

# Matthew G. Knepley

Associate Professor  
Department of Computer Science and Engineering

Dept. of Computer Science and Engineering  
University at Buffalo  
211A Capen Hall  
Box 602000  
Buffalo, NY 14260, USA

Office: +1 716 645 0747  
Mobile: +1 773 413 8537  
Email: [knepley@buffalo.edu](mailto:knepley@buffalo.edu)  
Web: <https://www.cse.buffalo.edu/~knepley>

## Education

Ph.D. Computer Science, Purdue University, 2000 (Advisor: Prof. Ahmed H. Sameh).  
M.S. Computer Science, University of Minnesota, 1996.  
B.S. Mathematical Physics, *summa cum laude*, Case Western Reserve University, 1994.

## Professional Experience

**Associate Professor**, Computer Science and Engineering, University at Buffalo, 2017–*Present*  
**Visiting Researcher**, Department of Earth Science and Engineering, Imperial College London, 2018–2020  
**Adjunct Professor**, Computational and Applied Mathematics, Rice University, 2018–*Present*  
**Assistant Professor**, Computational and Applied Mathematics, Rice University, 2015–2018  
**Assistant Professor**, Computer Science, Rice University, 2017–2018  
**Affiliated Faculty**, Systems, Synthetic and Physical Biology Graduate Program, Rice University, 2017–*Present*  
**Director**, Intel Parallel Computing Center, Rice University, 2016–*Present*  
**Senior Research Associate**, Computation Institute, University of Chicago, 2009–2015  
**Fellow**, Computation Institute, University of Chicago, 2008–2015  
**Visiting Assistant Professor**, Molecular Biophysics and Physiology, Rush Univ. Medical Center, 2006–2014  
**Adjunct Senior Research Fellow**, School of Mathematical Sciences, Monash University, 2010–2013  
**Assistant Computational Mathematician**, Mathematics and Computer Science, Argonne National Laboratory, 2005–2009  
**Postdoctoral Researcher**, Mathematics and Computer Science, Argonne National Laboratory, 2001–2004  
**Research Scientist**, Distributed Data Collection, Akamai Technologies Inc., 2000–2001  
**Research Assistant**, Purdue University 1997–2000  
**Teaching Assistant**, University of Chicago 1994–1995, University of Minnesota 1995–1996

## Academic Awards and Honors

[SIAM/ACM Prize](#) in Computational Science and Engineering (as part of PETSc team) (2015)

Lindbergh Lecture, Department of Mechanical Engineering, UW Madison, (2011)  
 R&D 100 Award (as part of the PETSc team) (2009)  
 J. T. Oden Faculty Research Fellow, ICES, UT Austin (2008)  
 Elected to Upsilon Pi Epsilon (2000)  
 Elected to Golden Key (1994)  
 Elected to Phi Beta Kappa (1994)  
 Elected to Sigma Xi (1993)  
 Tuition scholarship, Case Western Reserve University (1990–1994)

## Grants and Contracts

Funding Category	Total Direct	Candidate's Share
External Sources	10,804,744	3,451,123
Internal Sources	50,000	10,000
Total Funded Research	10,854,744	3,461,123

