \Omega_{\mathcal{I}})$ is equivalent to $H^s_c(\Omega \cup \Omega_{\mathcal{I}})$ and $L^2_c(\Omega \cup \Omega_{\mathcal{I}})$ for Case 1 and Case 2, respectively. The following result demonstrates that the minimization problem (4.1) has a unique minimizer if the constraint functional $E_c(u; 0)$ satisfies the general requirement (4.14).

THEOREM 4.9. *The nonlocal variational problem of minimizing $E(u; b, 0, 0)$ over $V_c(\Omega \cup \Omega_{\mathcal{I}})$ has a unique solution u for any $b \in V_c^*(\Omega \cup \Omega_{\mathcal{I}})$. Moreover, the Euler–Lagrange equation is given by* (4.7) *for $E_c(u; g) = E^d_c(u; 0)$ and* (4.8) *for $E_c(u; g) = E^n_c(u; 0)$. Furthermore, there exists a constant $C > 0$, independent of b, such that*

$$|||u||| \le C\|b\|_{V_c^*(\Omega \cup \Omega_{\mathcal{I}})}. \tag{4.20}$$

Proof. The theorem is established via a direct application of the Lax–Milgram theorem; see, e.g., [8, sec. 3.6]. ∎

The upper bounds in (4.10) and (4.12b) are not needed to prove Theorem 4.9, i.e., to show well-posedness with respect to space $V_c(\Omega \cup \Omega_{\mathcal{I}})$ and the nonlocal energy norm $|||\cdot|||$. However, those bounds are needed to show the equivalence of that norm to standard Sobolev norms and so establish well-posedness with respect to standard Sobolev spaces.

In section 4.3, we established the equivalence of the nonlocal constrained energy space $V_c(\Omega \cup \Omega_{\mathcal{I}})$ to $H^s_c(\Omega \cup \Omega_{\mathcal{I}})$ or $L^2_c(\Omega \cup \Omega_{\mathcal{I}})$ for Case 1 and Case 2, respectively. Thus, for problems for which the function γ satisfies the assumptions of Case 1 or Case 2, the estimate (4.20) implies that

$$\|u\|_{H^s(\Omega \cup \Omega_{\mathcal{I}})} \le C\|b\|_{H^{-s}(\Omega \cup \Omega_{\mathcal{I}})} \quad \text{for } 0 < s < 1 \quad \text{or} \tag{4.21a}$$

$$\|u\|_{L^2(\Omega \cup \Omega_{\mathcal{I}})} \le C\|b\|_{L^2(\Omega \cup \Omega_{\mathcal{I}})} \tag{4.21b}$$

hold, respectively. These should be contrasted with the analogous result for, e.g., (1.3b) with homogeneous Dirichlet boundary conditions, for which we have

$$\|u\|_{H^1_0(\Omega)} \le C\|b\|_{H^{-1}(\Omega)}. \tag{4.22}$$

The inequalities (4.21a) and (4.21b) show that a gain in regularity of $2s$ and 0, respectively, occurs for Case 1 and Case 2, respectively. In contrast, the inequality (4.22) results in a gain in regularity of 2. In other words, solutions of the nonlocal volume-constrained problems have at most $2s$ more derivatives than the data b, whereas solutions of the boundary-value problem (1.3b) can have two more derivatives. These regularity conditions are analogous to those established in [51] for restricted classes of one- and two-dimensional peridynamic models with constraints suggestive of nonlocal volume-constrained conditions.

5. Additional Comments about Nonlocal Volume-Constrained Problems.

In this section, we briefly discuss the well-posedness of nonlocal evolution problems, vanishing nonlocality, and nonlocal advection-diffusion problems.

5.1. Well-Posedness for Nonlocal Evolution Equations. Using the results about nonlocal operators and variational problems established in this paper, we may use standard techniques to establish well-posedness for nonlocal evolution equations such as the diffusion equation (1.2a) and the nonlocal wave equation (B.2). As an illustration, we consider the special case for which the constrained energy space $V_c(\Omega \cup \Omega_{\mathcal{I}})$ associated with the functional (4.2) is established to be a Hilbert space with its dual space $V_c^*(\Omega \cup \Omega_{\mathcal{I}})$ and where the operator $\mathcal{D}\big(\mathbf{\Theta} \cdot \mathcal{D}^*\big)$ is bounded and coercive in $V_c(\Omega \cup \Omega_{\mathcal{I}})$. For that case, we have the following result.

THEOREM 5.1. *Assume that* $b \in L^2(0, T; V_c^*(\Omega))$ *and* $u_0 \in V_c(\Omega)$*; then the initial volume-constrained problem* (1.2a) *has a unique solution* $u \in C(0, T; V_c(\Omega \cup \Omega_{\mathcal{I}})) \cap H^1(0, T; V_c^*(\Omega \cup \Omega_{\mathcal{I}}))$. *Moreover, assume instead that* $b \in L^2(0, T; V_c^*(\Omega))$ *with* $u_0 \in V_c(\Omega)$ *and* $u_1 \in L^2(\Omega)$*; then the initial volume-constrained problem* (B.2) *has a unique solution* $u \in L^2(0, T; V_c(\Omega \cup \Omega_{\mathcal{I}})) \cap L^2(0, T; L^2(\Omega \cup \Omega_{\mathcal{I}})) \cap H^1(0, T; V_c^*(\Omega \cup \Omega_{\mathcal{I}}))$.

