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U.S. Citizen

Research Interests

- Computational mathematics, Numerical analysis
- Scientific machine learning
- Multiscale mathematics, Atomistic-to-continuum coupling
- Nonlocal models and mathematics
- Numerical linear algebra, Linear solvers

Education

Ph.D., Computer Science, May 2005

University of Illinois at Urbana-Champaign, Urbana, IL.

GPA: 3.92/4.00

Completed Computational Science and Engineering degree option (demonstrating proficiency in numerical computation)

The Iterative Solution of a Sequence of Linear Systems Arising From Nonlinear Finite Element Analysis Ph.D. Dissertation

Eric de Sturler (chair), Michael T. Heath, Paul E. Saylor, Keith D. Hjelmstad

M.S., Computer Science, May 2000

Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, VA.

GPA: 3.96/4.00

Efficient Numeric Computation of a Phase Diagram in Biased Diffusion of Two Species Masters Thesis

Calvin J. Ribbens (chair), Donald Allison, Royce K. P. Zia, Beate Schmittmann

B.S., Computer Science, Summa Cum Laude, May 1998

B.S., Physics, Summa Cum Laude, In Honors, May 1998

Minor, Mathematics

Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, VA.

GPA: 3.87/4.00

The Construction and Analysis of Factorial Experiments: Application to Tribochemical Vapor Deposition Honors Thesis (Physics)

Jimmy Ritter (chair), Beate Schmittmann, Jerome Long

Research and Technical Experience

2014Present	Manager, Computational Mathematics, Org. 1442, Sandia National Laboratories
2013 – 2014	Acting Manager, Computational Mathematics, Org. 1442, Sandia National Laboratories
2013–2014	Principal Member of the Technical Staff, Computing Research Center, Sandia National Laboratories
2007–2013	Senior Member of the Technical Staff, Computing Research Center, Sandia National Laboratories
2004–2007	Postdoctoral Employee, Sandia National Laboratories Conducted research in multiscale modeling and analysis
2001–2004	Research Assistant, Dept. of Computer Science, University of Illinois Developed new solvers and preconditioners for ill-conditioned sparse linear systems
Summer 1998	Applications Programmer, Dept. of Physics, Virginia Tech Constructed custom interactive laboratory software for use in undergraduate physics labs
1996-1997	Research Assistant, Dept. of Physics, Virginia Tech Developed software to drive experimental apparatus; Aided in experiment design, data collection, and analysis

Teaching Experience

$Summer\ 1999$	Instructor, Dept. of Computer Science, Virginia Tech
	Taught Object-Oriented Software Design and Construction course (60 students)
	Managed teaching assistants
	Prepared lectures, homework, programming assignments, and exams
Fall 2000	Teaching Assistant, Dept. of Computer Science, University of Illinois
	Graded assignments and exams, held office hours
	Assisted with Programming Languages and Compilers course (300 students)
1998–2000	Teaching Assistant, Dept. of Computer Science, Virginia Tech
	Graded assignments and exams, held office hours, and taught lab sections
	Assisted with Object-Oriented Software Design and Construction and Numerical Methods
	courses

Selected Honors, Awards and Fellowships

2021	Sandia Award for Excellence (for outstanding leadership and professionalism in handling additional management responsibilities during the COVID-19 pandemic.)
2016	Sandia Award for Excellence (for exceptional leadership and programmatic service.)
2016	Sandia Center for Computing Research Exceptional Service Award (for organizing an outstanding experience for CCR's 2016 summer interns)
2010	Sandia Award for Excellence (for creating the PDLAMMPS code)
2009	Sandia Employee Recognition Award (for <i>Peridynamics as a Rigorous Coarse-Graining of Atomistics for Multiscale Materials Design</i> Project)
2008	Sandia Award for Excellence (for Technical and Programmatic Leadership in Multiscale Simulation)
2006	Sandia Award for Excellence (for Organizing CSRI-NECIS Special Seminar Series on Predictive Science for Nanotechnology)

2003 – 2004	Computational Science and Engineering Fellow, University of Illinois (10 awarded per year)
2002-2003	Computational Science and Engineering Fellow, University of Illinois (10 awarded per year)
2000	Outstanding Graduate Teaching Award, Department of Computer Science, Virginia Tech
1997-1998	Barry M. Goldwater Scholar (300 awarded nationally per year)
1997	Phi Beta Kappa
1997	Upsilon Pi Epsilon, the International Honor Society for the Computing and Information Disciplines
1997	Sigma Pi Sigma, the National Physics Honor Society

Publications

All papers can be downloaded from http://www.sandia.gov/-mlparks/.

Journal Articles

- N.E. Buczkowski, M.D. Foss, M.L. Parks, and P. Radu, Sensitivity analysis for solutions to heterogeneous nonlocal systems: Theoretical and numerical studies. Journal of Peridynamics and Nonlocal Modeling, 4, pp. 367–397, 2022.
- M. Bolten, E. De Sturler, C. Hahn, and M.L. Parks, Krylov Subspace Recycling for Evolving Structures. Computer Methods in Applied Mechanics and Engineering, 114222, 2022.
- G. Pang, M. D'Elia, M.L. Parks, and G.E. Karniadakis, nPINNs: nonlocal Physics-Informed Neural Networks for a parametrized nonlocal universal Laplacian operator. Algorithms and Applications. Journal of Computational Physics, 422, 109760, 2020.
- N. Trask, H. You, Y. Yu, and M.L. Parks, An asymptotically compatible meshfree quadrature rule for non-local problems with applications to peridynamics. Computer Methods in Applied Mechanics and Engineering, 343, pp. 151–165, 2019.
- Y. Yu, F.F. Bargos, H. You, M.L. Parks, M.L. Bittencourt, and G.E. Karniadakis, A partitioned coupling framework for peridynamics and classical theory: Analysis and simulations. Computer Methods in Applied Mechanics and Engineering, 340, pp. 905–931, 2018.
- S.A. SILLING, M.L. PARKS, J.R. KAMM, O. WECKNER, AND M. RASSAIAN, *Modeling shockwaves* and impact phenomena with Eulerian peridynamics. International Journal of Impact Engineering, 107, pp. 47–57, 2017.
- R. Panchadhara, P.A. Gordon, and M. L. Parks, *Modeling propellant-based stimulation of a borehole with peridynamics*. International Journal of Rock Mechanics and Mining Sciences, 93, pp. 330–343, 2017.
- W. Pan, K. Kim, M. Perego, A.M. Tartakovsky, and M. L. Parks, *Modeling Electrokinetic Flows by Consistent Implicit Incompressible Smoothed Particle Hydrodynamics*. Journal of Computational Physics, 334, pp. 125–144, 2017.
- P. Seleson, Q. Du, and M. L Parks, On the consistency between nearest-neighbor peridynamic discretizations and discretized classical elasticity models. Computer Methods in Applied Mechanics and Engineering, 311, pp. 698–722, 2016.
- P. Lindsay, M.L. Parks, and A. Prakash, *Enabling fast, stable and accurate peridynamic computations using multi-time-step integration*. Computer Methods in Applied Mechanics and Engineering, 306, pp. 386–405, 2016.
- D. Turner, B. van Bloemen Waanders, and M. L Parks, *Inverse problems in heterogeneous and fractured media using peridynamics*. Journal of Mechanics of Materials and Structures, 10(5), pp. 573–590, 2015.