### *Current Funding*

Co-PI, DOE, *PSAAPIII CHREST Center*, \$8,530,200 (\$1,176.579), 2020-2025  
 Co-PI, SUNY, *Grant in aid of research*, \$50,000, 2019  
 PI, PPPL, *ECP-WDMApp*, \$112,333, 2020-2022  
 Co-PI, NSF SI2 Framework: [Multiphase Fluid-Structure Interaction Software Infrastructure to Enable Applications in Medicine, Biology, and Engineering](#), \$504,431, 2020–2025  
 co-PI, NSF SI2-SSI: [Scalable Infrastructure for Enabling Multiscale and Multiphysics Applications in Fluid Dynamics, Solid Mechanics, and Fluid-Structure Interaction](#), \$215,715, 2015–2020  
 Subcontract, NSF [Computational Infrastructure for Geodynamics](#), \$585,000, 2016–2021  
 Co-PI, DOE Basic Energy Sciences, *Development of Terrestrial Dynamical Cores for the ACME to Simulate Water Cycle*, \$160,000, 2018–2021  
 Co-PI, DOE Applied Math Research, *Extending PETSc's Composable Hierarchically Nested Linear Solvers*, \$247,000, 2018–2021  
 Subcontract, DOE SciDAC FES, *Support for SCREAM and EPSI*, \$100,000, 2018–2020  
 Co-PI, NSF SI2-SSE: [Extending the Practicality and Scalability of LibMesh-Based Unstructured, Adaptive Finite Element Computations](#), \$350,065, 2017–2020

### *Previous Funding*

PI, Intel Parallel Computing Center, *Extending PETSc with Adaptive Mesh Refinement and Optimal Solvers, Applied to PFLOTRAN, and Optimized for Modern Intel Processors*, \$400,000, 2015–2017  
 Co-PI, DOE Applied Math Research, *Extending PETSc's Composable Hierarchically Nested Linear Solvers*, \$240,000, 2015–2018  
 Co-PI, NSF SI2-SSE: [SPIKE — An Implementation of a Recursive Divide-and-Conquer Parallel Strategy for Solving Large Systems of Linear Equations](#), \$117,710, 2012–2015  
 Co-PI, DOE Applied Math Research, *Extending PETSc's Composable Hierarchically Nested Linear Solvers*, \$240,000, 2012–2015

Co-PI, DOE Math-CS Institute, *Nonlinear Algorithms to Circumvent the Memory Bandwidth Limitations of Implicit PDE Simulations*, \$550,000, 2009–2014

Co-PI, NSF STCI, *Mechanical Transformation of Knowledge to Libraries*, \$90,000, 2009–2011

Co-PI, DOE SciDAC ISIC, *Towards Optimal Petascale Simulations*, \$1,200,000, 2001–2011

Subcontract, NSF *Computational Infrastructure for Geodynamics*, \$650,000, 2010–2015

Subcontract, NSF *Computational Infrastructure for Geodynamics*, \$650,000, 2005–2010

Subcontract, Army Research Office W911NF-09-1-0488, *Classical Density Functional Theory of Fluids: Ions at a Dielectric Interface*, \$45,000, 2010–2012

Subcontract, DOE Reactor Core Modeling, \$210,000, 2005–2007

## Research Areas

Scalable linear and nonlinear solvers for multiphysics problems

Bioelectrostatics and molecular modeling for ion channels

Geophysical modeling in crustal deformation, mantle convection, and magma dynamics

Scientific library development and automated scientific computing

Libraries and code generation for high performance computing

Efficient solvers and preconditioners for GPUs and accelerators

Finite element and boundary element discretizations for nonlinear problems

Classical density functional theory, theory and numerics

## Research Achievements

Matthew Knepley has made substantial and innovative contributions to the scalable solution of PDE and BIE problems. Through PETSc, his work has been used to model complex phenomena in a wide array of science and engineering research, including bioelectrostatics and molecular modeling, climate science, geodynamics, both fission and fusion, nanosimulations, subsurface flow, oil-reservoir modeling and optimization, combustion, fracture mechanics, real-time surgery, and micromagnetics. He has produced lasting software artifacts which form a solid foundation for the development of leading scientific applications and industrial simulators. Both Cray and Microsoft distribute versions of PETSc tuned to their platforms, and several commercial simulation packages, including FIDAP 8.5, TigerCAD, and RF3P, use PETSc for their algebraic solvers. PETSc has been used by Boeing and CFD Research for computational fluid dynamics simulations, by Shell for solving inverse problems for oil reservoir management, and by the South Florida Water Management District modeling the Everglades. He has published over 70 journal and proceedings articles, ranging from Molecular Based Mathematical Biology to the Journal of Geophysical Research to Journal of Chemical Physics to Transactions on Mathematical Software. His work has received almost 10,000 citations according to Google Scholar with an H-index of 25, and more than 20,000 reads on ResearchGate.

