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Nonlocal diffusion and peridynamic models with Neumann type constraints and their numerical approximations☆

Yunzhe Tao, Xiaochuan Tian, Qiang Du*

Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027, USA

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ABSTRACT

This paper studies nonlocal diffusion models associated with a finite nonlocal horizon parameter δ that characterizes the range of nonlocal interactions. The focus is on the variational formulation associated with Neumann type constraints and its numerical approximations. We establish the well-posedness for some variational problems associated and study their local limit as $\delta \to 0$. A main contribution is to derive a second order convergence to the local limit. We then discuss the numerical approximations including standard finite element methods and quadrature based finite difference methods. We study their convergence in the nonlocal setting and in the local limit.

1. Introduction

Nonlocal diffusion equations and their numerical approximations have been subjects of recent studies. Such models arise in the studies of stochastic jump processes [10,18] and they also share common features with the peridynamic model of continuum mechanics proposed by S. Silling [29]. The latter has been shown to be effective in modeling material singularities [4,8,13,27,31,32] since the model avoids the explicit use of spatial derivatives. Nonlocal models such as peridynamics are often parametrized by a parameter δ that is called the horizon measuring the range of nonlocal interactions.

A feature of nonlocal models, different from the local PDEs, is the treatment of interfaces and domain boundaries. Unlike local boundary conditions, the nonlocal analog may be attributed to how the law of nonlocal interactions gets modified in the presence of physical boundary. Discussions on a variety of nonlocal constraints has been given in [17]. It is known that Neumann type problems presents substantial differences from that on Dirichlet type problems for nonlocal equations, see [2,3,5,6,12,14,17,25,37] for various studies devoted to nonlocal Neumann type problems. Our study here provides new understanding to the proper formulation of Neumann conditions. In particular, we demonstrate how a suitable formulation leads to the second order convergence of the nonlocal models to their local limit in the horizon parameter δ as $\delta \to 0$. Such results are new and are expected to be of optimal order while previous studies have provided at most linear (first order) convergence [19]. Neumann problems are not only interesting on their own but also play important roles in interface problems, free boundary problems, the coupling and domain decomposition of nonlocal problems.

Parallel to the derivation of Neumann problems and their mathematical analysis, it is natural to consider their numerical approximations. For nonlocal models characterized by the parameter δ, it has been known in the literature that as

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* Corresponding author.
E-mail addresses: y.tao@columbia.edu (Y. Tao), xt2156@columbia.edu (X. Tian), qd2125@columbia.edu (Q. Du).

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$\delta \to 0$, one often encounter consistency issues at both continuum and discrete levels between the nonlocal models and the local PDEs, when the latter remain valid. On the continuum level, the consistency has been established either formally using Taylor expansions of sufficiently smooth solutions [29,30], or more rigorously via functional analytic means without extra regularity assumptions [23,25,34]. With the increasing interests in developing efficient codes for nonlocal models, it is often asked if numerical schemes developed for nonlocal models would produce results consistent with that produced by the local limit models when the horizon is small and with sufficient numerical resolution. Answering such questions on the discrete level is an important task of code validation and verification. In [34], a theory of asymptotically compatible schemes was developed. It was successfully applied to nonlocal models with Dirichlet type nonlocal volumetric constraints. Given the extra complications involved in the nonlocal Neumann type problems, a separate study of similar issues in the Neumann setting is worthwhile. Hence, another contribution of this paper is to demonstrate the applicability of the theory on asymptotically compatible scheme for Neumann type problems.

To highlight the main issues addressed in this manuscript, we summarize several different limiting processes that are of our particularly concern, namely: (1) limit of nonlocal continuum models as the horizon $\delta \to 0$; (2) limit of discrete schemes for nonlocal models as $\delta \to 0$ for a fixed mesh parameter h; (3) limit of discrete schemes of nonlocal models as $h \to 0$ for fixed δ; (4) limit of the discrete schemes for the nonlocal models with both $\delta \to 0$ and $h \to 0$. We present findings on these processes in this work. A one-dimensional model is used for the simplicity in presentation. Our results offer a rigorous mathematical theory behind the nonlocal Neumann type problems and an optimal order error bound between the solutions of nonlocal models and their local limit. They also demonstrate the general applicability of the framework on asymptotically compatible scheme to the numerical discretization of Neumann type problems.