• X. Yang, Y. Mehmani, W. A. Perkins, A. Pasquali, M. Schönherr, K. Kim, M. Perego, M. L. Parks, N. Trask, M. T. Balhoff, M. C. Richmond, M.Geier, M. Krafczyk, L. Luo, A. M. Tartakovsky, and T. D. Scheibe, *Intercomparison of 3D Pore-scale Flow and Solute Transport Simulation Methods*. Advances in Water Resources, 95, pp. 176–189, 2016.

- N. Trask, M. Maxey, K. Kim, M. Perego, M. L. Parks, K. Yang, and J. Xu, A scalable consistent second-order SPH solver for unsteady low Reynolds number flows. Computer Methods in Applied Mechanics and Engineering, 289, pp. 155–178, 2015.
- A. L. Frischknecht, D. O. Halligan and M. L. Parks, *Electrical double layers and differential capacitance in molten salts from density functional theory*. The Journal of Chemical Physics, 141(5), 054708, 2014.
- P. Seleson, M. L. Parks, and M. Gunzburger, *Peridynamic state-based models and the embedded-atom model*. Communications in Computational Physics, 15(1), pp. 179–205, 2014.
- P. Seleson, M. Gunzburger, and M. L. Parks, *Interface problems in nonlocal diffusion and sharp transitions between local and nonlocal domains*. Computer Methods in Applied Mechanics and Engineering, 266, pp. 185–204, 2013.
- L. J. D. Frink, A. L. Frischknecht, M. A. Heroux, M. L. Parks, and A. G. Salinger, Towards Quantitative Coarse-Grained Models of Lipids with Fluids Density Functional Theory. Journal of Chemical Theory and Computation, 8(4), pp. 1393–1408, 2012.
- Q. Du, J. R. Kamm, R. B. Lehoucq, and M. L. Parks, A New Approach for a Nonlocal, Nonlinear Conservation Law. SIAM Journal on Applied Mathematics, 72(1), pp. 464–487, 2012.
- P. Seleson, and M. L. Parks, On the Role of the Influence Function in the Peridynamic Theory. International Journal for Multiscale Computational Engineering, 9(6), pp. 689–706, 2011.
- B. Aksoylu, and M. L. Parks, Variational Theory and Domain Decomposition for Nonlocal Problems. Applied Mathematics and Computation, 217, pp. 6498–6515, 2011.
- P. Seleson, M. L. Parks, M. Gunzburger, and R. B. Lehoucq, *Peridynamics as an Upscaling of Molecular Dynamics*. Multiscale Modeling and Simulation, 8(1), pp. 204–227, 2009.
- M. L. Parks, R. B. Lehoucq, S. J. Plimpton, and S. A. Silling, *Implementing Peridynamics within a Molecular Dynamics Code*. Computer Physics Communications, 179(11), pp. 777–783, 2008.
- G. J. WAGNER, R. E. JONES, J. A. TEMPLETON, M. L. PARKS, An Atomistic-to-Continuum Coupling Method for Heat Transfer in Solids. Computer Methods in Applied Mechanics and Engineering, 197, pp. 3351–3365, 2008.
- M. L. Parks, P. B. Bochev, and R. B. Lehoucq, Connecting Atomistic-to-Continuum Coupling and Domain Decomposition. Multiscale Modeling and Simulation, 7, pp. 362–380, 2008.
- S. Badia, M. L. Parks, P. B. Bochev, M. Gunzburger, and R. B. Lehoucq, *On Atomistic-to-Continuum Coupling by Blending*. Multiscale Modeling and Simulation, 7, pp. 381–406, 2008.
- S. Badia, P. B. Bochev, J. Fish, M. D. Gunzburger, R. B. Lehoucq, M. A. Nuggehally, M. L. Parks, *A Force-Based Blending Model for Atomistic-to-Continuum Coupling*. International Journal for Multiscale Computational Engineering, 5, pp. 387-406, 2007.
- J. Fish, M. A. Nuggehally, M. S. Shephard, C. R. Picu, S. Badia, M. L. Parks, and M. Gunzburger, *Concurrent AtC coupling based on a blend of the continuum stress and the atomistic force*, Computer Methods in Applied Mechanics and Engineering, 196, pp. 4548-4560, 2007.
- M. L. Parks, L. A. Romero, and P. B. Bochev, *A Novel Lagrange-Multiplier Based Method for Consistent Mesh Tying*, Computer Methods in Applied Mechanics and Engineering, 196, pp. 3335-3347, 2007.

• M. L. Parks and L. A. Romero, Taylor-Aris Dispersion in High Aspect Ratio Columns of Nearly Rectangular Cross Section, Mathematical and Computer Modelling, 46, pp. 699–717, 2007.

• M. L. Parks, E. de Sturler, G. Mackey, D. Johnson, and S. Maiti, Recycling Krylov Subspaces for Sequences of Linear Systems, SIAM Journal on Scientific Computation, 28(5), pp. 1651-1674, 2006.