Four of his most noteworthy contributions are highlighted here. **1** Development of a scalable preconditioning strategy for the cohesive element formulation of Ortiz. This block, multilevel preconditioner was used in PyLith to solve quasi-static crustal deformation problems with complex fault rheologies on large parallel machines. It is generally applicable to the saddle-point problems arising from this discretization. **2** Development, with Jaydeep Bardhan, of a theory for approximation of the boundary integral operators describing molecular electrostatics which is used to precondition the high-fidelity system, but also to provide extremely efficient low-fidelity solutions for use in optimization and design iterations. This strategy has recently been employed to model protein-ligand binding, and favorably compared with experimental results. **3** Creation of the first 3D classical density functional theory simulation for ion channels using a new scalable, efficient

algorithm for hard sphere interaction and electrostatic correlations. The electrostatic formulation of Gillespie allowed for much more accurate determination of channel fields than the standard bulk theory, but all previous implementations scaled as  $\mathcal{O}(N^3)$ . We developed a comprehensive  $\mathcal{O}(N \log N)$ , with Peter Brune, for the entire simulation, and applied the code to ryanodine receptor transport. **4** Development of the unstructured mesh component of PETSc. This reformulation allows physics routines to be formulated independently of the mesh dimension and cell shape, so that simulator code is written once, but multiple meshes even of different dimension may be compared dynamically. This component has been used in bioelectrostatic calculations, in PyLith for crustal deformation, and in magma dynamics, fracture mechanics, crop modeling, and airfoil simulation.

## Publications

My Advisees are **bold**, Student Collaborators are underlined

### Book Chapters

- [6] Satish Balay, Jed Brown, Matthew G. Knepley, Lois McInnes, and Barry Smith. *Software Engineering for Science*, chapter Providing Mixed Language and Legacy Support within a Library. Taylor & Francis, 2015.
- [5] Shijie Zhong, David A. Yuen, Louis N. Moresi, and Matthew G. Knepley. Numerical methods for mantle convection. In Gerald Schubert, editor, *Treatise on Geophysics*, volume 7. Elsevier, second edition edition, 2015.
- [4] Matthew G. Knepley. Programming languages for scientific computing. In Björn Engquist, editor, *Encyclopedia of Applied and Computational Mathematics*. Springer, 2012.
- [3] **Andy R. Terrel**, Robert C. Kirby, Matthew G. Knepley, L. Ridgway Scott, and Garth N. Wells. Finite elements for incompressible fluids. In *Automated solutions of differential equations by the finite element method*, volume 84 of *Lecture Notes in Computational Science and Engineering*, pages 163–169. Springer-Verlag, 2012.
- [2] Robert C. Kirby, Matthew G. Knepley, Anders Logg, L. Ridgway Scott, and **Andy R. Terrel**. Discrete optimization of finite element matrix evaluation. In *Automated solutions of differential equations by the finite element method*, volume 84 of *Lecture Notes in Computational Science and Engineering*, pages 385–397. Springer-Verlag, 2012.
- [1] Matthew G. Knepley, Richard F. Katz, and Barry Smith. Developing a geodynamics simulator with PETSc. In Are Magnus Bruaset and Aslak Tveito, editors, *Numerical Solution of Partial Differential Equations on Parallel Computers*, volume 51 of *Lecture Notes in Computational Science and Engineering*, pages 413–438. Springer Berlin Heidelberg, 2006.

