

# SANDIA REPORT

Printed



Sandia  
National  
Laboratories

## **Mathematical Foundations for Nonlocal Interface Problems: Multiscale Simulations of Heterogeneous Materials Final LDRD Report**

Marta D'Elia, Pavel Bochev, John T. Foster, Christian Glusa, Mamikon Gulian, Max Gunzburger, Jeremy Trageser, Kristopher Kuhlman, Mario Martinez, Habib Najm, Stewart Silling, Michael Tupek, Xiao Xu

Prepared by  
Sandia National Laboratories  
Albuquerque, New Mexico 87185  
Livermore, California 94550

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology & Engineering Solutions of Sandia, LLC.

**NOTICE:** This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from

U.S. Department of Energy  
Office of Scientific and Technical Information  
P.O. Box 62  
Oak Ridge, TN 37831

Telephone: (865) 576-8401  
Facsimile: (865) 576-5728  
E-Mail: reports@osti.gov  
Online ordering: <http://www.osti.gov/scitech>

Available to the public from

U.S. Department of Commerce  
National Technical Information Service  
5301 Shawnee Road  
Alexandria, VA 22312

Telephone: (800) 553-6847  
Facsimile: (703) 605-6900  
E-Mail: orders@ntis.gov  
Online order: <https://classic.ntis.gov/help/order-methods>



## **ABSTRACT**

Nonlocal models provide a much-needed predictive capability for important Sandia mission applications, ranging from fracture mechanics for nuclear components to subsurface flow for nuclear waste disposal, where traditional partial differential equations (PDEs) models fail to capture effects due to long-range forces at the microscale and mesoscale. However, utilization of this capability is seriously compromised by the lack of a rigorous nonlocal interface theory, required for both application and efficient solution of nonlocal models. To unlock the full potential of nonlocal modeling we developed a mathematically rigorous and physically consistent interface theory and demonstrate its scope in mission-relevant exemplar problems.



# CONTENTS

<b>1. Introduction</b>	<b>7</b>
<b>2. Technical Highlights</b>	<b>9</b>
2.1. Mathematical Foundations .....	9
2.2. Learning and parameter identification .....	11
2.3. Implementation issues .....	12
2.4. Applications in mechanics and subsurface transport .....	14
2.5. Coupling and domain decomposition methods .....	15
<b>3. Project Metrics</b>	<b>19</b>
3.1. Staffing .....	19
3.2. Publications .....	19
3.3. Presentations .....	21
3.4. Conference organization .....	24
3.5. Team building and partnerships .....	25
3.6. Mentoring and training .....	26
<b>4. Project Legacy</b>	<b>27</b>
4.1. PyNucleus .....	27
4.2. Fractional-Order Models for Sea Ice (FOMSI) .....	28
4.3. Project files .....	28
<b>Bibliography</b>	<b>29</b>

## LIST OF FIGURES

Figure 2-1. From [26]: Solution for constant forcing, finite horizon and fractional order with four layers. As expected, the solution behavior is more diffusive for layers with larger fractional order, at the top of the domain, than for layers with lower fractional order at the bottom. . . . .	10
Figure 2-2. From [35]: Illustration of a two-dimensional configuration of a nonlocal interface problem with different horizons. . . . .	10
Figure 2-3. From [35]: Numerical solution of the nonlocal two-dimensional interface problem with solution and flux jumps and constant kernels of different horizons on both sides of the interface. . . . .	11
Figure 2-4. From [25]: Cost functional evaluations (●) and BFGS iterates (–) for a 2D test problem and regularization $\mathcal{R}(s, \delta) = \frac{\alpha}{s(1-s)} + \beta \frac{e^\delta}{\delta}$ with $\alpha = 5 \times 10^{-7}$ and $\beta = 10^{-6}$ . The final iterate is marked with ×, the parameters $q^*$ used to generate the data $u_d$ is marked with +. . . . .	12
Figure 2-5. From [29]: Different approaches to approximate the integration domain in the assembly of nonlocal operators with finite horizon. (a) An inscribed polygonal approximation of the ball. (b) Subdivision of the ball into the polygon of (a) and circular caps. An inscribed polygonal approximation of the ball is defined by approximating the green caps by triangles. (c) Approximation of the ball by whole finite element triangles that intersect the ball and for which the barycenter lies within the ball. (d) Approximation of the ball by all whole finite element triangles that intersect the ball. . . . .	13
Figure 2-6. From [32]: Validation results on the displacement for influence functions learned with and without energy constraint. The importance of the imposed energy constraint is apparent. . . . .	15
Figure 2-7. From [36]: Breakthrough curve prediction by nonlocal dynamic kernel learned from sparse data and blackbox neural network surrogate (the green dashed line is used to separate training and testing). The proposed model using a learned nonlocal dynamic kernel manages to correctly reproduce the tail behavior in the testing regime, whereas the blackbox neural network fails. . . . .	16
Figure 2-8. From [23]: Top left: domain configuration for 2D numerical test. Top right: numerical solution of the local coupling problem in $\Omega_1 \cup \Omega_2$ . Bottom left: numerical solution of the nonlocal coupling problem in $\Omega_1 \cup \Omega_2$ with $(\delta_1, \delta_2) = (2^{-8}, 2^{-7})$ . Bottom right: numerical solution of the nonlocal coupling problem in $\Omega_1 \cup \Omega_2$ with $(\delta_1, \delta_2) = (2^{-4}, 2^{-3})$ . . . . .	17
Figure 2-9. From [33]: Weak scaling of the substructuring solver for constant horizon and different local problem sizes $L/p$ . Dirichlet preconditioner, Cholesky solvers in the operator and preconditioner. . . . .	18

# 1. INTRODUCTION

Nonlocal models (NLMs) employ integral rather than differential operators which allows them to capture effects arising from long-range forces at the microscale and mesoscale, not accounted for by partial-differential equations (PDEs). Consequently, NLMs provide exceptional simulation fidelity for a broad spectrum of mission applications such as fracture mechanics [3, 14, 12], anomalous subsurface transport [2, 4, 6, 20], phase transitions [1, 5], image processing [11, 7, 9, 13], multiscale and multiphysics systems [8, 15], MHD [10], and stochastic processes [16, 21, 18].

However, wider deployment of NLMs at Sandia is hindered by the lack of a mathematically rigorous and physically consistent interface theory because successful utilization of NLMs in mission applications requires handling of both physical and virtual interfaces. The former arise from material discontinuities, whereas the latter are needed for the design of scalable domain-decomposition NL solvers.

We proposed to develop a NL interface theory to unlock the full potential of NLMs in mission applications such as fracture mechanics and subsurface flow. This made our project fundamentally different from previous nonlocal projects at Sandia, which focused on NL discretizations for single-material simulation purposes, but did not address the modeling, analysis, or numerics of NL interface problems involving multiple materials. Furthermore, our project was not tied to any discretization. In PDEs this difference corresponds to research focused solely on PDE discretization (e.g. FEM) versus modeling and analysis of PDE interface problems (e.g. contact, heat transfer).

The key technical challenge was to discover NL transmission conditions yielding physically consistent well-posed interface problems that also recover classical formulations in the local limit. We posited that the treatment of local entities (interfaces) in nonlocal terms together with minimization of the (nonlocal) energy of the system provides a mathematically sound foundation to identify transmission conditions leading to well-posed NL interface problems (NIP). The combination of energy minimization and enforcement of the equivalence with classical interface conditions at the local limit provides governing equations and NL interface conditions that are mathematically and physically consistent, regardless of the discretization.

The treatments of NL interfaces in SNL mechanics codes are ad hoc and heuristic, compromising physical consistency. Existing mathematical approaches [19, 17] failed to establish rigorous theoretical foundations either because they do not ensure uniqueness of solutions or they do not rigorously analyze convergence to local limits, undermining both mathematical and physical consistency. We addressed these shortcomings by establishing a mathematical theory for NL interfaces mirroring that available for PDEs.

Our approach 1) applied to existing algorithms and software, requiring modest implementation efforts; 2) enabled new scalable domain-decomposition NL solvers; 3) provided a foundation for data-driven discovery of interfaces. By providing physically faithful solutions our work advanced the state of the art of mission-relevant applications such as treating heterogeneity in nuclear devices and subsurface geosciences, and impacted the fast-growing NL modeling community by providing a new in-demand tool.