Conference Proceedings Articles

- S. Badia, P. B. Bochev, M. D. Gunzburger, R. B. Lehoucq, M. L. Parks, *Bridging Methods for Coupling Atomistic and Continuum Models*, in Large-Scale Scientific Computing 6th International Conference, Sozopol, Bulgaria, June 5-9, 2007, I. Lirkov, S. Margenov, and J. Wasniewski, eds., vol. 4818 of Lecture Notes in Computer Science, pp. 16–27, 2009.
- E. ASKARI, F. BOBARU, R. B. LEHOUCQ, M. L. PARKS, S. A. SILLING, O. WECKNER, *Peridynamics for multiscale materials modeling*, in SciDAC 2008, Seattle, Washington, vol. 125 of Journal of Physics: Conference Series, (012078) 2008.

Book Chapters

- P. Seleson and M.L. Parks, "Links to Atomistic Modeling", in *Handbook of Peridynamic Modeling*, ed. by F. Bobaru, J.T. Foster, P. Geubelle, and S.A. Silling, CRC Press, 2016.
- P. Bochev, R. Lehoucq, M. Parks, S. Badia, and M. Gunzburger, "Blending methods for coupling atomistic and continuum models", in *Multiscale Methods: Bridging the Scales in Science and Engineering*, ed. by J. Fish, Oxford University Press, pp. 165–191, 2009.

Technical Reports

- N.E. Buczkowski, M.D. Foss, M.L. Parks, J. Trageser, and P. Radu, *Two Nonlocal Bi-harmonic Operators*, in Computer Science Research Institute Summer Proceedings 2021, J.D. Smith and E. Galvan, eds., Sandia National Laboratories, 2021, pp. 3–15. Available as Sandia National Laboratories Technical Report SAND2022-0653R.
- N.E. Buczkowski, M. D'Elia and M.L. Parks, *Nonlocal Physics-Informed Neural Networks*,, in Computer Science Research Institute Summer Proceedings 2019, M. Powell and M. L. Parks, eds., Sandia National Laboratories, 2020, pp. 29–40. Available as Sandia National Laboratories Technical Report SAND2020-9969R.
- D.J. LITTLEWOOD, S.A. SILLING, J.A. MITCHELL, P.D SELESON, S.D. BOND, M.L. PARKS, D.Z. TURNER, D.J. BURNETT, J. OSTIEN, M. GUNZBURGER, Strong Local-Nonlocal Coupling for Integrated Fracture Modeling, Technical Report SAND2015-7998, Sandia National Laboratories, September 2015.
- P.E. LINDSAY AND M.L. PARKS, A Multi-Timestepping Extension to the Peridynamic Theory, in CSRI Summer Proceedings 2014, D.P. Kouri and M.L. Parks, eds., Sandia National Laboratories, 2014, pp. 15–25. Available as Sandia National Laboratories Technical Report SAND2015-3829O.
- M.L. Parks, D.J. Littlewood, J.A. Mitchell, and S.A. Silling, *Peridigm Users' Guide*. *V1.0.0.*, Available as Sandia National Laboratories Technical Report SAND2012-7800.
- K. Ahuja, M. L. Parks, E. T. Phipps, A. G. Salinger, and E. De Sturler, *Krylov Recycling for Climate Modeling and Uncertainty Quantification*, in CSRI Summer Proceedings 2010, E. C. Cyr and S. S. Collis, eds., Sandia National Laboratories, 2010, pp. 103–111. Available as Sandia National Laboratories Technical Report SAND2010-8783P.
- M. L. Parks, P. Seleson, S. J. Plimpton, R. B. Lehoucq, and S. A. Silling, *Peridynamics with LAMMPS: A User Guide*, Technical Report SAND2010-5549, Sandia National Laboratories, August 2010.

• P. Seleson, M. L. Parks, and M. Gunzburger, *Peridynamics as an upscaling of Molecular Dynamics*, in CSRI Summer Proceedings, D. Ridzal and S. S. Collis, eds., Sandia National Laboratories, 2008, pp. 177–184. Available as Sandia National Laboratories Technical Report SAND2008-8257P.

- P. B. Bochev, S. S. Collis, R. E. Jones, R. B. Lehoucq, M. L. Parks, G. Scovazzi, S. A. Silling, J. A. Templeton, G. J. Wagner, A Mathematical Framework for Multiscale Science and Engineering: the Variational Multiscale Method and Interscale Transfer Operators, Technical Report SAND2007-6179, Sandia National Laboratories, October 2007.
- S. Badia, P. Bochev, M. Gunzburger, R. Lehoucq, and M. L. Parks, *Blended Atomistic-to-Continuum Coupling Analyses and Methods*, Technical Report SAND2007-0905, Sandia National Laboratories, February 2007.
- E. B. Vanderzee, M. L. Parks, and P. Knupp, Numerical experiments for local quasicontinuum analysis, in NECIS Summer Proceedings, S. S. Collis, J. Lee, and J. Zimmerman, eds., Sandia National Laboratories, 2006, pp. 194–202. Available as Sandia National Laboratories Technical Report SAND2006-6564.
- M. L. Parks, L. A. Romero, and J. Whiting, A Reduced Order Model for the Study of Asymmetries in Linear Gas Chromatography for Homogeneous Tubular Columns, Technical Report SAND2005-4868, Sandia National Laboratories, August 2005.
- M. L. Parks, The Iterative Solution of a Sequence of Linear Systems Arising From Nonlinear Finite Element Analysis, Ph.D. Dissertation, Dept. of Computer Science at the University of Illinois at Urbana-Champaign, 2005. Available as University of Illinois Technical Report UIUCDCS-R-2005-2497.
- M. L. Parks, Efficient Numeric Computation of a Phase Diagram in Biased Diffusion of Two Species, Master's Thesis, Dept. of Computer Science at the Virginia Polytechnic Institute and State University (Virginia Tech), 2000. Available as Virginia Tech Electronic Thesis etd-05172000-14430029.

Books Co-Edited

• G.Z. Voyiadjis, et al., editors. *Handbook of Nonlocal Continuum Mechanics for Materials and Structures*, Springer, Switzerland, 2018.