### Journal Articles

- [54] Mark F. Adams, Dylan P. Brennan, Matthew G. Knepley, and Peng Wang. Exascale Landau collision operator in the CUDA programming model applied to thermal quench plasmas. 2021. Submitted.
- [53] Albert Mollén, Mark F. Adams, Matthew G. Knepley, Robert Hager, and C. S. Chang. Implementation of higher-order velocity mapping between marker particles and grid in the particle-in-cell code xgc. *Journal of Plasma Physics*, 2021. accepted.
- [52] Junchao Zhang, Jed Brown, Satish Balay, Jacob Faibussowitsch, Matthew G. Knepley, Oana Marin, Richard Tran Mills, Todd Munson, Barry F. Smith, and Stefano Zampini. The petscscf scalable communication layer. *IEEE Transactions on Parallel and Distributed Systems*, 2021. Accepted.

- [51] **Hannah Morgan**, **Patrick Sanan**, Matthew G. Knepley, and Richard Tran Mills. Understanding performance variability in standard and pipelined parallel Krylov solvers. *The International Journal of High Performance Computing Applications*, 35, 2020.
- [50] Patrick E Farrell, Matthew G Knepley, Florian Wechsung, and Lawrence Mitchell. PCPATCH: software for the topological construction of multigrid relaxation methods. *ACM Transaction on Mathematical Software*, 2020. accepted.
- [49] Vaclav Hapla, Matthew G. Knepley, **Michael Afanasiev**, Christian Boehm, Martin van Driel, Lion Krischer, and Andreas Fichtner. Fully parallel mesh I/O using PETSc DMPlex with an application to waveform modeling. *SIAM Journal on Scientific Computing*, 2020. accepted.
- [48] **Maurice S. Fabien**, Matthew G. Knepley, and Béatrice M. Rivière. A high order hybridizable discontinuous galerkin method for incompressible miscible displacement in heterogeneous media. *Results in Applied Mathematics*, 8, 2020.
- [47] **Maurice S. Fabien**, Matthew G. Knepley, and Béatrice M. Rivière. Families of interior penalty hybridizable discontinuous galerkin methods for second order elliptic problems. *Journal of Numerical Mathematics*, 2019.
- [46] **M. S. Joshaghani**, **Justin Chang**, Kalyana B. Nakshatrala, and Matthew G. Knepley. Composable solvers for the four-field double porosity/permeability model. *Journal of Computational Physics*, 386:428–466, 2019.
- [45] Travis Thompson, Béatrice M. Rivière, and Matthew G. Knepley. An implicit discontinuous galerkin method for modeling acute edema and resuscitation in the small intestine. *Mathematical Medicine and Biology*, 2019.
- [44] **Maurice S. Fabien**, Matthew G. Knepley, and Béatrice M. Rivière. A hybridizable discontinuous galerkin method for two-phase flow in heterogeneous porous media. *International Journal for Numerical Methods in Engineering*, 2018.
- [43] **Justin Chang**, **Maurice S. Fabien**, Matthew G. Knepley, and Richard T. Mills. Comparative study of finite element methods using the time-accuracy-size (TAS) spectrum analysis. *SIAM Journal on Scientific Computing*, 40(6):C779–C802, 2018.
- [42] **Michael Afanasiev**, Christian Boehm, Martin van Driel, Lion Krischer, Max Rietmann, Dave A. May, Matthew G. Knepley, and Andreas Fichtner. Modular and flexible spectral-element waveform modelling in two and three dimensions. *Geophysical Journal International*, 216(3):1675–1692, 2019.
- [41] **Jonas Actor** and Matthew G. Knepley. An algorithm for computing Lipschitz inner functions in Kolmogorov’s Superposition Theorem. *SIAM Journal on Numerical Analysis*, 2018. In review.
- [40] **Thomas S. Klotz**, Jaydeep Bardhan, and Matthew G. Knepley. Efficient evaluation of ellipsoidal harmonics for potential modeling. *Communications in Applied Mathematics and Computational Science*, 2018. In review.
- [39] **Justin Chang**, Kalyana B. Nakshatrala, Matthew G. Knepley, and Lennart Johnsson. A performance spectrum for parallel computational frameworks that solve PDEs. *Concurrency: Practice and Experience*, 30(11), 2017.
- [38] Mark F. Adams, Eero Hirvijoki, Matthew G. Knepley, Jed Brown, **Tobin Isaac**, and Richard Mills. Landau collision integral solver with adaptive mesh refinement on emerging architectures. *SIAM Journal on Scientific Computing*, 39(6):C452–C465, 2017.