These results are consequences of standard semigroup theory or Galerkin-type arguments. We refer the reader to [51] for more detailed proofs of these results in a special case for which the techniques used are directly generalizable to the problems considered here.

5.2. Vanishing Nonlocality. The local limit of the operator $\mathcal{L} = -\mathcal{D}(\mathbf{\Theta} \cdot \mathcal{D}^*)$ was examined in [27]. It was demonstrated that the free-space operator, i.e., $\mathcal{L}$ with $\Omega = \mathbb{R}^n$, converges to $-\nabla \cdot (\mathbf{C} \cdot \nabla)$ as $\varepsilon \to 0$ under suitable conditions on the kernel function. More recently, in [4, 28], for kernel functions of radial type $\gamma(\mathbf{x}, \mathbf{y}) = \gamma(|\mathbf{x} - \mathbf{y}|)$ with γ an element of $L^1(\Omega \cup \Omega_{\mathcal{I}})$ satisfying (4.9), the local limit of the nonlocal diffusion equation has been studied. Further, in [28], finite element solutions for nonlocal diffusion and the peridynamic model are also investigated.

As an example of a local limit, let Ω denote a bounded domain independent of ε and $\mathbf{C} := \lim_{\varepsilon \to 0} \mathbf{C}_\varepsilon$, where

$$(\mathbf{C}_\varepsilon)_{ij} = \int_{B_\varepsilon(0)} \gamma(|\mathbf{z}|)\, z_i z_j \, d\mathbf{z} \quad \text{for} \quad i, j = 1, 2, \ldots, n.$$

Then, recalling that γ satisfies (4.9) so that $\gamma(|\mathbf{z}|) = 0$ for $|\mathbf{z}| > \varepsilon$, a particular consequence of the results in [28] is

$$\begin{aligned} &\lim_{\varepsilon \to 0} \int_{\Omega \cup \Omega_{\mathcal{I}}} \int_{\Omega \cup \Omega_{\mathcal{I}}} \mathcal{D}^* v \cdot \big(\mathbf{\Theta} \cdot \mathcal{D}^* u\big)\, d\mathbf{y}\, d\mathbf{x} \\ &\quad = \lim_{\varepsilon \to 0} \int_{\Omega \cup \Omega_{\mathcal{I}}} \int_{\Omega \cup \Omega_{\mathcal{I}}} \big(u(\mathbf{y}) - u(\mathbf{x})\big)\big(v(\mathbf{y}) - v(\mathbf{x})\big) \gamma(|\mathbf{x} - \mathbf{y}|)\, d\mathbf{y}\, d\mathbf{x} \\ &\quad = \int_\Omega \nabla v \cdot \big(\mathbf{C} \cdot \nabla u\big)\, d\mathbf{x} \end{aligned} \tag{5.1}$$

for any $u, v \in H^1(\Omega \cup \Omega_{\mathcal{I}})$ with support in Ω. A more general form of the above limit was given in [28] for piecewise smooth functions with respect to a triangulation of the domain that was used to examine the limiting properties of finite element approximations and the corresponding error estimators.

By setting $u = v$, we see from (5.1) that

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

This establishes the relationship between the nonlocal norms and the standard local Sobolev space norms in the local limit. Moreover, it has also been shown in [51] that, albeit for special nonlocal boundary conditions, the solutions of nonlocal diffusion equations converge, in such a limit, to the solution of the local diffusion equation in suitable spaces. This result relies on a key estimate showing that when $\mathbf{\Theta}$ is positive definite, the smallest eigenvalue of the nonlocal diffusion operator $\mathcal{D}(\mathbf{\Theta}\cdot\mathcal{D}^*)$ 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 [51]. When such a property holds for more general volume-constrained problems considered here, we may also see that the solutions u_ε of (4.4) converge, at least weakly in $L^2(\Omega\cup\Omega_{\mathcal{I}})$, to the unique weak solution u of (2.8) 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 obtain

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

One may draw analogies between the above results and 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

$$\lim_{m\to\infty}\int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}}\frac{\big(u(\mathbf{x})-u(\mathbf{y})\big)^2}{|\mathbf{y}-\mathbf{x}|^2}\rho_m(|\mathbf{y}-\mathbf{x}|)\,d\mathbf{y}\,d\mathbf{x}\propto|u|_{H^1(\Omega)}$$

for a sequence of radial mollifiers $\{\rho_m\}$. In particular, in [7], it is demonstrated that the norm induced by $\int_{\Omega\cup\Omega_{\mathcal{I}}}\int_{\Omega\cup\Omega_{\mathcal{I}}}\frac{(u(\mathbf{x})-u(\mathbf{y}))^2}{|\mathbf{y}-\mathbf{x}|^2}\rho_m(|\mathbf{y}-\mathbf{x}|)\,d\mathbf{y}\,d\mathbf{x}$ 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.