Proceedings Edited

- A. A. Rushdi and M. L. Parks, editors. Computer Science Research Institute Summer Proceedings 2020, The Computer Science Research Institute at Sandia National Laboratories, Albuquerque, NM, 2020. Available as Sandia National Laboratories Technical Report SAND2020-12580R.
- M. POWELL AND M. L. PARKS, editors. Computer Science Research Institute Summer Proceedings 2019, The Computer Science Research Institute at Sandia National Laboratories, Albuquerque, NM, 2019. Available as Sandia National Laboratories Technical Report SAND2020-9969R.
- A. CANGI AND M. L. PARKS, editors. Center for Computing Research Summer Proceedings 2018, The Center for Computing Research at Sandia National Laboratories, Albuquerque, NM, 2018. Available as Sandia National Laboratories Technical Report SAND2019-5093R.
- A. D. BACZEWSKI AND M. L. PARKS, editors. Center for Computing Research Summer Proceedings 2017, The Center for Computing Research at Sandia National Laboratories, Albuquerque, NM, 2018. Available as Sandia National Laboratories Technical Report SAND2018-2780O.
 - J. B. Carleton and M. L. Parks, editors. *Center for Computing Research Summer Proceedings* 2016, The Center for Computing Research at Sandia National Laboratories, Albuquerque, NM, 2016. Available as Sandia National Laboratories Technical Report SAND2017-1294R.

• A. M. Bradley and M. L. Parks, editors. *Center for Computing Research Summer Proceedings* 2015, The Center for Computing Research at Sandia National Laboratories, Albuquerque, NM, 2015. Available as Sandia National Laboratories Technical Report SAND2016-0830R.

- D. P. Kouri and M. L. Parks, editors. *Center for Computing Research Summer Proceedings* 2014, The Center for Computing Research at Sandia National Laboratories, Albuquerque, NM, 2014. Available as Sandia National Laboratories Technical Report SAND2015-3829O.
- S. RAJAMANICKAM, M. L. PARKS, AND S. S. COLLIS, editors. *CSRI Summer Proceedings 2013*, The Computer Science Research Institute at Sandia National Laboratories, Albuquerque, NM, 2013. Available as Sandia National Laboratories Technical Report SAND2014-20409R.
- M. L. Parks and S. S. Collis, editors. CSRI Summer Proceedings 2007, The Computer Science Research Institute at Sandia National Laboratories, Albuquerque, NM, 2007. Available as Sandia National Laboratories Technical Report SAND2007-7977.

Other

• M. L. Parks and R. B. Lehoucq, Researchers Discuss Atomistic-to-Continuum (AtC) Coupling, SIAM News, Vol. 39, No. 7 (September 2006).

Invited Presentations

- The Peridigm Meshfree Peridynamics Code: Mathematics, Numerics, and Computation, Joint Mathematics Meetings 2023, Boston, Massachusetts, January 4, 2023.
- On Neumann-type Boundary Conditions for Nonlocal Models, Workshop on Theoretical and Applied Aspects for Nonlocal Models, Banff International Research Station for Mathematical Innovation and Discovery, Banff, Canada, July 18, 2022.
- On Neumann-type Boundary Conditions for Nonlocal Models, 9th U.S. National Congress on Theoretical and Applied Mechanics, Austin, Texas, June 21, 2022.
- Research and Opportunities in the Mathematical Sciences at Sandia National Laboratories, Joint Mathematics Meetings (JMM 2022), virtual, April 8, 2022.
- On Neumann-type Boundary Conditions for Nonlocal Models, Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology (MMLDT-CSET), San Diego, California (virtual), September 27, 2021.
- On Neumann-type Boundary Conditions for Nonlocal Models, Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology (MMLDT-CSET), San Diego, California (virtual), September 27, 2021.
- nPINNS: Nonlocal Physics-Informed Neural Networks, 16th U.S. National Congress on Computational Mechanics, Chicago, Illinois (virtual), July 29, 2021.
- Computational Aspects of Nonlocal Models, Center for Nonlinear Analysis, Department of Mathematical Sciences MCS, Carnegie Mellon University, Virtual, April 13, 2021.
- nPINNS: Nonlocal Physics-Informed Neural Networks, One Nonlocal World, Virtual, January 23, 2021.
- On Neumann-type Boundary Conditions for Nonlocal Models, The 5th Annual Meeting of SIAM Central States Section, Ames, Iowa, October 19, 2019.
- On Neumann-type Boundary Conditions for Nonlocal Models, 9th International Congress on Industrial and Applied Mathematics, Valencia, Spain, July 16, 2019.
- Subsurface Applications for Peridynamics, SIAM Conference on Computational Science and Engineering, Spokane, Washington, February 27, 2019.
 Subsurface Applications for Peridynamics, Workshop on Dynamics, Control, and Numerics for Fractional PDEs, San Juan, Puerto Rico, December 6, 2018.

Solving Real-World Problems with Mathematics and Computing, Department of Mathematics Colloquium, University of Nebraska-Lincoln, Lincoln, Nebraska, November 30, 2018.