- [37] **Maurice S. Fabien**, Matthew G. Knepley, Richard Mills, and Béatrice M. Rivière. Manycore parallel computing for a hybridizable discontinuous Galerkin nested multigrid method. *SIAM Journal on Scientific Computing*, 41(2):C73–C96, 2018.
- [36] Amneet Pal Singh Bhalla, Boyce E. Griffith, Matthew G. Knepley, Mark F. Adams, and Robert D. Guy. Scalable smoothing strategies for a geometric multigrid method for the immersed boundary equations. *Advances in Computational Mathematics*, 2017. In review.
- [35] Amirhossein Molavi Tabrizi, Spencer Goossens, Ali Mehdizadeh Rahimi, Matthew G. Knepley, and Jaydeep P. Bardhan. Predicting solvation free energies and thermodynamics in polar solvents and mixtures using a solvation-layer interface condition. *Journal of Chemical Physics*, 146(9):094103, 2017. PMID: PMC5336475.
- [34] Amirhossein Molavi Tabrizi, Spencer Goossens, Christopher D. Cooper, Matthew G. Knepley, and Jaydeep P. Bardhan. Extending the solvation-layer interface condition (SLIC) continuum electrostatic model to linearized Poisson-Boltzmann solvent. *Journal of Chemical Theory and Computation*, 2017.
- [33] **Tobin Isaac** and Matthew G. Knepley. Support for non-conformal meshes in PETSc’s DMPlex interface. *ACM Transaction on Mathematical Software*, 2017. In review.
- [32] Matthew G. Knepley, Michael Lange, and Gerard J. Gorman. Unstructured overlapping mesh distribution in parallel. *ACM Transactions on Mathematical Software*, 2017. submitted.
- [31] Amirhossein Molavi Tabrizi, Matthew G. Knepley, and Jaydeep P. Bardhan. Generalising the mean spherical approximation as a multiscale, nonlinear boundary condition at the solute-solvent interface. *Molecular Physics*, 114(16-17):2558–2567, 2016.
- [30] Mark F. Adams, Jed Brown, Matthew G. Knepley, and Ravi Samtaney. Segmental refinement: A multigrid technique for data locality. *SIAM Journal on Scientific Computing*, 8(4):C426–C440, 2016.
- [29] **Hannah Morgan**, Matthew G. Knepley, Patrick Sanan, and L. Ridgway Scott. A stochastic performance model for pipelined Krylov methods. *Concurrency and Computation: Practice and Experience*, 28:4532–4542, 2016.
- [28] Michael Lange, Lawrence Mitchell, Matthew G. Knepley, and Gerard J. Gorman. Efficient mesh management in Firedrake using PETSc-DMPlex. *SIAM Journal on Scientific Computing*, 38(5):S143–S155, 2016.
- [27] **Peter R. Brune**, Matthew G. Knepley, Barry F. Smith, and Xuemin Tu. Composing scalable nonlinear algebraic solvers. *SIAM Review*, 57(4):535–565, 2015. <http://www.mcs.anl.gov/papers/P2010-0112.pdf>.
- [26] Jaydeep P. Bardhan, Matthew G. Knepley, and **Peter R. Brune**. Analytical nonlocal electrostatics using eigenfunction expansions of boundary-integral operators. *Molecular Based Mathematical Biology*, 3(1):1–22, 2015.
- [25] Jaydeep P. Bardhan and Matthew G. Knepley. Multiscale models and approximation algorithms for protein electrostatics. In *Boundary Elements and Other Mesh Reduction Methods XXXVIII*, volume 61, pages 163–174. WIT Press, 2015.
- [24] Jaydeep P. Bardhan and Matthew G. Knepley. Modeling charge-sign asymmetric solvation free energies with nonlinear boundary conditions. *Journal of Chemical Physics*, 141(13):131103, 2014.
- [23] Brad T. Aagaard, Matthew G. Knepley, and Charles A. Williams. A domain decomposition approach to implementing fault slip in finite-element models of quasi-static and dynamic crustal deformation. *Journal of Geophysical Research: Solid Earth*, 118(6):3059–3079, 2013.