## 2. TECHNICAL HIGHLIGHTS

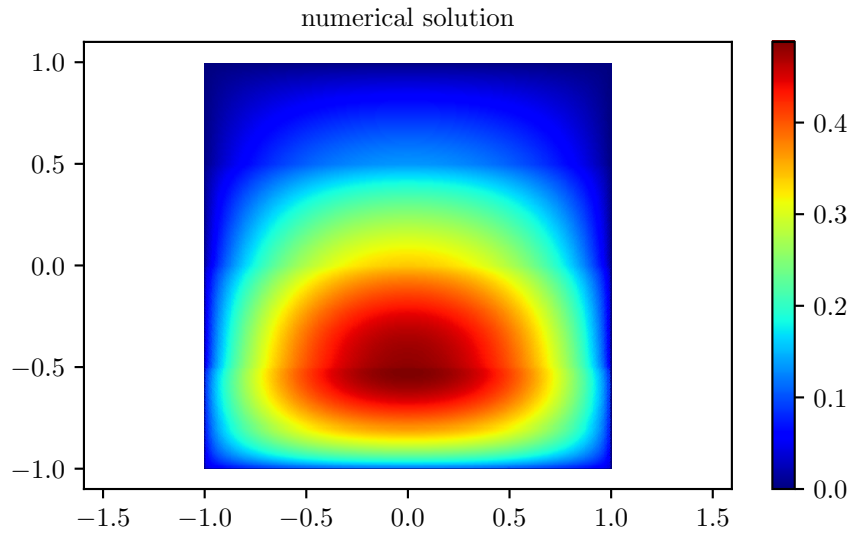
### 2.1. Mathematical Foundations

Fractional equations have become the model of choice in several applications where heterogeneities at the microstructure result in anomalous diffusive behavior at the macroscale. In [26] we introduce a new fractional operator characterized by a doubly-variable fractional order and possibly truncated interactions. Under certain conditions on the model parameters and on the regularity of the fractional order we show that the corresponding Poisson problem is well-posed. We also introduce a finite element discretization and describe an efficient implementation of the finite-element matrix assembly in the case of piecewise constant fractional order. Through several numerical tests, we illustrate the improved descriptive power of this new operator across media interfaces. Furthermore, we present one-dimensional and two-dimensional  $h$ -convergence results that show that the variable-order model has the same convergence behavior as the constant-order model.

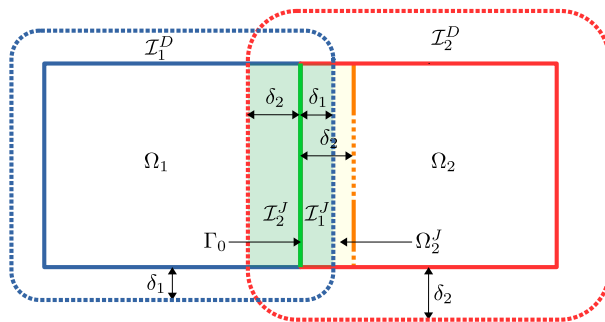
In [27] we analyze the well-posedness of an anisotropic, nonlocal diffusion equation. Establishing an equivalence between weighted and unweighted anisotropic nonlocal diffusion operators in the vein of unified nonlocal vector calculus, we apply our analysis to a class of fractional-order operators and present rigorous estimates for the solution of the corresponding anisotropic anomalous diffusion equation. Furthermore, we extend our analysis to the anisotropic diffusion-advection equation and prove well-posedness for fractional orders  $s$  in  $[0.5, 1)$ . We also present an application of the advection-diffusion equation to anomalous transport of solutes.

In [28], we present an optimization-based coupling method for local and nonlocal continuum models. Our approach couches the coupling of the models into a control problem where the states are the solutions of the nonlocal and local equations, the objective is to minimize their mismatch on the overlap of the local and nonlocal problem domains, and the virtual controls are the nonlocal volume constraint and the local boundary condition. We present the method in the context of Local-to-Nonlocal diffusion coupling. Numerical examples illustrate the theoretical properties of the approach.

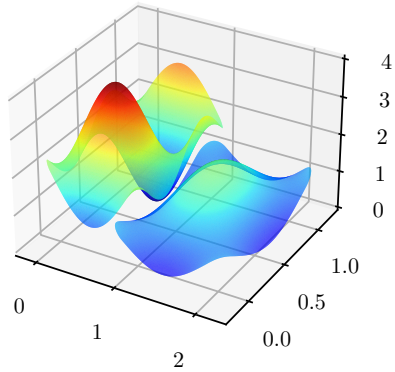
In [35] we introduce a mathematically rigorous formulation for a nonlocal interface problem with jumps and propose an asymptotically compatible finite element discretization for the weak form of the interface problem. After proving the well-posedness of the weak form, we demonstrate that solutions to the nonlocal interface problem converge to the corresponding local counterpart when the nonlocal data are appropriately prescribed. Several numerical tests in one and two dimensions show the applicability of our technique, its numerical convergence to exact nonlocal solutions, its convergence to the local limit when the horizons vanish, and its robustness with respect to the patch test.



**Figure 2-1.** From [26]: Solution for constant forcing, finite horizon and fractional order with four layers. As expected, the solution behavior is more diffusive for layers with larger fractional order, at the top of the domain, than for layers with lower fractional order at the bottom.



**Figure 2-2.** From [35]: Illustration of a two-dimensional configuration of a nonlocal interface problem with different horizons.

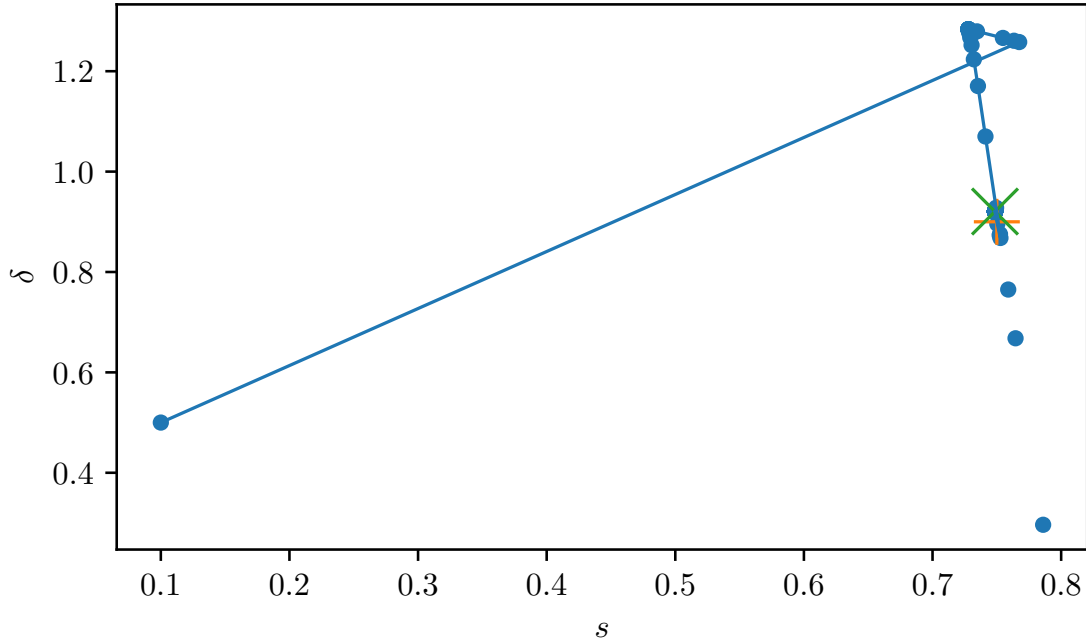


**Figure 2-3. From [35]: Numerical solution of the nonlocal two-dimensional interface problem with solution and flux jumps and constant kernels of different horizons on both sides of the interface.**

## 2.2. Learning and parameter identification

In [31] we consider the integral definition of the fractional Laplacian and analyze a linear-quadratic optimal control problem for the so-called fractional heat equation; control constraints are also considered. We derive existence and uniqueness results, first order optimality conditions, and regularity estimates for the optimal variables. To discretize the state equation we propose a fully discrete scheme that relies on an implicit finite difference discretization in time combined with a piecewise linear finite element discretization in space. We derive stability results and a novel  $L^2(0, T; L^2(\Omega))$  a priori error estimate. On the basis of the aforementioned solution technique, we propose a fully discrete scheme for our optimal control problem that discretizes the control variable with piecewise constant functions, and we derive a priori error estimates for it. We illustrate the theory with one- and two-dimensional numerical experiments.