5.3. Nonlocal Advection-Diffusion Problems. Nonlocal advection-diffusion problems can be defined from (3.12) by letting $\boldsymbol{\nu}$ account for an advective flux in addition to a diffusive flux. To this end, we now set, for a given symmetric vector function $\boldsymbol{\mu}(\mathbf{x},\mathbf{y})$,[7]

$$\begin{aligned}\boldsymbol{\nu}(\mathbf{x},\mathbf{y})&=\mathbf{\Theta}(\mathbf{x},\mathbf{y})\cdot\mathcal{D}^*(u)(\mathbf{x},\mathbf{y})+\frac{u(\mathbf{x})+u(\mathbf{y})}{2}\boldsymbol{\mu}(\mathbf{x},\mathbf{y})\\&=-\big(u(\mathbf{y})-u(\mathbf{x})\big)\mathbf{\Theta}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})+\frac{u(\mathbf{x})+u(\mathbf{y})}{2}\boldsymbol{\mu}(\mathbf{x},\mathbf{y}).\end{aligned}\tag{5.2}$$

The term $\frac{1}{2}\big(u(\mathbf{x})+u(\mathbf{y})\big)\boldsymbol{\mu}$ is used to model a nonlocal convective flux (see [29]) and is analogous to the use of $u(\mathbf{x})\mathbf{v}(\mathbf{x})$ as a model for the conventional local advective flux. Substitution of (5.2) into (3.13) results in the *nonlocal advection-diffusion equation*

$$u_t+\mathcal{D}\big(\mathbf{\Theta}\cdot\mathcal{D}^*u\big)+\frac{1}{2}\mathcal{D}(\boldsymbol{\mu}u)=b\qquad\forall\,\mathbf{x}\in\Omega,\ t>0.\tag{5.3}$$

We have that, using the symmetry of $\boldsymbol{\mu}$,

$$\begin{aligned}\mathcal{D}(\boldsymbol{\mu}u)(\mathbf{x})&=\int_{\mathbb{R}^n}\big(u(\mathbf{x})+u(\mathbf{y})\big)\boldsymbol{\mu}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,d\mathbf{y}\\&=u(\mathbf{x})\int_{\mathbb{R}^n}\big(\boldsymbol{\mu}(\mathbf{x},\mathbf{y})+\boldsymbol{\mu}(\mathbf{y},\mathbf{x})\big)\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,d\mathbf{y}\\&\qquad+\int_{\mathbb{R}^n}\big(u(\mathbf{y})-u(\mathbf{x})\big)\boldsymbol{\mu}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\,d\mathbf{y},\end{aligned}$$

[7] We again suppress explicit reference to dependences on t.

so that

$$\mathcal{D}(\boldsymbol{\mu}u) = u\mathcal{D}(\boldsymbol{\mu}) - \int_{\mathbb{R}^n} \boldsymbol{\mu}\cdot\mathcal{D}^*(u)\,d\mathbf{y},$$

which is the nonlocal analogue of the local product formula $\nabla\cdot(u\mathbf{v}) = u\nabla\cdot\mathbf{v}+\mathbf{v}\cdot\nabla u$. Selecting the special kernel $\alpha(\mathbf{x},\mathbf{y}) = -\nabla_{\mathbf{y}}\delta(\mathbf{y}-\mathbf{x})$ results in

$$\mathcal{D}(\boldsymbol{\mu}u)(\mathbf{x}) = \nabla\cdot\big(u(\mathbf{x})\boldsymbol{\mu}(\mathbf{x},\mathbf{x})\big),$$

i.e., in conventional advection, so that the nonlocal product rule is equivalent to the conventional product rule in a distributional sense.

The one-dimensional case of a nonlinear advective conservation law is the subject of [29] and nonlocal convection-diffusion is investigated in [36].

6. Finite-Dimensional Approximations.

Given the variational formulation (4.1) of the nonlocal volume-constrained problem (1.2b), one may naturally consider its finite-dimensional approximations within that variational framework. Here, for both Case 1 and Case 2, we establish a priori error and condition number estimates for finite-dimensional approximations of the nonlocal volume-constrained problem (1.2b). These results are analogous to those established in [51] for a restricted class of one- and two-dimensional volume-constrained problems associated with linear peridynamic models.

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

$$|||v-v_N|||\to 0 \quad \text{as} \quad N\to\infty. \tag{6.1}$$

Throughout the remainder of this section, we let $u\in V_c(\Omega\cup\Omega_{\mathcal{I}})$ denote the solution of the variational problem (4.1) posed on $V_c(\Omega\cup\Omega_{\mathcal{I}})$, or equivalently, of (4.4). We seek the Ritz–Galerkin approximation $u_N\in V_c^N$ of u determined by posing the variational problem (4.1) on $V_c^N\subset V_c(\Omega\cup\Omega_{\mathcal{I}})$; this approximation falls within the class of "internal" (see [9, p. 86]) or "conforming" approximations.

For the sake of brevity, throughout this section we again confine the discussion to the homogeneous nonlocal "Dirichlet" and "Neumann" problems (4.7) and (4.8), respectively.

6.1. Convergence and Error Estimates.

We first state an abstract convergence result that gives the best approximation property of the finite-dimensional Ritz–Galerkin solution.