- [22] Amy Kreienkamp, Lucy Y. Liu, Mona S. Minkara, Matthew G. Knepley, Jaydeep P. Bardhan, and Mala L. Radhakrishnan. Analysis of fast boundary-integral approximations for modeling electrostatic contributions of molecular binding. *Molecular Based Mathematical Biology*, 1:124–150, June 2013. <http://www.degruyter.com/view/j/mlbmb.2012.1.issue/mlbmb-2013-0007/mlbmb-2013-0007.xml>.
- [21] **Peter R. Brune**, Matthew G. Knepley, and L. Ridgway Scott. Unstructured geometric multigrid in two and three dimensions on complex and graded meshes. *SIAM Journal on Scientific Computing*, 35(1):A173–A191, 2013. <http://arxiv.org/abs/1104.0261>.
- [20] Liang Zheng, Taras Gerya, Matthew G. Knepley, David A. Yuen, Huai Zhang, and Yaolin Shi. Implementation of a multigrid solver on GPU for Stokes equations with strongly variable viscosity based on Matlab and CUDA. *IJHPCA*, 28(1):50–60, 2013.
- [19] Matthew G. Knepley and **Andy R. Terrel**. Finite element integration on GPUs. *ACM Transactions on Mathematical Software*, 39(2), 2013. no. 10, <http://arxiv.org/abs/1103.0066>.
- [18] Jaydeep P. Bardhan and Matthew G. Knepley. Computational science and re-discovery: open-source implementations of ellipsoidal harmonics for problems in potential theory. *Computational Science & Discovery*, 5:014006, 2012. <http://arxiv.org/abs/1204.0267>.
- [17] David I. Ketcheson, Kyle T. Mandli, Aron J. Ahmadi, Amal Alghamdi, Manuel Quezada de Luna, Matteo Parsani, Matthew G. Knepley, and Matthew Emmett. PyClaw: Accessible, extensible, scalable tools for wave propagation problems. *SIAM Journal on Scientific Computing*, 34(4):C210–C231, 2012. <http://arxiv.org/abs/1111.6583>.
- [16] Jaydeep P. Bardhan and Matthew G. Knepley. Mathematical analysis of the BIBEE approximation for molecular solvation: Exact results for spherical inclusions. *Journal of Chemical Physics*, 135(12):124107–124117, 2011. <http://arxiv.org/abs/1109.0651>.
- [15] Dave A. May and Matthew G. Knepley. Optimal, scalable forward models for computing gravity anomalies. *Geophysical Journal International*, 187(1):161–177, 2011. <http://arxiv.org/abs/1107.5951>.
- [14] Rio Yokota, Jaydeep P. Bardhan, Matthew G. Knepley, L.A. Barba, and Tsuyoshi Hamada. Biomolecular electrostatics using a fast multipole BEM on up to 512 GPUs and a billion unknowns. *Computer Physics Communications*, 182(6):1272–1283, 2011.
- [13] Felipe A Cruz, Matthew G Knepley, and L A Barba. PetFMM – a dynamically load-balancing parallel fast multipole library. *International Journal of Numerical Methods in Engineering*, 85(4):403–428, 2010. <http://arxiv.org/abs/0905.2637>.
- [12] Rio Yokota, L A Barba, and Matthew G Knepley. PetRBF – a parallel  $O(N)$  algorithm for radial basis function interpolation. *Computer Methods in Applied Mechanics and Engineering*, 199(25-28):1793–1804, 2010. <http://arxiv.org/abs/0909.5413v1>.
- [11] Matthew G. Knepley, Dmitry A. Karpeev, **Seth Davidovits**, Robert S. Eisenberg, and Dirk Gillespie. An efficient algorithm for classical density functional theory in three dimensions: Ionic solutions. *Journal of Physical Chemistry*, 132(12):124101–124111, 2010.
- [10] V. Stodden, M. G. Knepley, C. Wiggins, R. J. LeVeque, D. Donoho, S. Fomel, M. P. Friedlander, M. Gerstein, I. Mitchell, L. L. Ouellette, N. W. Bramble, P. O. Brown, V. Carey, L. DeNardis, R. Gentleman, D. Gezelter, J. A. Goodman, J. E. Moore, F. A. Pasquale, J. Rolnick, M. Seringhaus, and R. Subramanian. Reproducible Research: addressing the need for data and code sharing in computational science. *Computing in Science and Engineering*, 12(5):8–13, 2010.
- [9] Matthew G. Knepley and Dmitry A. Karpeev. Mesh algorithms for PDE with Sieve I: Mesh distribution. *Scientific Programming*, 17(3):215–230, 2009. <http://arxiv.org/abs/0908.4427>.