Nonlocal operators of fractional type are a popular modeling choice for applications that do not adhere to classical diffusive behavior; however, one major challenge in nonlocal simulations is the selection of model parameters. In [25] we propose an optimization-based approach to parameter identification for fractional models with an optional truncation radius. We formulate the inference problem as an optimal control problem where the objective is to minimize the discrepancy between observed data and an approximate solution of the model, and the control variables are the fractional order and the truncation length. For the numerical solution of the minimization problem we propose a gradient-based approach, where we enhance the numerical performance by an approximation of the bilinear form of the state equation and its derivative with respect to the fractional order. Several numerical tests in one and two dimensions illustrate the theoretical results and show the robustness and applicability of our method.

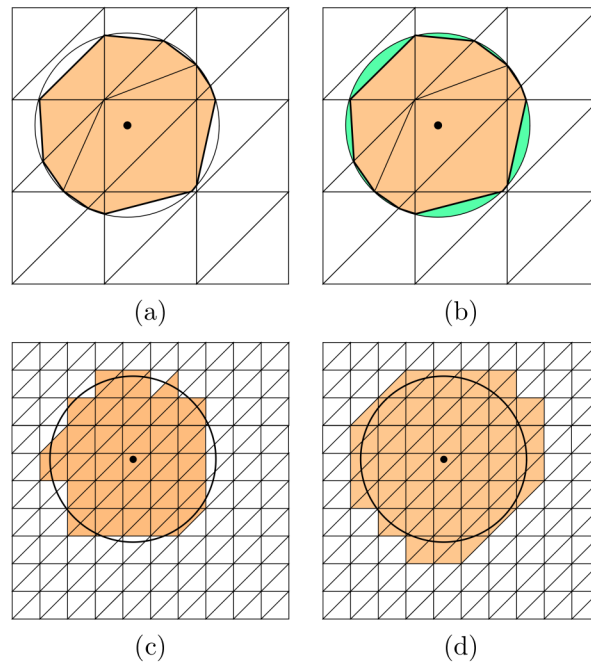


**Figure 2-4. From [25]: Cost functional evaluations (•) and BFGS iterates (–) for a 2D test problem and regularization  $\mathcal{R}(s, \delta) = \frac{\alpha}{s(1-s)} + \beta \frac{e^\delta}{\delta}$  with  $\alpha = 5 \times 10^{-7}$  and  $\beta = 10^{-6}$ . The final iterate is marked with  $\times$ , the parameters  $q^*$  used to generate the data  $u_d$  is marked with  $+$ .**

### 2.3. Implementation issues

The implementation of finite element methods (FEMs) for nonlocal models with a finite range of interaction poses challenges not faced in the partial differential equations (PDEs) setting. For example, one has to deal with weak forms involving double integrals which lead to discrete systems having higher assembly and solving costs due to possibly much lower sparsity compared to that of FEMs for PDEs. In addition, one may encounter nonsmooth integrands. In many nonlocal models, nonlocal interactions are limited to bounded neighborhoods that are ubiquitously chosen to be Euclidean balls, resulting in the challenge of dealing with intersections of such balls with the finite elements. In [29], we focus on developing recipes for the efficient assembly of FEM stiffness matrices and on the choice of quadrature rules for the double integrals that contribute to the assembly efficiency and also possess sufficient accuracy. A major feature of our recipes is the use of approximate balls, e.g. several polygonal approximations of Euclidean balls, that, among other advantages, mitigate the challenge of dealing with ball-element intersections. We provide numerical illustrations of the relative accuracy and efficiency of the several approaches we develop.

In [24], we design efficient quadrature rules for finite element (FE) discretizations of nonlocal diffusion problems with compactly supported kernel functions. Two of the main challenges in nonlocal modeling and simulations are the prohibitive computational cost and the nontrivial implementation of discretization schemes, especially in three-dimensional settings. In this work,



**Figure 2-5. From [29]: Different approaches to approximate the integration domain in the assembly of nonlocal operators with finite horizon. (a) An inscribed polygonal approximation of the ball. (b) Subdivision of the ball into the polygon of (a) and circular caps. An inscribed polygonal approximation of the ball is defined by approximating the green caps by triangles. (c) Approximation of the ball by whole finite element triangles that intersect the ball and for which the barycenter lies within the ball. (d) Approximation of the ball by all whole finite element triangles that intersect the ball.**

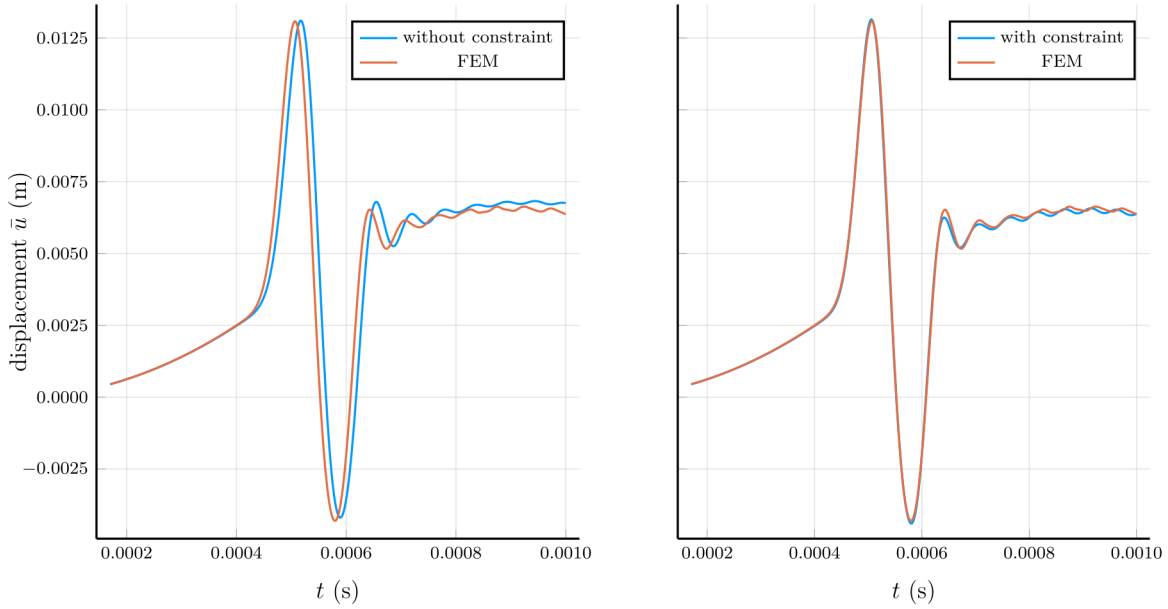
we circumvent both challenges by introducing a parametrized mollifying function that improves the regularity of the integrand, utilizing an adaptive integration technique, and exploiting parallelization. We first show that the “mollified” solution converges to the exact one as the mollifying parameter vanishes, then we illustrate the consistency and accuracy of the proposed method on several two- and three-dimensional test cases. Furthermore, we demonstrate the good scaling properties of the parallel implementation of the adaptive algorithm and we compare the proposed method with recently developed techniques for efficient FE assembly.

## 2.4. Applications in mechanics and subsurface transport

As a nonlocal extension of continuum mechanics, peridynamics has been widely and effectively applied in different fields where discontinuities in the field variables arise from an initially continuous body. An important component of the constitutive model in peridynamics is the influence function which weights the contribution of all the interactions over a nonlocal region surrounding a point of interest. Recent work has shown that in solid mechanics the influence function has a strong relationship with the heterogeneity of a material’s micro-structure. However, determining an accurate influence function analytically from a given micro-structure typically requires lengthy derivations and complex mathematical models. To avoid these complexities, in [32] we develop a data-driven regression algorithm to find the optimal bond-based peridynamic model to describe the macro-scale deformation of linear elastic medium with periodic heterogeneity. We generate macro-scale deformation training data by averaging over periodic micro-structure unit cells and add a physical energy constraint representing the homogenized elastic modulus of the micro-structure to the regression algorithm. We demonstrate this scheme for examples of one- and two-dimensional linear elastodynamics and show that the energy constraint improves the accuracy of the resulting peridynamic model.

In [34], we show that machine learning can improve the accuracy of simulations of stress waves in one-dimensional composite materials. We propose a data-driven technique to learn nonlocal constitutive laws for stress wave propagation models. The method is an optimization-based technique in which the nonlocal kernel function is approximated via Bernstein polynomials. The kernel, including both its functional form and parameters, is derived so that when used in a nonlocal solver, it generates solutions that closely match high-fidelity data. The optimal kernel therefore acts as a homogenized nonlocal continuum model that accurately reproduces wave motion in a smaller-scale, more detailed model that can include multiple materials. We apply this technique to wave propagation within a heterogeneous bar with a periodic microstructure. Several one-dimensional numerical tests illustrate the accuracy of our algorithm. The optimal kernel is demonstrated to reproduce high-fidelity data for a composite material in applications that are substantially different from the problems used as training data.