- Domain Decomposition Methods: Origins and Applications to Multiscale Modeling, Department of Mathematics Continuum Mechanics Seminar, University of Nebraska-Lincoln, Lincoln, Nebraska, November 29, 2018.
- Subsurface Applications for Peridynamics, 13th World Congress on Computational Mechanics, New York, New York, July 24, 2018.
- Subsurface Applications for Peridynamics, 6th European Conference on Computational Mechanics, Glasgow, United Kingdom, June 12, 2018.
- Computational and Mathematical Aspects of Nonlocal Models, Center for Shock Wave-processing of Advanced Reactive Materials Seminar, University of Notre Dame, South Bend, Indiana, April 27, 2018.
- A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics, Recent Trends in Pure and Applied Mathematics, "1 Decembrie 1918" University, Alba Iulia, Romania, August 2, 2017.
- A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics, 14th US National Congress on Computational Mechanics, Montreal, Canada, July 17, 2017.
- Computational and Mathematical Aspects of Nonlocal Models, Center for Computational & Applied Mathematics Seminar, Purdue University, West Lafayette, Indiana, April 24, 2017.
- A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics, SIAM Conference on Computational Science and Engineering, Atlanta, Georgia, March 2, 2017
- Nonlocal Models and Peridynamics, Applied Mathematics Seminar, Department of Mathematics, The George Washington University, Washington, DC, October 18, 2016.
- A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics, USACM Conference on Isogeometric Analysis and Meshfree Methods, La Jolla, California, October 11, 2016.
- A Massively Parallel Scalable Implicit SPH Solver, SIAM Conference on Nonlinear Waves and Coherent Structures, Philadelphia, Pennsylvania, August 10, 2016.
- Computational and Mathematical Aspects of Nonlocal Models, Department of Mathematics Colloquium, University of Nebraska-Lincoln, Lincoln, Nebraska, February 26, 2016.
- Nonlocal Models and Peridynamics, Applied Mathematics & Statistics Department Seminar, Colorado School of Mines, Golden, Colorado, January 29, 2016.
- A Massively Parallel Scalable Implicit SPH Solver, Joint Mathematics Meetings, Seattle, Washington, January 7, 2016.
- A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics, poster presentation.
 Workshop on Nonlocal Models in Mathematics, Computation, Science, and Engineering, Oak Ridge National Laboratory, Oak Ridge, Tennessee, October 27, 2015.
- A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics, 1st Pan-American Conference Computational Mechanics, Buenos Aires, Argentina, April 28, 2015.
- A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics, Conference on Recent Developments in Continuum Mechanics and PDEs, Lincoln, Nebraska, April 18, 2015.
- Quadrature Methods for Peridynamics, SIAM Conference on Analysis of Partial Differential Equations, Orlando, Florida, December 7, 2013.
- Peridigm: A New Paradigm in Computational Peridynamics, SIAM Conference on Analysis of Partial Differential Equations, Orlando, Florida, December 7, 2013.
- Peridigm: A New Paradigm in Computational Peridynamics, Workshop on Nonlocal Damage and Failure: Peridynamics and Other Nonlocal Models, San Antonio, Texas, March 11, 2013.
- Peridigm: A New Paradigm in Computational Peridynamics, Joint Mathematics Meetings, San Diego, California, January 10, 2013.

• Peridigm: A New Paradigm in Computational Peridynamics, ASME 2012 International Mechanical Engineering Congress & Exposition, Houston, Texas, November 14, 2012.

- Solving Real-World Problems with Mathematics and Computing, 6th Annual Pi Mu Epsilon Lecture, University of Nebraska-Lincoln, Lincoln, Nebraska, November 9, 2012.
- Computational Peridynamics, Dept. of Mathematics Continuum Mechanics Seminar, University of Nebraska-Lincoln, Lincoln, Nebraska, November 8, 2012.
- Peridigm: A New Paradigm in Computational Peridynamics, 10th World Congress on Computational Mechanics, Sao Paulo, Brazil, July 11, 2012.
- Computational Peridynamics, Workshop on Nonlocal Continuum Models for Diffusion, Mechanics, and Other Applications, The Statistical and Applied Mathematical Sciences Institute (SAMSI), Research Triangle Park, North Carolina, June 29, 2012.
- A New Approach for a Nonlocal, Nonlinear Conservation Law, Workshop on Nonlocal Continuum Models for Diffusion, Mechanics, and Other Applications, The Statistical and Applied Mathematical Sciences Institute (SAMSI), Research Triangle Park, North Carolina, June 28, 2012.
- Computational Peridynamics, Workshop on Peridynamics, Dissipative Particle Dynamics and the Mori-Zwanzig Formulation, Brown University, Providence, Rhode Island, April 10, 2012.
- Peridynamics for Material Failure, Los Alamos National Laboratory, Los Alamos, New Mexico, April 5, 2012.
- Computational Peridynamics, Dept. of Mathematics, Temple University, Philadelphia, Pennsylvania, March 26, 2012.
- Computational Materials Modeling with Peridynamics, 6Lab Meeting: Engineering & Materials at Extreme Conditions, Barcelona, Spain, October 26, 2011.
- Computational Peridynamics, International Center for Numerical Methods in Engineering (CIMNE), Universitat Politécnica de Catalunya, Barcelona, Spain, October 24, 2011.
- A New Peridynamic-Inspired Approach to Nonlocal Advection, 2011 AMS Fall Central Section Meeting, Lincoln, Nebraska, October 14, 2011.
- A New Approach to Nonlocal Advection, 11th US National Congress on Computational Mechanics (USNCCM), Minneapolis, Minnesota, July 26, 2011.
- Computational Peridynamics, SIAM Conference on Computational Science and Engineering, Reno, Nevada, February 28, 2011.
- Computational Peridynamics, MiniWorkshop: Mathematical Analysis of Peridynamics, Mathematisches Forschungsinstitut Oberwolfach, Oberwolfach, Germany, January 18, 2011.
- Computational Peridynamics, ExxonMobil Research and Engineering Company, Annandale, New Jersey, November 5, 2010.
- Peridynamics as an Upscaling of Molecular Dynamics, 16th US National Congress on Theoretical and Applied Mechanics (USNCTAM), State College, Pennsylvania, June 27–July 2, 2010.
- Atomistic-to-Continuum Coupling Methods Based on Domain Decomposition, 16th US National Congress on Theoretical and Applied Mechanics (USNCTAM), State College, Pennsylvania, June 27–July 2, 2010.
- Atomistic-to-Continuum Coupling Methods Based on Domain Decomposition, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, Pennsylvania, May 23-26, 2010.
- Mesoscale Simulations with Microscale Tools: Peridynamics in a Molecular Dynamics Code, 2010 LAMMPS User Workshop, Computer Science Research Institute, Sandia National Laboratories, Albuquerque, New Mexico, February 25, 2010.
- Mesoscale Simulations with Microscale Tools: Peridynamics in a Molecular Dynamics Code, IAMCS Workshops on Computational and Mathematical Challenges in Material Science and Engineering:

Multi-Scale Materials Modeling – Nano-Scale to Macro-Scale Materials Modeling and Hybrid Theories, Institute for Applied Mathematics and Computational Science, Texas A&M University, College Station, Texas, November 2, 2009.