- [8] Jaydeep P. Bardhan, Matthew G. Knepley, and Mihai Anitescu. Bounding the electrostatic free energies associated with linear continuum models of molecular solvation. *Journal of Chemical Physics*, 130(10):104108, 2008. Selected for the March 15, 2009 issue of Virtual Journal of Biological Physics Research.
- [7] **Andy R. Terrel**, L. Ridgway Scott, Matthew G. Knepley, and Robert C. Kirby. Automated FEM discretizations for the Stokes equation. *BIT*, 48(2), 2008.
- [6] Richard F. Katz, Matthew G. Knepley, Barry Smith, Marc Spiegelman, and Ethan Coon. Numerical simulation of geodynamic processes with the Portable Extensible Toolkit for Scientific Computation. *Phys. Earth Planet. In.*, 163:52–68, 2007.
- [5] Robert C. Kirby, Matthew G. Knepley, Anders Logg, and L. Ridgway Scott. Optimizing the evaluation of finite element matrices. *SIAM Journal on Scientific Computing*, 27(3):741–758, 2005.
- [4] Minimax Collaboration. Search for disoriented chiral condensate at the Fermilab Tevatron. *Physical Review D*, 61(3), 2000.
- [3] Minimax Collaboration. Analysis of charged particle/photon correlations in hadronic multiparticle production. *Physical Review D*, 55(9), 1997.
- [2] Mary E. Convery, W. L. Davis, Ken W. Del Signore, Tom L. Jenkins, Erik Kangas, Matthew G. Knepley, Ken L. Kowalski, Cyrus C. Taylor, C. H. Wang, S. H. Oh, W. D. Walker, P. L. Colestock, B. Hanna, M. Martens, J. Streets, R. C. Ball, H. R. Gustafson, L. W. Jones, M. J. Longo, J. D. Bjorken, N. Morgan, and C. A. Pruneau. Minimax: What has been learned thus far. *Nuovo Cimento*, 19(1):1045–1049, 1996.
- [1] Robert W. Brown, Mary Convery, Scott Hotes, Matthew G. Knepley, and Labros Petropoulos. Closed strings with low harmonics and kinks. *Physical Review D*, 48(6), 1993.