Anomalous behavior is ubiquitous in subsurface solute transport due to the presence of high degrees of heterogeneity at different scales in the media. Although fractional models have been extensively used to describe the anomalous transport in various subsurface applications, their application is hindered by computational challenges. Simpler nonlocal models characterized by integrable kernels and finite interaction length represent a computationally feasible alternative to

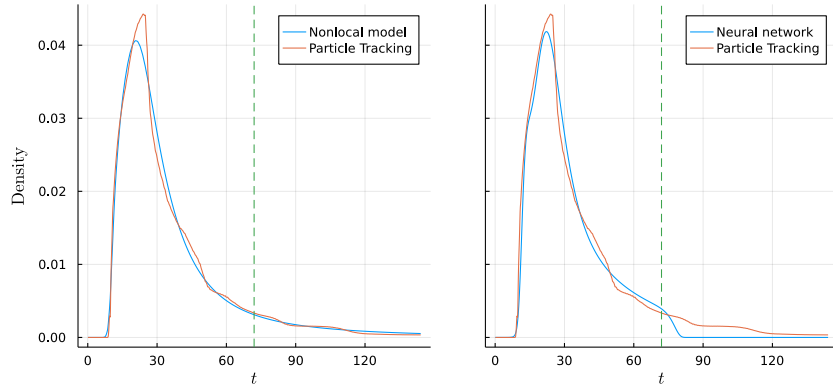


**Figure 2-6. From [32]: Validation results on the displacement for influence functions learned with and without energy constraint. The importance of the imposed energy constraint is apparent.**

fractional models; yet, the informed choice of their kernel functions still remains an open problem. In [36], we propose a general data-driven framework for the discovery of optimal kernels on the basis of very small and sparse data sets in the context of anomalous subsurface transport. Using spatially sparse breakthrough curves recovered from fine-scale particle-density simulations, we learn the best coarse-scale nonlocal model using a nonlocal operator regression technique. Predictions of the breakthrough curves obtained using the optimal nonlocal model show good agreement with fine-scale simulation results even at locations and time intervals different from the ones used to train the kernel, confirming the excellent generalization properties of the proposed algorithm. A comparison with trained classical models and with black-box deep neural networks confirms the superiority of the predictive capability of the proposed model.

## 2.5. Coupling and domain decomposition methods

Nonlocal models provide accurate representations of physical phenomena ranging from fracture mechanics to complex subsurface flows, settings in which traditional partial differential equation models fail to capture effects caused by long-range forces at the microscale and mesoscale. However, the application of nonlocal models to problems involving interfaces, such as multimaterial simulations and fluid-structure interaction, is hampered by the lack of a physically consistent interface theory which is needed to support numerical developments and, among other features, reduces to classical models in the limit as the extent of nonlocal interactions vanish. In [23], we use an energy-based approach to develop a formulation of a nonlocal interface problem which provides a physically consistent extension of the classical perfect interface formulation for

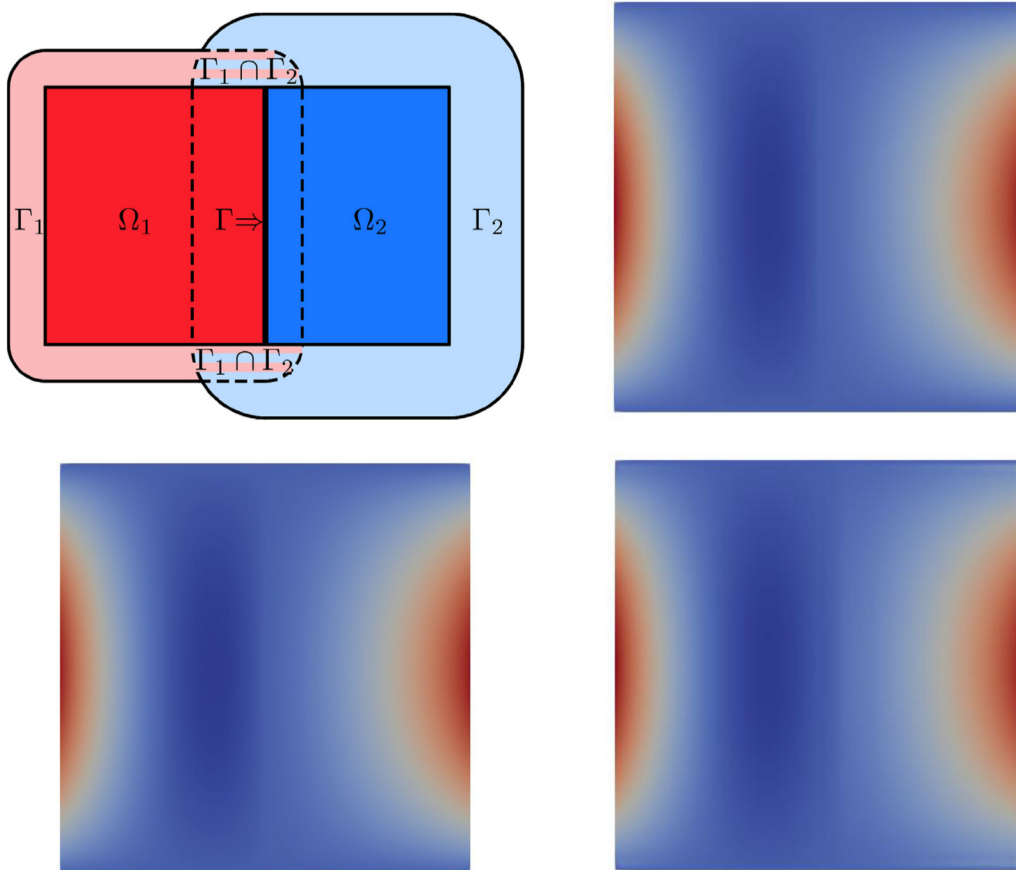


**Figure 2-7. From [36]: Breakthrough curve prediction by nonlocal dynamic kernel learned from sparse data and blackbox neural network surrogate (the green dashed line is used to separate training and testing). The proposed model using a learned nonlocal dynamic kernel manages to correctly reproduce the tail behavior in the testing regime, whereas the blackbox neural network fails.**

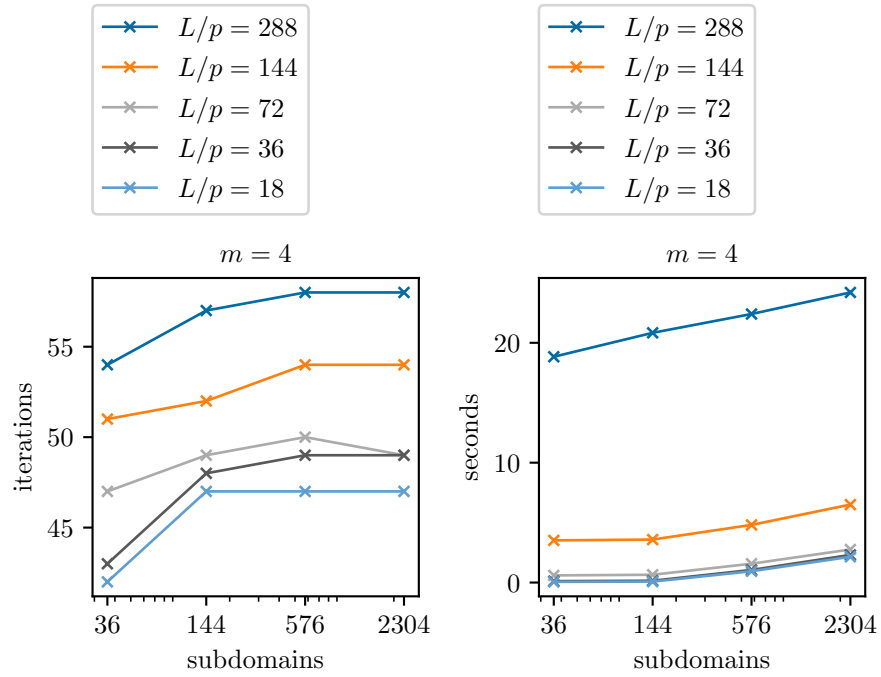
partial differential equations. Numerical examples in one and two dimensions validate the proposed framework and demonstrate the scope of our theory.