THEOREM 6.1. *If the function γ satisfies* (4.9) *and either* (4.10) *or* (4.12)*, then, for any $b\in V_c^*(\Omega)$, we have*

$$|||u-u_N|||\le \min_{v_N\in V_c^N}|||u-v_N|||\to 0 \quad \text{as } N\to\infty. \tag{6.2}$$

Proof. Standard variational arguments show that the Ritz–Galerkin approximation u_N is the best approximation to u in V_c^N with respect to the energy norm. This, together with (6.1), gives the result of the theorem. ∎

We now consider a concrete example of finite-dimensional approximations, namely, finite element approximations for the case that both $\Omega\cup\Omega_{\mathcal{I}}$ and Ω are polyhedral domains. For a given triangulation of $\Omega\cup\Omega_{\mathcal{I}}$ that simultaneously triangulates Ω, we let

V_c^N consist of those functions in $V_c(\Omega \cup \Omega_{\mathcal{I}})$ 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 quasi-uniform [18] as $h \to 0$, i.e., as N, the dimension of the approximation space V_c^N, goes to ∞; here h denotes the diameter of the largest element in the triangulation. Note that generally N is of order h^{-n} for small h. If the exact solution u is sufficiently smooth, we have the following result.

THEOREM 6.2. *Let m be a nonnegative integer and $0 < s < 1$.*

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

$$\|u - u_n\|_{H^s(\Omega\cup\Omega_{\mathcal{I}})} \leq Ch^{m+t-s}\|u\|_{H^{m+t}(\Omega\cup\Omega_{\mathcal{I}})}. \tag{6.3a}$$

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

$$\|u - u_n\|_{L^2(\Omega\cup\Omega_{\mathcal{I}})} \leq Ch^{m+t}\|u\|_{H^{m+t}(\Omega\cup\Omega_{\mathcal{I}})}. \tag{6.3b}$$

Proof. The proof follows similar derivations as given in [51] for a linear peridynamic model. We thus omit the details except for stating that, by Theorem 6.1 and the norm equivalence established by Corollaries 4.5 and 4.8, the error estimates (6.3a) and (6.3b) follow from standard approximation properties in Sobolev spaces [9, 18]. ∎

In particular, second-order convergence with respect to the L^2 norm can be expected for linear elements and for Case 2 when $m = 1$ and $t = 1$. The same order can also be established via a standard duality argument for Case 1 if the H^{2s} regularity holds for problems (4.7) and (4.8) with data b in L^2; see [51] for an illustration.

It is important to note that for Case 1 with $s < 1/2$ and for Case 2, *discontinuous* (across element boundaries) finite element spaces are conforming. This should be contrasted with discontinuous Galerkin methods for second-order elliptic partial differential equations that 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 $s < 1/2$.

6.2. Condition Number Estimates. For finite element approximations of the nonlocal operator $\mathcal{L}$ using basis functions $\{\phi_i\}_{i=1}^N$, consider the nonlocal $N \times N$ stiffness matrix $\mathbf{K}$, where the entries K_{ij} are defined by

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

The condition number of the stiffness matrix is an indicator of the sensitivity of the discrete solution with respect to 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 the inverse of $-\mathcal{L}$ smooths the data.

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

$$c_1 h^n \sum_{i=1}^N u_i^2 \leq \Big\| \sum_{i=1}^N u_N \phi_i \Big\|^2_{L^2(\Omega\cup\Omega_{\mathcal{I}})} \leq c_2 h^n \sum_{i=1}^n u_i^2$$

holds for any $u_h = \sum_{i=1}^N u_i\phi_i \in V_c^N$. We then have the following condition number estimates.

THEOREM 6.3. *For the nonlocal stiffness matrix* $\mathbf{K}$*, we have, for* h *small:*

(a) Case 1. *If* γ *satisfies* (4.9) *and* (4.10)*, then for some generic constant* $c > 0$*,*

$$\text{cond}(\mathbf{K}) \le ch^{-2s}. \tag{6.4a}$$

(b) Case 2. *If* γ *satisfies* (4.9) *and* (4.12)*, then for some generic constant* $c > 0$*,*

$$\text{cond}(\mathbf{K}) \le c. \tag{6.4b}$$

Proof. The proof again follows the same line of derivations as that given in [51] for a linear nonlocal peridynamic model. The main ingredients are the norm equivalences as established in earlier sections and, for any finite element function $u_h = \sum_{i=1}^N u_i\phi \in V_c^N(\Omega \cup \Omega_{\mathcal{I}})$, an inverse inequality of the type

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

for conventional Sobolev space norms [18]. ∎

These results are again consistent with those given in [51] for special boundary conditions corresponding to special peridynamic nonlocal models.

We again observe that if $s \in (0, 1/2)$, the error and condition number estimates also hold for discontinuous Galerkin approximations, because in this case all piecewise polynomial spaces with respect to the triangulation, whether globally continuous or not, are conforming for the internal discretization of the nonlocal problem; see [23, 51]. Moreover, note that for Case 1 with $s \in (0, 1)$, the condition number increases at a slower rate as h decreases than that for elliptic partial differential equations, for which the condition number increases with h^{-2}. In contrast, for Case 2, the condition number is bounded independently of h.

Interestingly, related to the discussion given in Appendix B.3, the finite-dimensional stiffness matrix may also be related to a graph Laplacian matrix. The inequality (6.4b) implies that the condition number is uniformly bounded with respect to the system size. Such results help explain why the development of preconditioners and solvers remains a challenge.

Appendix A. Relations between the Operator $\mathcal{L}$ and Fractional Laplacian and Fractional Derivative Operators. In this section, we discuss two approaches for the modeling of anomalous superdiffusion that replace $\nabla \cdot \nabla u$ with the fractional Laplacian or a fractional derivative operator. In section 3.1, we explained 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 diffusions over general domains in $\mathbb{R}^n$. In particular, here we demonstrate that *both the fractional Laplacian and fractional derivative operators are special cases of the integral operator* $\mathcal{L}$. Moreover, the notion of volume constraints and the nonlocal vector calculus has enabled us to discuss well-posedness over bounded domains in $\mathbb{R}^n$ for a more general class of diffusion problems.

