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Institution: Pennsylvania State University

Project Title:
Mathematical and Numerical Analyses of Peridynamics for Multiscale Materials Modeling

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Technical Progress:

Classical partial differential equation (PDE) models for diffusion (e.g., the heat equation) and mechanics (e.g., the Navier equation of linear elasticity) have been spectacularly successful in many scientific inquiry and technological design applications. Indeed, these models collectively represent some of the greatest triumphs in physics, engineering, and mathematics. A paradigm of classical PDE models is that interactions only occur though contact and infinitesimally in time. Still, in an ever-growing number of settings, classical models are found to fail to adequately describe the phenomena they purportedly model. An alternative approach is to replace the classical PDEs with integral operators that avoid spatial derivatives. Peridynamics is one of such theory that has attracted much attention in recent years. The peridynamic mechanic balance laws (momentum and energy) are instances of the nonlocal balance laws. Combining the nonlocal balance laws with a kinematic model leads to the peridynamic mechanics mechanic balance laws of momentum and energy.

Supported by the project *Mathematical and Numerical Analyses of Peridynamics for Multiscale Materials Modeling.* significant progress has been made in the areas of peridynamic mathematical and numerical analyses and in an unplanned foray into nonlocal diffusion and its probabilistic interpretations. This impressive body of work includes a SIAM review paper and numerous high quality publications and Ph.D theses. Our work has manifold DOE applications of interest, ranging from the design of composite materials, soft matter to flows in porous media.

–*Nonlocal vector calculus.*

We have developed a vector calculus for those operators that mimics the classical vector calculus for differential operators. The new nonlocal vector calculus is then used to define nonlocal balance laws where subregions not in direct contact may have a nonzero interaction. This is accomplished by defining a nonlocal flux in terms of interactions between regions having positive measure, possibly not sharing a common boundary. We have discussed necessary and sufficient condition for the resulting balance laws to be additive, an action-reaction principle to hold, and that the nonlocal flux is an alternating form. As a result, the nonlocal vector calculus provides an alternative to standard approaches for circumventing the technicalities associated with the lack of sufficient regularity in local balance laws by avoiding the use of derivatives. The nonlocal calculus is applied to diffusion, transport, and mechanics problems involving nonlocal interactions. Specific nonlocal field equations for these types of problems are developed by choosing, in the aforementioned balance laws, specific constitutive relations relating flux densities to intensive variables. An example is a nonlocal analogue of Fourier's heat law which yields a field equation for the temperature.

–*Numerical analysis and algorithms.*

For multiscale problems, adaptive computation is a key approach to obtain reliable and efficient numerical solutions. We have presented an a posteriori error analysis of conforming finite element methods for solving linear nonlocal diffusion and peridynamic mechanics models. A general abstract framework is developed for a posteriori error analysis of nonlocal volume constrained problems for scalar equations. A posteriori error estimators are provided for integrable kernels and the reliability and efficiency of the estimators is proved. Relationships between nonlocal classical local a posteriori error estimation are also studied.

We have further developed an adaptive finite element algorithm for the numerical solution of scalar nonlocal models. For problems involving certain non-integrable kernel functions, the convergence of the adaptive algorithm is rigorously derived with the help of several basic ingredients, such as an upper bound of the estimator, the estimator reduction, and the orthogonality property. This represents the first time in the literature that the convergence of adaptive finite element methods for nonlocal problems is rigorously proved. Moreover, we also consider how the results are affected by the horizon parameter.

–*Nonlocal diffusion and mechanics*,

In our SIAM review paper we have built upon the nonlocal vector calculus to present a comprehensive overview of nonlocal diffusion, demonstrating that the nonlocal diffusion equations are well-posed on bounded domains and also emphasizing the compelling analogy that can be drawn with classical diffusion, including that of a conforming finite element discretization. In addition, we demonstrate that some well-known models for nonlocal diffusion such as fractional Laplacian and a particular instance of a fractional derivative model are instances within of our more general theory.

Using the nonlocal vector calculus, we have provided the first rigorous mathematical formulation of the linear peridynamic Navier equation and associated volume constrained problem. The paper also demonstrates that in free space, the local limit of the nonlocal peridynamic Navier operator recovers the conventional Navier operator of linear elasticity with the entire range of allowable constants, e.g., Poisson ratio in the interval $(-1, 1/2)$. Moreover, the peridynamic Navier equation is shown to be well-posed over the space of square integrable functions for a locally integrable tensor kernel. Because the trace operator on this space is unbounded, traditional boundary conditions are not, in general, defined and so are replaced by a constraint on the displacement field over a volume of nonzero measure.