In [22], a mathematical framework is provided for a substructuring-based domain decomposition (DD) approach for nonlocal problems that features interactions between points separated by a finite distance. Here, by substructuring it is meant that a traditional geometric configuration for local partial differential equation (PDE) problems is used in which a computational domain is subdivided into non-overlapping subdomains. In the nonlocal setting, this approach is substructuring-based in the sense that those subdomains interact with neighboring domains over interface regions having finite volume, in contrast to the local PDE setting in which interfaces are lower dimensional manifolds separating abutting subdomains. Key results include the equivalence between the global, single-domain nonlocal problem and its multi-domain reformulation, both at the continuous and discrete levels. These results provide the rigorous foundation necessary for the development of efficient solution strategies for nonlocal DD methods.

In [33], we propose a domain decomposition method for the efficient simulation of nonlocal problems. Our approach is based on a multi-domain formulation of a nonlocal diffusion problem where the subdomains share “nonlocal” interfaces of the size of the nonlocal horizon. This system of nonlocal equations is first rewritten in terms of minimization of a nonlocal energy, then discretized with a meshfree approximation and finally solved via a Lagrange multiplier approach in a way that resembles the finite element tearing and interconnect method. Specifically, we propose a distributed projected gradient algorithm for the solution of the Lagrange multiplier system, whose unknowns determine the nonlocal interface conditions between subdomains. Several two-dimensional numerical tests on problems as large as 191 million unknowns illustrate the strong and the weak scalability of our algorithm, which outperforms the standard approach to the distributed numerical solution of the problem. This work is the first rigorous numerical study in a two-dimensional multi-domain setting for nonlocal operators with finite horizon and, as such,



**Figure 2-8. From [23]: Top left: domain configuration for 2D numerical test. Top right: numerical solution of the local coupling problem in  $\Omega_1 \cup \Omega_2$ . Bottom left: numerical solution of the nonlocal coupling problem in  $\Omega_1 \cup \Omega_2$  with  $(\delta_1, \delta_2) = (2^{-8}, 2^{-7})$ . Bottom right: numerical solution of the nonlocal coupling problem in  $\Omega_1 \cup \Omega_2$  with  $(\delta_1, \delta_2) = (2^{-4}, 2^{-3})$ .**



**Figure 2-9. From [33]: Weak scaling of the substructuring solver for constant horizon and different local problem sizes  $L/p$ . Dirichlet preconditioner, Cholesky solvers in the operator and preconditioner.**

it is a fundamental step towards increasing the use of nonlocal models in large scale simulations.

### 3. PROJECT METRICS

#### 3.1. Staffing

The team was composed of Marta D’Elia (8734, PI, until 6/2022), Christian Glusa (1465, PI since 6/2022), Pavel Bochev (1400), Jeremy Trageser (1444, now 1542, FY20&FY21) and Mamikon Gulian (8734, FY22).

Kristopher Kuhlman (8864), Mario Martinez (1516), Habib Najm (8300), Stewart Silling (1444) and Michael Tupek (previously 1542) and supported the project as consultants.

During the full duration of the project, a subcontract was in place with Professor Max Gunzburger from Florida State University. Giacomo Capodaglio (now Los Alamos National Laboratory) worked under this contract for FY 20.

For FY 21 and FY 22, a subcontract was in place with Professor John Foster from University of Texas, Austin. Xiao Xu worked under this contract for both years.

#### 3.2. Publications

During the lifetime of the project, we published 15 papers. 3 more manuscripts have been accepted for publication. 2 manuscripts are currently in peer review. Moreover, we are working on 5 draft manuscripts that are to be submitted before the end of the project.

Giacomo Capodaglio, Marta D’Elia, Max Gunzburger, Pavel Bochev, Manuel Klar, and Christian Vollmann. “A general framework for substructuring-based domain decomposition methods for models having nonlocal interactions”. In: *Numerical Methods for Partial Differential Equations* (2020). DOI: <https://doi.org/10.1002/num.22832>.

Giacomo Capodaglio, Marta D’Elia, Pavel Bochev, and Max Gunzburger. “An energy-based coupling approach to nonlocal interface problems”. In: *Computers & Fluids* 207 (2020), p. 104593. DOI: <https://doi.org/10.1016/j.compfluid.2020.104593>.

Marta D’Elia, Qiang Du, Christian Glusa, Max Gunzburger, Xiaochuan Tian, and Zhi Zhou. “Numerical methods for nonlocal and fractional models”. In: *Acta Numerica* 29 (2020), pp. 1–124. DOI: [10.1017/S096249292000001X](https://doi.org/10.1017/S096249292000001X).

Eugenio Aulisa, Giacomo Capodaglio, Andrea Chierici, and Marta D’Elia. “Efficient quadrature rules for finite element discretizations of nonlocal equations”. In: *Numerical Methods for Partial Differential Equations* (2021). DOI: [10.1002/num.22833](https://doi.org/10.1002/num.22833).

- Olena Burkovska, Christian Glusa, and Marta D’Elia. “An optimization-based approach to parameter learning for fractional type nonlocal models”. In: *Computers & Mathematics with Applications* (2021). DOI: 10.1016/j.camwa.2021.05.005.
- Marta D’Elia and Christian Glusa. “A fractional model for anomalous diffusion with increased variability: Analysis, algorithms and applications to interface problems”. In: *Numerical Methods for Partial Differential Equations* (2021). DOI: 10.1002/num.22865.
- Marta D’Elia and Mamikon Gulian. “Analysis of anisotropic nonlocal diffusion models: Well-posedness of fractional problems for anomalous transport”. In: *arXiv preprint arXiv:2101.04289* (2021).
- Marta D’Elia, David Littlewood, Jeremy Trageser, Mauro Perego, and Pavel Bochev. “An optimization-based strategy for peridynamic-FEM coupling and for the prescription of nonlocal boundary conditions”. In: *arXiv preprint arXiv:2110.04420* (2021).
- Marta D’Elia and Pavel Bochev. “Formulation, analysis and computation of an optimization-based local-to-nonlocal coupling method”. In: *Results in Applied Mathematics* 9 (2021), p. 100129. DOI: 10.1016/j.rinam.2020.100129.
- Marta D’Elia, Max Gunzburger, and Christian Vollmann. “A cookbook for approximating Euclidean balls and for quadrature rules in finite element methods for nonlocal problems”. In: *Mathematical Models and Methods in Applied Sciences* 31.08 (2021), pp. 1505–1567. DOI: 10.1142/S0218202521500317.
- Marta D’Elia, Xingjie Li, Pablo Seleson, Xiaochuan Tian, and Yue Yu. “A review of local-to-nonlocal coupling methods in nonlocal diffusion and nonlocal mechanics”. In: *Journal of Peridynamics and Nonlocal Modeling* (2021), pp. 1–50.
- Christian Glusa and Enrique Otárola. “Error Estimates for the Optimal Control of a Parabolic Fractional PDE”. In: *SIAM Journal on Numerical Analysis* 59.2 (2021), pp. 1140–1165. DOI: 10.1137/19M1267581.
- Jorge Suzuki, Mamikon Gulian, Mohsen Zayernouri, and Marta D’Elia. “Fractional modeling in action: A survey of nonlocal models for subsurface transport, turbulent flows, and anomalous materials”. In: *arXiv preprint arXiv:2110.11531* (2021).
- Xiao Xu, Marta D’Elia, and John T Foster. “A machine-learning framework for peridynamic material models with physical constraints”. In: *Computer Methods in Applied Mechanics and Engineering* 386 (2021), p. 114062. DOI: <https://doi.org/10.1016/j.cma.2021.114062>.
- Xiao Xu, Christian Glusa, Marta D’Elia, and John T. Foster. “A FETI approach to domain decomposition for meshfree discretizations of nonlocal problems”. In: *Computer Methods in Applied Mechanics and Engineering* 387 (2021), p. 114148. DOI: 10.1016/j.cma.2021.114148.
- Huaiqian You, Yue Yu, Stewart Silling, and Marta D’Elia. “Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws”. In: *Proceedings of the AAAI 2021 Spring Symposium on Combining Artificial Intelligence and Machine Learning with Physical Sciences*. 2021.

Eric Darve, Marta D’Elia, Roberto Garrappa, Andrea Giusti, and Natalia L Rubio. “On the fractional Laplacian of variable order”. In: *Fractional Calculus and Applied Analysis* 25.1 (2022), pp. 15–28.

Christian Glusa, Marta D’Elia, Giacomo Capodaglio, Max Gunzburger, and Pavel B Bochev. “An asymptotically compatible coupling formulation for nonlocal interface problems with jumps”. In: *arXiv preprint arXiv:2203.07565* (2022).