A.1. The Fractional Laplacian as a Special Case of the Operator $\mathcal{L}$. The fractional Laplacian is the pseudodifferential operator with Fourier symbol $\mathcal{F}$ satisfying [5]

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

where $\widehat{u}$ denotes the Fourier transform of u. Suppose that $u \in L^2(\mathbb{R}^n)$ and that $\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}(u(\mathbf{x})-u(\mathbf{y}))^2|\mathbf{y}-\mathbf{x}|^{-(n+2s)}d\mathbf{y}\,d\mathbf{x} < \infty$; the vector space of such functions defines, for $0 < s < 1$, the fractional Sobolev space $H^s(\mathbb{R}^n)$ defined by (4.15). The Fourier transform can be used to show that an equivalent characterization of the fractional Laplacian is given by [5]

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

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

$$-\mathcal{D}\mathcal{D}^* = \mathcal{L} = -\big(-\Delta\big)^s, \qquad 0<s<1, \tag{A.1}$$

thus establishing that, when $\Omega = \mathbb{R}^n$, *the fractional Laplacian is the special case of the operator* $\mathcal{L}$ *defined in* (1.1) for the choice of $\gamma(\mathbf{x},\mathbf{y})$ proportional to $1/|\mathbf{y}-\mathbf{x}|^{n+2s}$.

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

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

However, in order for the constrained minimization problem

$$\min_{u\in H^s(\Omega)} \frac{1}{2}\int_\Omega\int_\Omega \frac{\big(u(\mathbf{x})-u(\mathbf{y})\big)^2}{|\mathbf{y}-\mathbf{x}|^{n+2s}}\,d\mathbf{y}\,d\mathbf{x} - \int_\Omega ub\,d\mathbf{x} \quad \text{subject to} \quad u=0 \text{ on } \partial\Omega \tag{A.2}$$

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

$$u = 0 \quad \text{on } \Omega_{\mathcal{I}},$$

where $\Omega_{\mathcal{I}}$ has nonzero volume, results in a well-posed minimization problem for $0 < s < 1$. This in turn demonstrates that the volume-constrained problem (1.2b) is a well-posed reformulation of constrained value problems involving the fractional Laplacian operator on bounded domains for $0 < s < 1$.

As an added bonus, note that (A.1) shows that by introducing the nonlocal operator $\mathcal{D}$ and its adjoint operator $\mathcal{D}^*$, we are able to provide, for $0 < s < 1$, the decomposition $(-\Delta)^s = \mathcal{D}\mathcal{D}^*$ of the fractional Laplacian operator analogous to the decomposition $-\Delta = -\nabla\cdot\nabla = \nabla\cdot(\nabla\cdot)^*$ for the Laplacian operator. Having such a decomposition available has useful consequences. First, in addition to the fact that the fractional Laplacian operator is a special case of the operator $\mathcal{L} = -\mathcal{D}\mathcal{D}^*$, we can define more general operators $-\mathcal{D}(\mathbf{\Theta}\cdot\mathcal{D}^*)$, where $\mathbf{\Theta}(\mathbf{x},\mathbf{y})$ denotes a second-order tensor function, that have similar properties to the fractional Laplacian. Furthermore, for $0 < s < 1$, we are able to define the weak formulation (4.4) for problems involving the fractional Laplacian; this itself is useful for the analysis of such problems and for developing finite element discretizations, as we have demonstrated in this paper.

A.2. Fractional Derivative Operators as a Special Case of the Operator $\mathcal{L}$. In [43], the free-space fractional dispersion problem

$$\begin{cases} u_t(\mathbf{x},t) = c\nabla_M^{2s}u(\mathbf{x},t), & \mathbf{x}\in\mathbb{R}^n, t>0,\\ u(\mathbf{x},0) = u_0(\mathbf{x}), & \mathbf{x}\in\mathbb{R}^n, \end{cases} \tag{A.3}$$

is proposed for $0 < s \leq 1$, where the Fourier symbol of ∇_M^{2s} is given by

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

where $M(d\theta)$ denotes an arbitrary probability measure on the unit sphere, and $\widehat{u}$ denotes the Fourier transform of u. The authors of [43] describe M as a mixing measure, because the integral involves directional derivatives over all radial directions on the unit sphere; the authors also explain that the solutions to (A.3) yield every possible multivariable Levy motion of index $2s$, $s \neq 1$. 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. In [42], a fractional divergence operator is introduced that enables the consideration of a fractional flux.

In the special case when $M(d\theta)$ corresponds to a symmetric measure $\omega(d\theta)$, i.e., $\omega(d\theta) = \omega(-d\theta)$, the Fourier symbol of ∇_ω^{2s} is given by [43, Eq. (8)]

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

The inverse Fourier transform may then be used to determine a kernel γ so that when $\Omega \equiv \mathbb{R}^n$,

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

for a constant $C_{n,s,\omega}$. In other words, the fractional derivative operator ∇_ω^{2s} and the nonlocal operator $\mathcal{L}$ are equivalent on all of space, i.e., for $\Omega = \mathbb{R}^n$.