- Peridynamics for Multiscale Materials Modeling, Workshop on Scale Transitions in Space and Time for Materials, Lorentz Center, Leiden, Netherlands, October 21, 2009.
- Towards Multiscale Material Modeling with Peridynamics, Dept. of Engineering Mechanics, University of Nebraska-Lincoln, Lincoln, Nebraska, October 6, 2009.
- Molecular dynamics at larger scales: Peridynamics as an upscaling of molecular dynamics, 10th US National Congress on Computational Mechanics, Columbus Ohio, July 16-19, 2009.
- Mesoscale Simulations with Microscale Tools: Peridynamics in a Molecular Dynamics Code, The 2009
 Joint ASCE-ASME-SES Conference on Mechanics and Materials, Virginia Tech, Blacksburg, Virginia,
 June 27, 2009.
- Towards Multiscale Materials Modeling With Peridynamics, Center for Computation and Technology, Louisiana State University, Baton Rouge, Louisiana, November 14, 2008.
- Molecular dynamics at larger scales: Peridynamics as an upscaling of molecular dynamics, Fourth International Conference on Multiscale Materials Modeling, Tallahassee Florida, October 27-31, 2008.
- Mesoscale Simulations with Microscale Tools: Peridynamics in a Molecular Dynamics Code, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, Pennsylvania, May 11-14, 2008.
- The Fast Solution of Sequences of Linear Systems via Subspace Recycling, School of Computational Science, Florida State University, Tallahassee, Florida, October 13, 2007.
- Analysis of Krylov-subspace recycling for sequences of linear systems, 6th International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 16-20, 2007.
- Connecting Domain Decomposition and Atomistic-to-Continuum (AtC) Coupling, Oak Ridge National Laboratories, Oak Ridge, Tennessee, May 1-2, 2007.
- Connections Between Domain Decomposition and Atomistic-to-Continuum (AtC) Coupling, Department of Mathematics, Virginia Tech, October 4-6, 2006.
- Fast Solution of Long Sequences of Linear Systems in Computational Mechanics, 7th World Congress on Computational Mechanics, Los Angeles, California, July 16-22, 2006. (Filled in for Eric de Sturler, who was unable to attend.)
- Relating Atomistic-to-Continuum Coupling and Domain Decomposition, 7th World Congress on Computational Mechanics, Los Angeles, California, July 16-22, 2006.
- Analysis of Krylov Subspace Recycling for Sequences of Linear Systems, SIAM Conference on Computational Science and Engineering, Orlando, Florida, February 12-15 2005.
- Recycling Krylov Subspaces for Sequences of Linear Systems, Annual Computational Science and Engineering Research Symposium, University of Illinois, Urbana, Illinois, April 27, 2004.
- Robust Preconditioners and Solvers for Ill-Conditioned Equations from Nonlinear Finite Element Analysis, Annual Computational Science and Engineering Research Symposium, University of Illinois, Urbana, Illinois, April 25, 2003.

Contributed Presentations

- Peridynamics for Material Failure, NECDC2012, Lawrence Livermore National Laboratory, Livermore, California, October 24, 2012.
- Peridynamics for multiscale materials modeling, Applied Mathematics Principal Investigators Meeting, Argonne National Laboratory, Argonne, Illinois., October 15-17, 2008.

• Relating atomistic-to-continuum coupling and domain decomposition, 6th International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 16-20, 2007.

- The Fast Solution of Sequences of Linear Systems via Subspace Recycling, Seventh Biennial Tri-Laboratory Engineering Conference, Albuquerque New Mexico, May 7-10, 2007.
- Analysis of Krylov Subspace Recycling for Sequences of Linear Systems, 7th IMACS International Symposium of Iterative Methods in Scientific Computing, Toronto, Canada, May 5-6 2005.
- Recycling Krylov Subspaces for Sequences of Linear Systems, Midwest Numerical Analysis Day, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin, April 24, 2004.
- Improved Krylov Methods and a Framework for the Analysis of Preconditioners for Ill-Conditioned Equations Arising from Nonlinear Finite Element Analysis, 2003 International Conference On Preconditioning Techniques For Large Sparse Matrix Problems In Scientific And Industrial Applications, Napa, California., October 27-29, 2003.

Software

I am a developer or co-developer of the following software packages. They have been developed under funding from the U.S. Government and are distributed via an open-source license.

• Peridigm

- Peridynamics is a nonlocal extension of classical continuum mechanics, and is principally used for simulations involving fracture, failure, and fragmentation. Peridigm is Sandia's primary open-source computational peridynamics code. It is a massively-parallel simulation code for implicit and explicit multi-physics simulations centering on solid mechanics and material failure. Peridigm utilizes foundational software components from Sandia's Trilinos project, and is fully compatible with the Cubit mesh generator and Paraview visualization code. Peridigm is used as a collaboration vehicle by Sandia for interactions with private industry and universities. See https://github.com/peridigm/peridigm.
- PDLAMMPS (Peridynamics-in-LAMMPS)
 A particular discretization of the peridynamics has the same computational structure as classical molecular dynamics. PDLAMMPS is implemented as a module within LAMMPS, Sandia's massively parallel molecular dynamics code. See http://lammps.sandia.gov and http://www.sandia.gov/-mlparks/software.
- Belos (Next-generation iterative linear solver package within Trilinos)
 Many problems in engineering and physics require the solution of a large sequence of linear systems. We can reduce the cost of solving subsequent systems in the sequence by recycling information from previous systems. I develop a family of solvers based upon a technique known as "Krylov Subspace Recycling". Belos currently contains a recycling GMRES solver (GCRODR) and a recycling CG solver (RCG). See http://trilinos.sandia.gov/packages/belos/ and http://www.sandia.gov/-mlparks/software.

Students

Nicole Buczkowski I co-supervised Nicole during the 2019 Sandia CCR summer student program,

and also in 2021 summer program and parts of 2022. During this time, Nicole worked on nonlocal physics-informed neural networks and mathematical analysis

and computational modeling of nonlocal biharmonic operators.

Cory Wright I supervised Cory during the 2017 Sandia CCR summer student program, and also

for the spring semester of 2018. During this time, Cory performed mathematical

analysis of various discretizations of peridynamics.

Payton Lindsay With Arun Prakash, Payton's Ph.D. advisor at Purdue, I co-supervised Payton

from 2013-2016, including summers Payton spent at Sandia as a summer student intern. During this time, Payton developed the first multi-time-stepping method for a nonlocal model, peridynamics. I also served as a member of Payton's Ph.D.

committee.