In a number of subsequent papers, we have further developed the nonlocal calculus of variations based on the nonlocal vector calculus. These works can be used in the analysis of variational problems associated with nonlocal models. For example, we have generalized the analysis of linear nonlocal models to include a nonintegrable tensor kernel and to cases where the kernel may change signs. This latter generalization is important because it is necessary for dealing with material instability within the peridynamic mechanics theory. In addition, these papers provide basic ingredients for the functional analysis of nonlocal energy spaces and nonlocal variational problems with general kernels for both scalar equations and for systems.

In addition, we have introduces the notion of a nonlinear, nonlocal conservation law in one-dimension. The model serves as a fundamental building block for the future study of more general nonlocal conservation law systems. Thus, instead of the usual second-order in time peridynamic equation corresponding to, say, elastic waves, we consider a first-order in time, nonlocal, nonlinear advection equation. Our ultimate goal is to develop a consistent approach to nonlocal conservation laws that is congruent with the existing peridynamic mechanics framework.

Key Accomplishments:

• *We have developed a vector calculus for nonlocal operators* that mimics in every way the classical vector calculus for differential operators; this includes the definition of nonlocal divergence, gradient, and curl operators, derivation of their adjoint operators, of nonlocal theorems such as Gauss' theorem and of Green's identities.

• We have used the nonlocal vector calculus to develop a theory of nonlocal calculus of variations which serves as the underpinning for *the rigorous analysis of the well-posedness and of finite element error estimates for linear nonlocal diffusion and* (both bond- and state-based) *peridynamics problems.*

• We have developed effective a posterior error estimators and developed convergent finite element methods for variational problems associated with linear nonlocal diffusion and nonlocal mechanical models.

Students and postdocs supported:

Tadele Mengesha (postdoc) - working on mathematical analysis of peridynamic models.

Li Tian (postdoc) - working on numerical analysis and simulations of peridynamic models.

Kun Zhou (Ph.D. in Mathematics awarded in 2011) - Dissertation title: The Peridynamic Theory of Solid Mechanics

Selected presentations by Qiang Du on research funded by grant:

Invited talk at the Workshop on Mathematical Analysis for Peridynamics, Oberwolfach, Germany, January, 2011.

Invited talk at the Workshop on Peridynamics, Dissipative Particle Dynamics and the Mori-Zwanzig Formulation, Brown University, 2012.

Invited talk at the Workshop on Nonlocal Models and Peridynamics, Institute of mathematics, Technische Universitat Berlin, 2012.

Invited minisymposium talk at the SIAM Materials Science Conference, Philadelphia, 2013.

Invited talk at the Seventh International Workshop on Meshfree Methods for Partial Differential Equations, Univ. Bonn, 2013.

List of publications resulted from the grant:

Q. Du, M. Gunzburger, R. Lehoucq, and K. Zhou, *Analysis and approximation of nonlocal diffusion problems with volume constraints*; SIAM Review, 54, 627-657, 2012.

Q. Du, J. Kamm, R. Lehoucq, and M. Parks, *A new approach for a nonlocal, nonlinear conservation law*, SIAM Journal on Applied Mathematics, 72 464–487, 2012.

Q. Du, M. Gunzburger, R. Lehoucq, and K. Zhou, *A nonlocal vector calculus, nonlocal volume-constrained problems, and nonlocal balance laws*; Math. Mod. Meth. Appl. Sci., 23, 493-540, 2013.

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. of Computation, 1889-1922, 2013.

Q. Du, L. Tian, and X. Zhao, *A convergent adaptive finite element algorithm for nonlocal diffusion & peridynamic models*, SIAM J. Numer. Anal. 51, 1211-1234, 2013

Q. Du, M. Gunzburger, R. Lehoucq, and K. Zhou, *Analysis of the volume-constrained peridynamic Navier equation of linear elasticity*, Journal of Elasticity, 113, 193-217, 2013.

T. Mengesha and Q. Du, *Analysis of a scalar peridynamic model with a sign changing kernel*, Disc. Cont. Dyn. Sys. B 18, 1415-1437, 2013.

T. Mengesha and Q. Du, *The bond-based peridynamic system with Dirichlet-type volume constraint*, Proc. Roy. Soc. Edin. A, 144, 161-186, 2014.

T. Mengesha and Q. Du, *Nonlocal constrained value problems for a linear peridynamic Navier equation*, J. Elasticity, 116, 27-51, 2014.

Q. Du, Z. Huang, and R. Lehoucq, *Nonlocal convection-diffusion volume-constrained problems and jump processes*, Disc. Cont. Dyn. Sys. B., 19, 373-389, 2014.