Xiao Xu, Marta D’Elia, Christian Glusa, and John T Foster. “Machine-learning of nonlocal kernels for anomalous subsurface transport from breakthrough curves”. In: *arXiv preprint arXiv:2201.11146* (2022).

Xiao Xu, Marta D’Elia, Christian Glusa, and John T Foster. “Machine-learning of nonlocal kernels for anomalous subsurface transport from breakthrough curves”. In: *Numerical Algebra, Control and Optimization* (2022).

Alessandro Alla, Marta D’Elia, Christian Glusa, and Hugo Oliveira. “Control of fractional diffusion problems via dynamic programming equations”.

Giacomo Capodaglio, Marta D’Elia, Christian Glusa, Max Gunzburger, Manuel Klar, and Christian Vollmann. “A scalable substructuring approach for peridynamics”.

Marta D’Elia, Yiming Fan, Habib Najm, Stewart Silling, and Yue Yu. “Bayesian nonlocal operator regression”.

Marta D’Elia, Christian Glusa, Mamikon Gulian, and Jeffrey Hyman. “Calibrating Fractional-Order Models for Anomalous Subsurface Flow through Fractures”.

Christian Glusa and Pierre Marchand. “Two-level overlapping Schwarz method with GenEO coarse grid for the fractional Laplacian”.

### 3.3. Presentations

During the lifetime of the project (FY20-22) our team presented a total of 50 conference, workshop and colloquia talks. In particular, we highlight that we gave 5 plenary talks. A list of presentations follows.

Marta D’Elia. *Mathematical foundations of Nonlocal Interface Problems*. MULTIMAT2019, Trento, Italy. Sept. 9–14, 2019.

Marta D’Elia. *Nonlocal models in computational science and engineering*. University of California at Berkeley. Nov. 14, 2019.

Marta D’Elia. *Nonlocal models in computational science and engineering*. Michigan State University. Oct. 1, 2019.

Christian Glusa. *Multigrid for fractional Laplacians*. AMG Summit, Santa Fe. Oct. 2019.

Giacomo Capodaglio. *Modeling and approximation of interface problems in nonlocal diffusion*. JMM, Joint Mathematics Meeting, Denver, CO. Jan. 15–18, 2020.

Giacomo Capodaglio. *Substructuring-based domain decomposition methods for nonlocal problems*. SIAM TX-LA Section, Texas A&A University. Oct. 16–18, 2020.

Marta D’Elia. *Nonlocal models in computational science and engineering*. University of New Mexico, Albuquerque, NM. Feb. 24, 2020.

Marta D’Elia. *Nonlocal Models in Computational Science and Engineering: theory and challenges*. Summer School at Sapienza University of Rome, Aerospace Engineering Department. Sept. 2020.

Marta D’Elia. *Nonlocal Models in Computational Science and Engineering: theory and challenges*. GA Scientific Computing Symposium, Atlanta, GA. Feb. 29, 2020.

Giacomo Capodaglio. *An energy-based coupling approach to nonlocal interface problems*. USNCCM, Chicago. July 25–29, 2021.

Giacomo Capodaglio. *An energy-based coupling approach to nonlocal interface problems*. One Nonlocal World opening event. Jan. 20–21, 2021.

Giacomo Capodaglio. *Substructuring-Based Domain Decomposition Methods For Nonlocal Problems*. Center for Nonlinear Studies seminar, LANL. Oct. 14, 2021.

Andrea Chierici. *Efficient quadrature rules for finite element discretizations of nonlocal equations*. One Nonlocal World opening event. Jan. 20–21, 2021.

Marta D’Elia. *A FETI approach to domain decomposition for meshfree discretizations of nonlocal problems*. SIAM CSE21, Fort Worth. Mar. 1–5, 2021.

Marta D’Elia. *A fractional model for anomalous diffusion with increased variability. Analysis, algorithms and applications to interface problems*. SIAM MS21, Bilbao, Spain. June 17–28, 2021.

Marta D’Elia. *A Unified Theory of Fractional and Nonlocal Calculus*. INdAM workshop on Fractional Differential Equations: Modeling, Discretization, and Numerical Solvers. July 13, 2021.

Marta D’Elia. *Addressing micro-scale interfaces via nonlocal models using ML*. Coupled Problems. June 14, 2021.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. IMECE, ASME Conference. Nov. 4, 2021.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. Workshop Nonlocality in Analysis, Numerics and Applications, Lorentz Institute, Leiden University, the Netherlands. Oct. 27, 2021.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. Amerimech Symposium Series, Machine Learning in Heterogeneous Porous Materials. Oct. 4, 2021.

Marta D’Elia. *Challenges in nonlocal modeling: nonlocal boundary conditions and interfaces*. WCCM20. Jan. 11–15, 2021.

Marta D’Elia. *Data Driven Learning of Nonlocal Models*. Invited Lecture at CMU. Mar. 16, 2021.

Marta D’Elia. *Data Driven Learning of Nonlocal Models*. Invited Lecture at CalTech. Mar. 10, 2021.

Marta D’Elia. *Data-driven learning of nonlocal models*. ALOP workshop on nonlocal models. July 12–14, 2021.

Marta D’Elia. *Data-driven learning of nonlocal models*. Mechanistic Machine Learning and Digital Twins, San Diego, CA. Sept. 9, 2021.

Marta D’Elia. *Data-driven learning of nonlocal models*. DDPS Seminar Series, Lawrence Livermore National Lab, CA. July 20, 2021.

Marta D’Elia. *Data-driven learning of nonlocal models*. SIAM Annual Meeting 2021. July 21, 2021.

Marta D’Elia. *Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws*. USNCCM, Chicago. July 25–29, 2021.

Marta D’Elia. *Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws*. AAAI Spring Symposium: MLPS, 2021, Stanford University. Mar. 24, 2021.

Christian Glusa. *A fractional model for anomalous diffusion with increased variability. Analysis, algorithms and applications to interface problems*. USNCCM, Chicago. July 25–29, 2021.

Christian Glusa. *A fractional model for anomalous diffusion with increased variability. Analysis, algorithms and applications to interface problems*. Coupled Problems 2021, Chia Laguna, Italy. June 14–18, 2021.

Christian Glusa. *A fractional model for anomalous diffusion with increased variability. Analysis, algorithms and applications to interface problems*. One Nonlocal World opening event. Jan. 20–21, 2021.

Christian Glusa. *Optimal Control for the Fractional Laplacian*. IFIP TC7 Conference on System Modelling and Optimization. Aug. 2021.

Christian Glusa. *Optimal Control for the Fractional Laplacian*. SIAM CSE21, Fort Worth. Mar. 1–5, 2021.

Max Gunzburger. *Finite element methods for nonlocal problems, including quadrature rules and approximate Euclidean balls*. One Nonlocal World opening event. Jan. 20–21, 2021.

Xiao Xu. *A machine-learning framework for peridynamic material models with physical constraints*. SIAM CSE21, Fort Worth. Mar. 1–5, 2021.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. Joint MMHM-NAA-DMC seminar, Nottingham, UK. June 8, 2022.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. Seminar at the Hong Kong Polytechnic University, Department of applied mathematics, Hong Kong, China. May 10, 2022.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. Joint Mathematics Meeting, Seattle, WA. Apr. 8, 2022.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. Artificial Intelligence Research and Optimization seminar series, Louisiana State University, LA. Apr. 6, 2022.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. MICDE Seminar at the University of Michigan. Mar. 14, 2022.

Marta D’Elia. *Bridging scales with Nonlocality: data-driven learning of nonlocal models*. Oden Institute, University of Texas, Austin. Mar. 8, 2022.

Marta D’Elia. *Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws*. BIRS workshop: Theoretical and Applied Aspects for Nonlocal Models. July 18–22, 2022.

Christian Glusa. *Domain Decomposition Methods for Nonlocal Equations*. 27th International Conference on Domain Decomposition Methods. July 25–29, 2022.

Christian Glusa. *Domain Decomposition Solvers for Nonlocal Equations*. 15th World Congress on Computational Mechanics. July 31–Aug. 5, 2022.

Christian Glusa. *Domain Decomposition Solvers for Nonlocal Equations*. SIAM PP22. Feb. 23–26, 2022.

Christian Glusa. *Scalable methods for nonlocal models*. BIRS workshop: Theoretical and Applied Aspects for Nonlocal Models. July 18–22, 2022.

Christian Glusa. *Scalable methods for nonlocal models*. Nonlocal School on Fractional Equations, Iowa State University. June 9–11, 2022.

Christian Glusa. *Scalable methods for nonlocal models*. Computation, Analysis and Applications of PDEs with Nonlocal and Singular Operators, National University of Singapore. Feb. 7–11, 2022.