Canio Hoffarth With Dave Littlewood, I co-supervised Canio during the 2012 Sandia CSRI sum-

mer student program. During this time, Canio conducted numerical simulations of compaction of granular material using the peridynamic code *Peridigm*. Canio also developed and implemented several capabilities into Peridigm, including new compute classes, a new contact algorithm incorporating friction, and useful post-

processing tools.

Kirk Soodhalter I supervised Kirk Soodhalter during the 2011 Sandia CSRI summer student pro-

gram. During this time, Kirk developed and implemented a block version of the Krylov subspace recycling solver GCRODR within Trilinos, and tested it in the fluid-DFT code Tramonto. I also served as a member of Kirk's Ph.D. committee.

Kapil Ahuja I supervised Kapil Ahuja during the 2010 Sandia CSRI summer student program.

During this time, Kapil applied Krylov subspace recycling solvers to climate mod-

eling and uncertainty quantification applications.

Pablo Seleson I supervised Pablo Seleson during the 2008 Sandia CSRI summer student pro-

gram. I continued my collaborations with Pablo after his visit, and was a member of his Ph.D. committee, chaired by Prof. Max Gunzburger. Pablo won the student paper prize at the 33rd SIAM Southeastern-Atlantic Section Conference for our joint paper, *Peridynamics as an Upscaling of Molecular Dynamics*. Pablo graduated from the Dept. of Scientific Computing at Florida State University in

2010.

Sandia Projects

2018–2022 PhILMS: Collaboratory on Mathematics and Physics-Informed Learning Machines for

Multiscale and Multiphysics Problems Funding: ASCR/MMICC

Activities: Developing physics-informed learning machines

Collaborators: G.E. Karniadakis (Director, PNNL), A. Tartakovsky (PNNL),

M. Ainsworth (Brown University), Constantinos Daskalakis (MIT), E. Darve (Stanford University), Gregory Valiant (Stanford University),

P. Atzberger (UC Santa Barbara)

2012–2017 CM4: Collaboratory on Mathematics for Mesoscopic Modeling of Materials

Funding: ASCR/MMICC Activities: Large-scale fast solvers, concurrent coupling methods G.E. Karniadakis (Director, PNNL), T.P. Straatsma (PNNL), Collaborators: M. Maxey (Brown University), P. Stinis (University of Minnesota), E. Darve (Stanford University), Weinan E (Princeton University), P. Atzberger (UC Santa Barbara), and J. Xu (Penn State) 2012-2015 SLEEC: Semantics-rich Libraries for Effective Exascale Computation Funding: ASCR/X-Stack Activities: Develop semantics-aware compiler infrastructure Collaborators: M. Kulkarni, S. Midkiff, V.S. Pai, and A. Prakash (all Purdue University) 2012-2015 Strong Local-Nonlocal Coupling for Integrated Fracture Modeling Funding: LDRD Activities: Develop, analyze, and deploy capability for strong coupling of peridynamics with classical solid mechanics Collaborators: D. Littlewood, J. Ostien, S. Silling, P. Seleson (U. Texas), and M. Gunzburger (FSU) 2008-2010 Linear Algebra for Extreme Scale Computing of Nanoscale Fluids Funding: ASCR Extreme scale solvers for Fluid-DFTs Activities: Collaborators: D. Day, M. Heroux, L.J. Frink 2008-2010 Rapid Production Software Development for Multi-Physics Peridynamics Funding: CSRF Create production-quality component-based multiphysics peridynamics code Activities: Collaborators: D.J. Littlewood, J. Mitchell, and S.A. Silling 2007-2009 Peridynamics as a Rigorous Coarse-Graining of Atomistics for Multiscale Materials Design Funding: LDRD Activities: Develop simulation capability for next generation computational material science. Collaborators: S.M. Foiles, R.B. Lehoucq, M.P. Sears, and S.A. Silling 2006-2008 Analysis of Atomistic-to-Continuum (AtC) Coupling Funding: ASCR Activities: Numerical analysis of atomistic-to-continuum coupling algorithms Collaborators: R.B. Lehoucg, P.B. Bochev, M. Gunzburger (FSU), S. Badia D. Estep (CSU), J. Fish (RPI), and M. Shephard (RPI) 2006-2008 System Level Methods for Electrical and Microsystems Applications (Co-PI) Funding: CSRF Activities: Research on Krylov subspace recycling algorithms; Trilinos development Collaborators: E. de Sturler (Virginia Tech), H. Thornquist, D. Day, and T. Coffey 2005-2007 A Mathematical Framework for Multiscale Science and Engineering Funding: Activities: Development and analysis of atomistic/continuum thermal coupling algorithms Collaborators: R.B. Lehoucq, P.B. Bochev, G. Wagner, R. Jones, J. Templeton, and A. Slepoy 2005-2006 Generalized Domain Bridging Methods

Funding: CSRF

Activities: Development and analysis of mesh tying algorithms

for finite element subdomains with inconsistently meshed boundaries

Collaborators: P.B. Bochev, D. Day, L.A. Romero, and M. Gee

Funded Proposals

2018–2022 PhILMS: Collaboratory on Mathematics and Physics-Informed Learning Machines for

Multiscale and Multiphysics Problems (Co-PI)

Director: George E. Karniadakis (PNNL)

Other Co-PIs: A. Tartakovsky (PNNL), M. Ainsworth (Brown University), P. Stinis (University of Minnesota), E. Darve (Stanford University), Constantinos Daskalakis

(MIT), P. Atzberger (UC Santa Barbara)

Funding Requested: \$10.0M (DOE/ASCR/MMICC)

2012–2017 CM4: Collaboratory on Mathematics for Mesoscopic Modeling of Materials (Co-PI)

Director: George E. Karniadakis (PNNL)

Other Co-PIs: T. P. Straatsma (PNNL), M. Maxey (Brown University), P. Stinis (University of Minnesota), E. Darve (Stanford University), Weinan E (Princeton

University), P. Atzberger (UC Santa Barbara), J. Xu (Penn State)

Funding Requested: \$15.0M (DOE/ASCR/MMICC)

2012–2015 SLEEC: Semantics-rich Libraries for Effective Exascale Computation (Co-PI)

Joint Proposal with Purdue University (PI: Milind Kulkarni)

Collaborators: M. Kulkarni, S. Midkiff, V.S. Pai, and A. Prakash (all Purdue University)

Funding Requested: \$1.5M (DOE/ASCR/X-Stack)

2006–2008 Peridynamics as a Rigorous Coarse-Graining of Atomistics for Multiscale Materials Design

(Co-PI)

Funding Requested: \$1.95M (Sandia/LDRD)

2006–2008 System Level Methods for Electrical and Microsystems Applications (Co-PI)

Funding Requested: \$1.5M (Sandia/CSRF)

Professional Society Memberships

Society for Industrial and Applied Mathematics (SIAM) U.S. Association for Computational Mechanics (USACM)

Professional Service Activities

2019-Present Member, WNA Resource Advisory Panel (WRAP).