As was the case for fractional Laplacian operator equations, for $1/2 < s < 1$, a limitation of fractional derivative-based approaches for modeling anomalous diffusion occurs on general bounded domains in $\mathbb{R}^n$ whenever the field u is constrained, e.g., by boundary conditions. This limitation is apparent when developing numerical methods for fractional partial differential equations; see [46] for recent work including many citations to the literature. In [31], an impressive attempt is made to improve numerical methods for fractional partial differential equations; an equivalent reformulation of the fractional dispersion equation (A.3) on bounded domains in $\mathbb{R}^n$, including a systematic numerical method, is considered. A fractional derivative function space is defined and demonstrated to be equivalent to the fractional Sobolev space $H^s(\Omega)$ for $s > 0$, excluding integer multiples of $1/2$. However, instead of applying the volume-constraint operator $\mathcal{V}$ of (1.2b), homogeneous Dirichlet boundary conditions are used and thus the well-posedness over $H_0^s(\Omega)$ for only $1/2 < s < 1$ can be considered in [31]. Hence, a restricted notion of steady-state diffusion is addressed; see [31, Thm. 6.1]. In contrast, the volume-constrained problem (1.2b) is a well-posed reformulation of fractional derivative operator equations on bounded domains for $0 < s < 1$. Furthermore, the development of finite element methods follows naturally from the weak formulation (4.4) of such volume-constrained problems.

Appendix B. Other 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. Applications to nonlocal diffusion and advection-diffusion problems are discussed in sections 3.3 and 5.3, respectively, and to reformulations of fractional Laplacian and fractional derivative operator equations are discussed in sections A.1 and A.2, respectively.

B.1. The Peridynamic Continuum Model for Mechanics. In [48], the linearized peridynamic balance of linear momentum is derived as

$$\mathbf{u}_{tt}(\mathbf{x},t) = \mathbf{\Lambda u}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t), \qquad \mathbf{x} \in \mathbb{R}^n, t > 0, \tag{B.1}$$

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

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

The operators $\mathcal{L}$ and $\mathbf{\Lambda}$ coincide when $n = 1$ and $\gamma(x,y) = (y-x)^2/\big(2\sigma(|y-x|)\big)$. In [51], results are provided about the well-posedness of both (B.1) and the associated equilibrium equation $\mathbf{\Lambda u} + \mathbf{b} = \mathbf{0}$. In [30], 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 [30, 51] relies on the analytic properties of σ, showing how the kernel γ determines the regularity (or lack thereof) of the solution of volume-constrained problems involving the operator $\mathcal{L}$.

B.2. Nonlocal Wave Equation. The operator $\mathcal{L} = -\mathcal{D}(\mathbf{\Theta} \cdot \mathcal{D}^*)$ appears in the nonlocal wave equation

$$\begin{cases} u_{tt} + \mathcal{D}\big(\mathbf{\Theta} \cdot \mathcal{D}^* u\big) = 0 & \forall\, \mathbf{x} \in \Omega\,,\ t > 0, \\ \mathcal{V}u = 0 & \forall\, \mathbf{x} \in \Omega_{\mathcal{I}}\,,\ t > 0, \\ u(\mathbf{x},0) = u_0(\mathbf{x}) & \forall\, \mathbf{x} \in \Omega, \\ u_t(\mathbf{x},0) = u_1(\mathbf{x}) & \forall\, \mathbf{x} \in \Omega, \end{cases} \tag{B.2}$$

which can be viewed as a special case of the time-dependent peridynamic model. The one-dimensional free-space problem for the nonlocal wave equation was studied in [50].

Define the energy

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

Applying the nonlocal Green's first identity (3.10), we obtain

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

so that if the nonlocal wave equation is satisfied, i.e., if the first equation in (B.2) holds, we obtain

$$\frac{d}{dt}\mathcal{E}(t) = -\int_{\Omega_{\mathcal{I}}} \mathcal{N}(\mathbf{\Theta} \cdot \mathcal{D}^* u)\big) u_t \, d\mathbf{x}.$$

If the volume constraint $\mathcal{V}$ in (B.2) implies that the last integral vanishes, as it does for either of the volume constraints (4.7b) and (4.8b), then $d\mathcal{E}/dt = 0$ so that the nonlocal wave equation conserves energy. This is an instance of the peridynamic balance of energy; see, e.g., [48, sec. 4].

B.3. Graph Laplacians. In [41], a precise notion of the limit of a sequence of dense finite graphs[8] is introduced. The limit is a symmetric measurable function $W : [0,1] \times [0,1] \mapsto [0,1]$ and represents the continuum analogue of an adjacency matrix for a simple unweighted graph. When $\gamma = W$ and $\Omega = (0,1)$, the operator $\mathcal{L}$ represents the continuum analogue 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 or its connectivity. This includes a continuum analogue of diffusion on a graph, where Ω then corresponds to diffusion occurring on the limit of a sequence of dense finite graphs. See, for instance, [25, Chap. 8] for an introduction to "Dirichlet" and "Neumann" boundary conditions for a graph Laplacian.

We note that a discrete calculus has precedence in the graph theory and machine learning literature; see, e.g., [26, sec. 3] and [10, 38, 37] 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 fascinating results of [41] then suggest that a continuum analogue of a discrete vector calculus and its analysis and applications are of interest.