The paper is organized as follows. In Section 2, we introduce the nonlocal Neumann type constrained value problems associated to nonlocal variational problems. The well-posedness of the variational problem is given. A number of key results are stated in Section 3, we analyze the asymptotic compatibility of our nonlocal model. The convergence of nonlocal models to linear local problems is established. Furthermore, we formally estimate the convergence rate as the interaction horizon tends to zero, which is new with regards to previous works. Discussion on the inhomogeneous Neumann type constraints is also made. In Section 4, we present both quadrature based finite difference and finite element discretization schemes. In Section 5, we first discuss how to numerically impose the Neumann constraints and then give related numerical results to further substantiate our theoretical studies. Different limiting processes are examined numerically in this section. Finally, we give some conclusions and remarks in Section 6.

2. Nonlocal variational problems

In this section, we first introduce a nonlocal variational problem with Neumann type volume constraints, along with the associated nonlocal operators and the class of nonlocal interactions kernel to be focused on in this paper. Later, in Sections 2.3 and 2.5, the natural energy space and the well-posedness of nonlocal problems are studied. The studies here are parallel to the traditional analysis of local second order elliptic equations as well as the analysis of nonlocal diffusion models with Dirichlet type constraints, but with necessary modifications. We refer to [17] for more discussions on the differences and connections between local and nonlocal steady-state diffusion problems.

2.1. Nonlocal variational problems

Let $\Omega \subset \mathbb{R}^d$ denote a bounded, open domain with a piecewise planar boundary. Consider the nonlocal energy functional

$$E(u) = \frac{1}{2}\int_\Omega\int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})\big(u(\mathbf{x}') - u(\mathbf{x})\big)^2 d\mathbf{x}' d\mathbf{x}\,, \tag{1}$$

where $\rho_\delta(\mathbf{x}',\mathbf{x}) = \rho_\delta(\mathbf{x},\mathbf{x}')$ is a symmetric, nonnegative interaction kernel with the property that $\rho_\delta(\mathbf{x}',\mathbf{x}) = 0$ if $|\mathbf{x}'-\mathbf{x}| > \delta$. Here $|\mathbf{x}'-\mathbf{x}|$ denotes the distance between $\mathbf{x}'$ and $\mathbf{x}$.

Without loss of generality, for given data $f = f(\mathbf{x})$ defined on Ω, with the total net-flux assumed to be zero, the following compatibility condition is assumed:

$$\int_\Omega f(\mathbf{x}) d\mathbf{x} = 0\,. \tag{2}$$

This type of compatibility is also present in Neumann type problems associated with local elliptic operators. We then define the total energy

$$E_f(u) = \frac{1}{2}\int_\Omega\int_\Omega \rho_\delta(\mathbf{x}',\mathbf{x})\big(u(\mathbf{x}') - u(\mathbf{x})\big)^2 d\mathbf{x}' d\mathbf{x} - \int_\Omega f(\mathbf{x})u(\mathbf{x}) d\mathbf{x}\,. \tag{3}$$

2.2. Nonlocal kernel

We assume that the symmetric, non-negative kernel ρ satisfies, for all $\mathbf{x},\mathbf{x}' \in \mathbb{R}^d$,

$$\rho_\delta(\mathbf{x}',\mathbf{x}) = \begin{cases} \rho_\delta(|\mathbf{x}'-\mathbf{x}|) \ge 0, & \text{if } |\mathbf{x}'-\mathbf{x}| \le \delta, \\ 0, & \text{if } |\mathbf{x}'-\mathbf{x}| > \delta, \end{cases} \tag{4}$$