2018-Present Member, Editorial Board, Journal of Peridynamics and Nonlocal Modeling.

2015-Present Associate Editor, SIAM Journal on Numerical Analysis.

2023 Member, Organizing Committee, 17th U.S. National Congress on Computational

Mechanics, Albuquerque, New Mexico, July 23-27 2023. Congress Chairs: Joe Bishop

(SNL), Jim Stewart (SNL).

2022 Member, Scientific Committee, USACM Thematic Conference on Uncertainty

Quantification for Machine Learning Integrated Physics Modeling (MLIP), Crystal City,

Arlington, Virginia, August 18-19, 2022.

2008-2018 Associate Editor, Applied Mathematics and Computation.

2021	Minisymposium Co-organizer, Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering and Technology (MMLDT-CSET). Organized minisymposium with Petronela Radu (University of Nebraska-Lincoln) and Animesh Biswas (University of Nebraska-Lincoln) on Nonlocal Operators and Machine Learning in Multiscale Modeling.
2021	Minisymposium Co-organizer, 16th U.S. National Congress on Computational Mechanics. Organized minisymposium with Petronela Radu (University of Nebraska-Lincoln) and Animesh Biswas (University of Nebraska-Lincoln) on Nonlocal Models in Continuum Mechanics: Mathematical, Computational, Machine Learning Aspects.
2017	Member, Organizing Committee, 2017 ASCR Applied Mathematics Principal Investigators Meeting with Jeff Hittinger (co-chair, LLNL), Lois Curfman McInnes, (co-chair, ANL), Abani Patra (SUNY Buffalo), Nathan Baker (PNNL), Miranda Holmes-Cerfon (NYU), Barney Maccabe (ORNL), Esmond Ng (LBNL), Pieter Swart (LANL), and Karen Willcox (MIT).
2015	Workshop Co-organizer, Nonlocal Models in Mathematics, Computation, Science, and Engineering at Oak Ridge National Laboratory with Pablo Seleson (Oak Ridge National Laboratory), Clayton Webster (Oak Ridge National Laboratory), and Tadele Mengesha (U. Tennessee).
2015	Minisymposium Co-organizer, 1st Pan-American Conference on Computational Mechanics. Organized minisymposium with Pablo Seleson (Oak Ridge National Laboratory) and Diego Del-Castillo-Negrete (Oak Ridge National Laboratory) on Nonlocal Models for Mechanics and Diffusion.
2013	Minisymposium Co-organizer, 2013 SIAM Conference on Analysis of Partial Differential Equations. Organized minisymposium with Petronela Radu (U. Nebraska) on Nonlocal Models in PDEs and Applications.
2012	Minisymposium Co-organizer, 10th World Congress on Computational Mechanics. Organized minisymposium with Pablo Seleson (U. Texas) and Serge Prudhomme (U. Texas) on Mathematical and Computational Analysis of Concurrent Methods for Multiscale Material Modeling.
2011	Minisymposium Co-organizer, 11th US Congress on Computational Mechanics. Organized minisymposium with Pablo Seleson (U. Texas), Mitchell Luskin (U. Minnesota), and Serge Prudhomme (U. Texas) on <i>Mathematical Modeling and Analysis for Multiscale Materials</i> .
2011	Minisymposium Co-organizer, 11th US Congress on Computational Mechanics. Organized minisymposium with David Littlewood, Jay Foulk and Alejandro Mota (Sandia National Laboratories) on <i>Recent Advances in Nonlocal Computational Mechanics</i> .
2010	Minisymposium Co-organizer, 2010 SIAM Conference on Mathematical Aspects of Materials Science. Organized minisymposium with Burak Aksoylu (TOBB University) on Analytical and Numerical Methods for Nonlocal Problems.
2010	Minisymposium Co-organizer, 16th US National Congress on Theoretical and Applied Mechanics (USNCTAM). Organized minisymposium with Stewart Silling (Sandia), Youping Chen (U. Florida), and Xiantao Li (Penn State) on <i>Theoretical and Computational Methods for Critical Material Behavior</i> .

2007 **Editor**, Sandia CSRI Summer Proceedings. Edited (with Scott Collis) the proceedings from the annual summer internship program at Sandia's Computer Science Research Institute (CSRI).

2007

2006

Ongoing

Seminar Series Organizer, Sandia CSRI seminar series. Hosted Sandia staff and university faculty for talks on computational science and applications.

Seminar Series Organizer, Sandia NECIS special seminar series. Hosted university faculty for talks on predictive science for nanotechnology.

Reviewer, SIAM Review (SIREV), SIAM Journal on Scientific Computing (SISC), SIAM Journal on Numerical Analysis (SINUM), Multiscale Modeling and Simulation (MMS), Computer Methods in Applied Mechanics and Engineering (CMAME), International Journal for Numerical Methods in Engineering (IJNME), Journal of Computational Physics (JCP), Electronic Transactions on Numerical Analysis (ETNA), Discrete and Continuous Dynamical Systems, Journal of Computational Mathematics, Applied Mathematics and Computation, Advances in Engineering Software, IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems, European Journal of Mechanics - A/Solids, Journal of Mechanics of Materials and Structures (JoMMS), Computational Materials Science, Computational Methods in Engineering Science and Mechanics, Acta Mechanica, Parallel Computing, Journal of Mathematical Analysis and Applications, International Journal of Fracture, Numerical Methods for Partial Differential Equations, Journal of Peridynamics and Nonlocal Modeling.