B.4. Symmetric Jump Processes. The operator $\mathcal{L}$ is the infinitesimal generator for a symmetric jump process[9] and has been the subject of much recent interest. 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 [24] 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 example, a statistic of interest is the time for a process to exit a domain; see, e.g., [20, 21, 22] for further discussion. Our results complement these probabilistic analyses and provide a variational approach useful for numerical simulations.

REFERENCES

[1] H. Abels and M. Kassmann, *The Cauchy problem and the martingale problem for integro-differential operators with non-smooth kernels*, Osaka J. Math., 46 (2009), pp. 661–683.

[2] B. Aksoylu and T. Mengesha, *Results on nonlocal boundary value problems*, Numer. Funct. Anal. Optim., 31 (2010), pp. 1301–1317.

[3] B. Aksoylu and M. L. Parks, *Variational theory and domain decomposition for nonlocal problems*, Appl. Math. Comput., 217 (2011), pp. 6498–6515.

[4] F. Andreu, J. M. Mazón, J. D. Rossi, and J. Toledo, *Nonlocal Diffusion Problems*, Math. Surveys Monogr. 165, AMS, Providence, RI, 2010.

[5] D. Applebaum, *Lévy Processes and Stochastic Calculus*, Cambridge Stud. Adv. Math. 93, Cambridge University Press, Cambridge, UK, 2004.

[6] D. N. Arnold, F. Brezzi, B. Cockburn, and L. D. Marini, *Unified analysis of discontinuous Galerkin methods for elliptic problems*, SIAM J. Numer. Anal., 39 (2002), pp. 1749–1779.

[7] G. Aubert and P. Kornprobst, *Can the nonlocal characterization of Sobolev spaces by Bourgain et al. be useful for solving variational problems?*, SIAM J. Numer. Anal., 47 (2009), pp. 844–860.

[8] J. P. Aubin, *Applied Functional Analysis*, 2nd ed., Wiley, New York, 2000.

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

[9] The infinitesimal generator corresponds to the operator $\mathcal{L}$ with a singular kernel; see Case 1 in section 4.2.

[9] J. P. Aubin, *Approximation of Elliptic Boundary-Value Problems*, Dover, New York, 2007. Unabridged reproduction of the 1980 corrected reprint edition by Krieger Publishing. Original publication by Wiley-Interscience, New York, 1972.

[10] N. Badr and E. Russ, *Interpolation of Sobolev spaces, Littlewood-Paley inequalities and Riesz transforms on graphs*, Publ. Mat., 53 (2009), pp. 273–328.

[11] O. Bakunin, *Turbulence and Diffusion: Scaling versus Equations*, Springer-Verlag, New York, 2008.

[12] C. Bardos, R. Santos, and R. Sentis, *Diffusion approximation and computation of the critical size*, Trans. Amer. Math. Soc., 284 (1984), pp. 617–649.

[13] M. T. Barlow, R. F. Bass, Z.-Q. Chen, and M. Kassmann, *Non-local Dirichlet forms and symmetric jump processes*, Trans. Amer. Math. Soc., 361 (2009), pp. 1963–1999.

[14] R. F. Bass, M. Kassmann, and T. Kumagai, *Symmetric jump processes: Localization, heat kernels and convergence*, Ann. Inst. Henri Poincaré Probab. Stat., 46 (2010), pp. 59–71.

[15] P. W. Bates and A. Chmaj, *An integrodifferential model for phase transitions: Stationary solutions in higher space dimensions*, J. Statist. Phys., 95 (1999), pp. 1119–1139.

[16] F. Bobaru and M. Duangpanya, *The peridynamic formulation for transient heat conduction*, Internat. J. Heat Mass Transfer, 53 (2010), pp. 4047–4059.

[17] J. Bourgain, H. Brezis, and P. Mironescu, *Another look at Sobolev spaces*, in Optimal Control and Partial Differential Equations: In Honor of Professor Alain Bensoussan's 60th Birthday, J. L. Menaldi, E. Rofman, and A. Sulem, eds., IOS Press, 2001, pp. 439–455.

[18] S. C. Brenner and L. R. Scott, *The Mathematical Theory of Finite Element Methods*, 3rd ed., Texts Appl. Math., Springer-Verlag, New York, 2008.

[19] A. Buades, B. Coll, and J. M. Morel, *Image denoising methods. A new nonlocal principle*, SIAM Rev., 52 (2010), pp. 113–147.

[20] N. Burch and R. B. Lehoucq, *Classical, nonlocal, and fractional diffusion equations on bounded domains*, Internat. J. Multiscale Comput. Engrg., 9 (2011), pp. 661–674.

[21] N. Burch and R. B. Lehoucq, *Continuous-time random walks on bounded domains*, Phys. Rev. E, 83 (2011), 012105.

[22] N. Burch and R. B. Lehoucq, *Computing the Exit-Time for a Jump Process*, Tech. report 2012-2132J, Sandia National Laboratories, 2012.

[23] X. Chen and M. Gunzburger, *Continuous and discontinuous finite element methods for a peridynamics model of mechanics*, Comput. Methods Appl. Mech. Engrg., 200 (2011), pp. 1237–1250.

[24] Z.-Q. Chen, P. Kim, and R. Song, *Heat kernel estimates for the Dirichlet fractional Laplacian*, J. Eur. Math. Soc. (JEMS), 12 (2010), pp. 1307–1329.