Mamikon Gulian. *Calibrating Fractional-Order Models for Anomalous Subsurface Flow through Fractures*. 15th World Congress on Computational Mechanics. July 31–Aug. 5, 2022.

### 3.4. Conference organization

- Joint Mathematics Meeting 2019, Denver, Jan 15-18, 2019. Special Session on Analysis of nonlocal models.
- World Congress on Computational Mechanics, Paris, France, Jul 20-24, 2020. Special session on Computational aspects of nonlocal models. (Canceled due to COVID-19 outbreak)
- One Nonlocal World Opening Event (PI founder and organizer), Jan 20-21, 2021.
- SIAM CSE21, Fort Worth, TX, March 1-5, 2021. Two minisymposia titled "Nonlocal models in computational Science and Engineering" and on "Model learning and optimization for nonlocal models".
- Coupled Problems 2021. Chia Laguna, Italy, June 14-18, 2021. Invited special session on Nonlocal Interface problems.
- SIAM MS21, Bilbao, Spain, virtually. Nonlocality in data-driven and physics-based materials modeling.

- USNCCM16, Chicago, IL, July 25-29, 2021. Invited session on Nonlocal interface problems.
- World Congress on Computational Mechanics, Yokohama, Japan, July 31-August 5, 2022. Minisymposia on “Nonlocal models in computational mechanics” and “Model Learning and Optimization for Nonlocal and Fractional Equations”

### 3.5. Team building and partnerships

During the course of the project we have created a large number of collaborations with researchers in academia and at other national labs, both domestically and abroad. Below we list the different groups that we have worked with and the resulting publications.

- Manuel Klar, Christian Vollmann (University of Trier, Germany) [22] [29]
- Max Gunzburger (Florida State University), Giacomo Capodaglio (Los Alamos National Laboratory, previously Florida State University) [23] [22] [23] [35] [24]
- Yue Yu, Huaiqian You (Lehigh University)
- John Foster, Xiao Xu (University of Texas, Austin) [32] [33] [36]
- Olena Burkovska (Oak Ridge National Laboratory) [25]
- Pablo Seleson (Oak Ridge National Laboratory) [30]
- Eugenio Aulisa, Andrea Chierici (Texas Tech University) [24]
- Enrique Otárola (Universidad Tecnica Federico Santa Maria, Chile) [31]
- Pierre Marchand (INRIA, France)
- Jeffrey Hyman (Los Alamos National Laboratory)
- Alessandro Alla (Università Ca’ Foscari Venezia, Italy, previously PUC-Rio, Rio de Janeiro, Brazil), Hugo Oliveira (PUC-Rio, Rio de Janeiro, Brazil)

The groundwork that was laid during the MATNIP project lead to a number of tangential grant proposals:

- Discovery of Fractional-Order Models (DiFract); 3 year CIS LDRD; PI: Christian Glusa (not funded)
- Multiscale Learning via Integral Operators, improved homogenized surrogates for heterogeneous materials models beyond PDEs; ASCR Base Math proposal; PI: Marta D’Elia (not funded)
- Domain Decomposition Methods for Nonlocal Problems in a Finite Element Framework; 3 year LDRD at Los Alamos National Laboratory; PI: Giacomo Capodaglio (not funded)

- Fractional-Order Models for Sea Ice (FOMSI); 3 year CIS LDRD; PI: Christian Glusa (funded)
- Seamless data-driven modeling of corrosion through different phases of damage using integro-differential equations; ExEx LDRD; PI: Mamikon Gulian

### **3.6. Mentoring and training**

- Marta D'Elia got promoted from Senior Member of Technical Staff to Principal Member.
- Christian Glusa got converted from Limited Term Employee to Foreign National Interim Technical Staff.
- Giacomo Capodaglio took on a staff position at Los Alamos National Laboratory after his postdoc with Max Gunzburger at Florida State University.

The MATNIP project also actively engaged with the academic community and interacted with multiple graduate students:

- Hayley Olson 3 summers (University of Nebraska-Lincoln, graduated in spring 2022, now postdoc at Carnegie Mellon University)
- Xiao Xu (University of Texas, Austin, graduated in spring 2022)
- Yiming Fan (Lehigh University, 2 summers as an intern in Sandia CA)
- Hugo Oliveira (PUC-Rio, Rio de Janeiro, Brazil, graduation in fall 2022)
- Manuel Klar (University of Trier, Germany, graduation in spring 2023)

## 4. PROJECT LEGACY

### 4.1. PyNucleus

PyNucleus <https://github.com/sandialabs/PyNucleus> is a finite element code that specifically targets nonlocal operators of the form

$$\int_{\mathbb{R}^d} [u(x) - u(y)] \gamma(x, y) dy$$

for nonlocal kernels  $\gamma$  with finite or infinite horizon and of integrable or fractional type. Specific examples of such operators include the integral and regional fractional Laplacians, their truncated and tempered variants, and operators arising from peridynamics.

The package aims to provide efficient discretization and assembly routines with  $O(N \log N)$  quasi-optimal complexity. The resulting sets of equations can be solved using optimal linear solvers. The code is fully NumPy/SciPy compatible, allowing easy integration into application codes.

Features:

- Simplicial meshes in 1D, 2D, 3D
- Finite Elements:
  - continuous P1, P2, P3 spaces,
  - discontinuous P0 space
- Assembly of local operators
- Nonlocal kernels:
  - Finite and infinite horizon
  - Singularities: fractional, peridynamic, constant kernel
  - spatially variable kernels: variable fractional order and variable coefficients
- Nonlocal assembly (1D and 2D) into dense, sparse and hierarchical matrices
- Solvers/preconditioners:
  - LU,
  - Cholesky,
  - incomplete LU & Cholesky,

- Jacobi,
  - CG,
  - BiCGStab,
  - GMRES,
  - geometric multigrid
- Distributed computing using MPI
  - Computationally expensive parts of the code are compiled via Cython.
  - Partitioning using METIS / ParMETIS

## **4.2. Fractional-Order Models for Sea Ice (FOMSI)**

Modeling sea-ice deformation and drift is critical in climate simulation and prediction, as ocean, ice layers and atmosphere form a tightly coupled system. Sea ice has a strong influence on global climate by reflecting solar radiation, regulating heat transfer between ocean and atmosphere, and influencing ocean currents. On smaller scales, seasonal and subseasonal predictions of Arctic sea ice are critically important for navigation. In both cases, it is necessary to accurately capture the dynamics of sea ice to enable accurate predictions.

Current sea-ice descriptions cannot achieve accuracy at kilometer scale. By accurately reproducing experimentally observed behavior, the proposed fractional-order models will greatly improve the fidelity of sea-ice simulation, and consequently climate prediction as a whole.

The CIS LDRD FOMSI project will leverage solvers and expertise developed by MATNIP.

## **4.3. Project files**

Artifacts of the project are kept in several git repositories under the MATNIP project at <https://gitlab-ex.sandia.gov/matnip>.

## BIBLIOGRAPHY

- [1] Peter W Bates and Adam Chmaj. “An integrodifferential model for phase transitions: stationary solutions in higher space dimensions”. In: *Journal of statistical physics* 95.5 (1999), pp. 1119–1139.
- [2] David A Benson, Stephen W Wheatcraft, and Mark M Meerschaert. “Application of a fractional advection-dispersion equation”. In: *Water resources research* 36.6 (2000), pp. 1403–1412.
- [3] S. Silling. “Reformulation of elasticity theory for discontinuities and long-range forces”. In: *Journal of the Mechanics and Physics of Solids* 48 (2000), pp. 175–209.
- [4] Rina Schumer, David A Benson, Mark M Meerschaert, and Stephen W Wheatcraft. “Eulerian derivation of the fractional advection–dispersion equation”. In: *Journal of contaminant hydrology* 48.1-2 (2001), pp. 69–88.
- [5] Paul Fife. “Some nonclassical trends in parabolic and parabolic-like evolutions”. In: *Trends in nonlinear analysis* (2003), pp. 153–191.
- [6] Rina Schumer, David A Benson, Mark M Meerschaert, and Boris Baeumer. “Multiscaling fractional advection-dispersion equations and their solutions”. In: *Water Resources Research* 39.1 (2003).
- [7] G. Gilboa and S. Osher. “Nonlocal linear image regularization and supervised segmentation”. In: *Multiscale Model. Simul.* 6 (2007), pp. 595–630.
- [8] E Askari, F Bobaru, RB Lehoucq, ML Parks, SA Silling, and O Weckner. “Peridynamics for multiscale materials modeling”. In: *Journal of Physics: Conference Series*. Vol. 125. 1. IOP Publishing. 2008, p. 012078.
- [9] G. Gilboa and S. Osher. “Nonlocal operators with applications to image processing”. In: *Multi. Model. Simul.* 7 (2008), pp. 1005–1028.
- [10] Alexander A Schekochihin, Steven C Cowley, and Tarek A Yousef. “MHD turbulence: Nonlocal, anisotropic, nonuniversal?” In: *IUTAM Symposium on computational physics and new perspectives in turbulence*. Springer. 2008, pp. 347–354.
- [11] A. Buades, B. Coll, and J. Morel. “Image denoising methods. A new nonlocal principle”. In: *SIAM Review* 52 (2010), pp. 113–147.
- [12] David J Littlewood. “Simulation of dynamic fracture using peridynamics, finite element modeling, and contact”. In: *ASME International Mechanical Engineering Congress and Exposition*. Vol. 44465. 2010, pp. 209–217.
- [13] Y. Lou, X. Zhang, S. Osher, and A. Bertozzi. “Image Recovery via Nonlocal Operators”. In: *J. Sci. Comput.* 42 (2010), pp. 185–197.