[25] F. R. K. Chung, *Spectral Graph Theory*, CBMS Regional Conf. Ser. in Math. 92, AMS, Providence, RI, 1997.

[26] T. Coulhon and A. Grigoryan, *Random walks on graphs with regular volume growth*, Geom. Funct. Anal., 8 (1998), pp. 656–701.

[27] Q. Du, M. Gunzburger, R. B. Lehoucq, and K. Zhou, *A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws*, Math. Models Methods Appl. Sci., to appear.

[28] Q. Du, L. Ju, L. Tian, and K. Zhou, *A posteriori error analysis of finite element method for linear nonlocal diffusion and peridynamic models*, Math. Comp., to appear.

[29] Q. Du, J. R. Kamm, R. B. Lehoucq, and M. L. Parks, *A new approach for a nonlocal, nonlinear conservation law*, SIAM J. Appl. Math., 72 (2012), pp. 464–487.

[30] Q. Du and K. Zhou, *Mathematical analysis for the peridynamic nonlocal continuum theory*, ESAIM Math. Model. Numer. Anal., 45 (2011), pp. 217–234.

[31] V. J. Ervin and J. P. Roop, *Variational solution of fractional advection dispersion equations on bounded domains in* $\mathbb{R}^d$, Numer. Methods Partial Differential Equations, 23 (2007), pp. 256–281.

[32] P. Fife, *Some nonclassical trends in parabolic and parabolic-like evolutions*, in Trends in Nonlinear Analysis, M. Kirkilionis, S. Krömker, R. Rannacher, and F. Tomi, eds., Springer-Verlag, New York, 2003, pp. 153–191.

[33] G. Gilboa and S. Osher, *Nonlocal linear image regularization and supervised segmentation*, Multiscale Model. Simul., 6 (2007), pp. 595–630.

[34] G. Gilboa and S. Osher, *Nonlocal operators with applications to image processing*, Multiscale Model. Simul., 7 (2008), pp. 1005–1028.

[35] M. Gunzburger and R. B. Lehoucq, *A nonlocal vector calculus with application to nonlocal boundary value problems*, Multiscale Model. Simul., 8 (2010), pp. 1581–1598.

[36] L. I. Ignat and J. D. Rossi, *A nonlocal convection-diffusion equation*, J. Funct. Anal., 251 (2007), pp. 399–437.

[37] X. Jiang, L.-H. Lim, Y. Yao, and Y. Ye, *Statistical ranking and combinatorial Hodge theory*, Math. Program., 127 (2011), pp. 203–244.

[38] O. Lézoray, V.-T. Ta, and A. Elmoataz, *Partial differences as tools for filtering data on graphs*, Pattern Recognition Lett., 31 (2010), pp. 2201–2213.

[39] J.-G. Liu and L. Mieussens, *Analysis of an asymptotic preserving scheme for linear kinetic equations in the diffusion limit*, SIAM J. Numer. Anal., 48 (2010), pp. 1474–1491.

[40] Y. Lou, X. Zhang, S. Osher, and A. Bertozzi, *Image recovery via nonlocal operators*, J. Sci. Comput., 42 (2010), pp. 185–197.

[41] L. Lovász and B. Szegedy, *Limits of dense graph sequences*, J. Combin. Theory Ser. B, 96 (2006), pp. 933–957.

[42] M. Meerschaert, J. Mortensen, and S. Wheatcraft, *Fractional vector calculus for fractional advection-dispersion*, Phys. A, 367 (2006), pp. 181–190.

[43] M. M. Meerschaert, D. A. Benson, and B. Bäumer, *Multidimensional advection and fractional dispersion*, Phys. Rev. E, 59 (1999), pp. 5026–5028.

[44] R. Metzler and J. Klafter, *The restaurant at the end of the random walk: Recent developments in the description of anomalous transport by fractional dynamics*, J. Phys. A., 37 (2004), R161.

[45] S. P. Neuman and D. M. Tartakovsky, *Perspective on theories of non-Fickian transport in heterogeneous media*, Adv. Water Resources, 32 (2009), pp. 670–680.

[46] I. Podlubny, A. Chechkin, T. Skovranek, Y. Chen, and B. M. V. Jara, *Matrix approach to discrete fractional calculus* II: *Partial fractional differential equations*, J. Comput. Phys., 228 (2009), pp. 3137–3153.

[47] L. Rosasco, M. Belkin, and E. D. Vito, *On learning with integral operators*, J. Mach. Learn. Res., 11 (2010), pp. 905–934.

[48] S. A. Silling, *Reformulation of elasticity theory for discontinuities and long-range forces*, J. Mech. Phys. Solids, 48 (2000), pp. 175–209.

[49] S. A. Silling, M. Zimmermann, and R. Abeyaratne, *Deformation of a peridynamic bar*, J. Elasticity, 73 (2003), pp. 173–190.

[50] O. Weckner and R. Abeyaratne, *The effect of long-range forces on the dynamics of a bar*, J. Mech. Phys. Solids, 53 (2005), pp. 705–728.

[51] K. Zhou and Q. Du, *Mathematical and numerical analysis of linear peridynamic models with nonlocal boundary conditions*, SIAM J. Numer. Anal., 48 (2010), pp. 1759–1780.

[52] A. Zoia, A. Rosso, and M. Kardar, *Fractional Laplacian in bounded domains*, Phys. Rev. E, 76 (2007), 021116.