- [14] Youn Doh Ha and Florin Bobaru. “Characteristics of dynamic brittle fracture captured with peridynamics”. In: *Engineering Fracture Mechanics* 78.6 (2011), pp. 1156–1168.
- [15] Bacim Alali and Robert Lipton. “Multiscale dynamics of heterogeneous media in the peridynamic formulation”. In: *Journal of Elasticity* 106 (2012), pp. 71–103.
- [16] M. Meerschaert and A. Sikorskii. *Stochastic models for fractional calculus*. De Gruyter, Berlin-Boston, 2012.
- [17] Pablo Seleson, Max Gunzburger, and Michael L Parks. “Interface problems in nonlocal diffusion and sharp transitions between local and nonlocal domains”. In: *Computer Methods in Applied Mechanics and Engineering* 266 (2013), pp. 185–204.
- [18] N. Burch, M. D’Elia, and R Lehoucq. “The exit-time problem for a Markov jump process”. In: *The European Physical Journal Special Topics* 223 (2014), pp. 3257–3271.
- [19] Bacim Alali and Max Gunzburger. “Peridynamics and material interfaces”. In: *Journal of Elasticity* 120.2 (2015), pp. 225–248.
- [20] Amir H Delgoushaie, Daniel W Meyer, Patrick Jenny, and Hamdi A Tchelepi. “Non-local formulation for multiscale flow in porous media”. In: *Journal of Hydrology* 531 (2015), pp. 649–654.
- [21] Marta D’Elia, Qiang Du, Max Gunzburger, and Richard B. Lehoucq. “Nonlocal convection-diffusion problems on bounded domains and finite-range jump processes”. In: *Comput. Meth. in Appl. Math.* 17 (2017), pp. 707–722.
- [22] Giacomo Capodaglio, Marta D’Elia, Max Gunzburger, Pavel Bochev, Manuel Klar, and Christian Vollmann. “A general framework for substructuring-based domain decomposition methods for models having nonlocal interactions”. In: *Numerical Methods for Partial Differential Equations* (2020). DOI: <https://doi.org/10.1002/num.22832>.
- [23] Giacomo Capodaglio, Marta D’Elia, Pavel Bochev, and Max Gunzburger. “An energy-based coupling approach to nonlocal interface problems”. In: *Computers & Fluids* 207 (2020), p. 104593. DOI: <https://doi.org/10.1016/j.compfluid.2020.104593>.
- [24] Eugenio Aulisa, Giacomo Capodaglio, Andrea Chierici, and Marta D’Elia. “Efficient quadrature rules for finite element discretizations of nonlocal equations”. In: *Numerical Methods for Partial Differential Equations* (2021). DOI: [10.1002/num.22833](https://doi.org/10.1002/num.22833).
- [25] Olena Burkovska, Christian Glusa, and Marta D’Elia. “An optimization-based approach to parameter learning for fractional type nonlocal models”. In: *Computers & Mathematics with Applications* (2021). DOI: [10.1016/j.camwa.2021.05.005](https://doi.org/10.1016/j.camwa.2021.05.005).
- [26] Marta D’Elia and Christian Glusa. “A fractional model for anomalous diffusion with increased variability: Analysis, algorithms and applications to interface problems”. In: *Numerical Methods for Partial Differential Equations* (2021). DOI: [10.1002/num.22865](https://doi.org/10.1002/num.22865).
- [27] Marta D’Elia and Mamikon Gulian. “Analysis of anisotropic nonlocal diffusion models: Well-posedness of fractional problems for anomalous transport”. In: *arXiv preprint arXiv:2101.04289* (2021).

- [28] Marta D’Elia and Pavel Bochev. “Formulation, analysis and computation of an optimization-based local-to-nonlocal coupling method”. In: *Results in Applied Mathematics* 9 (2021), p. 100129. DOI: 10.1016/j.rinam.2020.100129.
- [29] Marta D’Elia, Max Gunzburger, and Christian Vollmann. “A cookbook for approximating Euclidean balls and for quadrature rules in finite element methods for nonlocal problems”. In: *Mathematical Models and Methods in Applied Sciences* 31.08 (2021), pp. 1505–1567. DOI: 10.1142/S0218202521500317.
- [30] Marta D’Elia, Xingjie Li, Pablo Seleson, Xiaochuan Tian, and Yue Yu. “A review of local-to-nonlocal coupling methods in nonlocal diffusion and nonlocal mechanics”. In: *Journal of Peridynamics and Nonlocal Modeling* (2021), pp. 1–50.
- [31] Christian Glusa and Enrique Otárola. “Error Estimates for the Optimal Control of a Parabolic Fractional PDE”. In: *SIAM Journal on Numerical Analysis* 59.2 (2021), pp. 1140–1165. DOI: 10.1137/19M1267581.
- [32] Xiao Xu, Marta D’Elia, and John T Foster. “A machine-learning framework for peridynamic material models with physical constraints”. In: *Computer Methods in Applied Mechanics and Engineering* 386 (2021), p. 114062. DOI: <https://doi.org/10.1016/j.cma.2021.114062>.
- [33] Xiao Xu, Christian Glusa, Marta D’Elia, and John T. Foster. “A FETI approach to domain decomposition for meshfree discretizations of nonlocal problems”. In: *Computer Methods in Applied Mechanics and Engineering* 387 (2021), p. 114148. DOI: 10.1016/j.cma.2021.114148.
- [34] Huaqian You, Yue Yu, Stewart Silling, and Marta D’Elia. “Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws”. In: *Proceedings of the AAAI 2021 Spring Symposium on Combining Artificial Intelligence and Machine Learning with Physical Sciences*. 2021.
- [35] Christian Glusa, Marta D’Elia, Giacomo Capodaglio, Max Gunzburger, and Pavel B Bochev. “An asymptotically compatible coupling formulation for nonlocal interface problems with jumps”. In: *arXiv preprint arXiv:2203.07565* (2022).
- [36] Xiao Xu, Marta D’Elia, Christian Glusa, and John T Foster. “Machine-learning of nonlocal kernels for anomalous subsurface transport from breakthrough curves”. In: *arXiv preprint arXiv:2201.11146* (2022).

## DISTRIBUTION

### Hardcopy—External

Number of Copies	Name(s)	Company Name and Company Mailing Address
1	Giacomo Capodaglio	CNLS, MS B258 Los Alamos National Laboratory Los Alamos, NM 87545
1	Marta D'Elia	Meta Reality Labs 900 5th Ave Sunnyvale, CA, 94089
1	John Foster	The University of Texas at Austin 200 E. Dean Keeton, Stop C0300 Austin, TX 78712-1585
1	Max Gunzburger	Dept. of Scientific Computing Florida State University 400 Dirac Science Library Tallahassee, FL 32306-4120

### Hardcopy—Internal

Number of Copies	Name	Org.	Mailstop
1	Pavel Bochev	1400	1320
1	John Feddema	1460	1324
1	Christian Glusa	1465	1318
1	Mamikon Gulian	8734	9060
1	David Littlewood	1444	1322
1	Habib Najm	8300	9051
1	Stewart Silling	1444	1322
1	James Stewart	1400	1318
1	Jeremy Trageser	1542	1322
1	L. Martin, LDRD Office	1910	0359

### Email—Internal (encrypt for OUO)

Name	Org.	Sandia Email Address
Technical Library	1911	sanddocs@sandia.gov





Sandia  
National  
Laboratories

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.