## Peer-Reviewed Conference Papers

- [25] Jaydeep P. Bardhan and Matthew G. Knepley. Accurate atom-by-atom predictions of solvation electrostatics using a hydration-shell Poisson-Boltzmann model. *Biophysical Journal*, 110(3), 2017. Fall Meeting Supplemental, Abstract DI14A-08.
- [24] Dave A May and Matthew G Knepley. DMSwarm: Particles in PETSc. In *EGU General Assembly Conference Abstracts*, volume 19, page 10133, 2017.
- [23] Nicolas Barral, Matthew G. Knepley, Michael Lange, Matthew D. Piggott, and Gerard J. Gorman. Anisotropic mesh adaptation in Firedrake with PETSc DMPlex. In Steve Owen and Hang Si, editors, *25th International Meshing Roundtable*, pages 1–5, Washington, DC, September 2016.
- [22] Dave A. May, Patrick Sanan, Karl Rupp, Matthew G. Knepley, and Barry F. Smith. Extreme-scale multigrid components within PETSc. In *Proceedings of the Platform for Advanced Scientific Computing Conference*, PASC '16, pages 5:1–5:12, New York, NY, USA, 2016. ACM.
- [21] Jaydeep P. Bardhan and Matthew G. Knepley. Multiscale models and approximation algorithms for protein electrostatics. In *Boundary Elements and Other Mesh Reduction Methods XXXVIII*, volume 61, pages 163–174. WIT Press, 2015.
- [20] Matthew G. Knepley and Jaydeep P. Bardhan. Work/precision tradeoffs in continuum models of biomolecular electrostatics. In *Proceedings of ASME 2015 International Mechanical Engineering Congress & Exposition*, volume 9, page V009T12A04, 2015.



- [19] Michael Lange, Matthew G. Knepley, and Gerard J. Gorman. Flexible, scalable mesh and data management using PETSc DMPlex. In *Proceedings of the Exascale Applications and Software Conference*, April 2015.
- [18] Jaydeep P. Bardhan, D. A. Tejani, N. S. Wiecekowsky, A. Ramaswamy, and Matthew G. Knepley. A nonlinear boundary condition for continuum models of biomolecular electrostatics. In *Proceedings of PIERS*, pages 1215–1221, July 2015.
- [17] Jed Brown, Matthew G. Knepley, and Barry Smith. Run-time extensibility and librarization of simulation software. *IEEE Computing in Science and Engineering*, 17(1):38–45, Jan 2015.
- [16] **Victor Minden**, Barry F. Smith, and Matthew G. Knepley. Preliminary implementation of PETSc using GPUs. In David A. Yuen, Long Wang, Xuebin Chi, Lennart Johnsson, Wei Ge, and Yaolin Shi, editors, *GPU Solutions to Multi-scale Problems in Science and Engineering*, Lecture Notes in Earth System Sciences, pages 131–140. Springer Berlin Heidelberg, 2013.
- [15] Dmitry A. Karpeev, Matthew G. Knepley, and **Peter R. Brune**. Accurate evaluation of local averages on GPGPUs. In David A. Yuen, Long Wang, Xuebin Chi, Lennart Johnsson, Wei Ge, and Yaolin Shi, editors, *GPU Solutions to Multi-scale Problems in Science and Engineering*, Lecture Notes in Earth System Sciences, pages 487–501. Springer Berlin Heidelberg, 2013.
- [14] Mark F. Adams, Jed Brown, and Matthew G. Knepley. Low-communication techniques for extreme-scale multilevel solvers. In *Exascale Mathematics Workshop, Aug 21–22, Washington, DC*. DOE Office of Advanced Scientific Computing Research, 2013.
- [13] Liang Zheng, Taras Gerya, Matthew G. Knepley, David A. Yuen, Huai Zhang, and Yaolin Shi. GPU implementation of multigrid solver for Stokes equation with strongly variable viscosity. In David A. Yuen, Long Wang, Xuebin Chi, Lennart Johnsson, Wei Ge, and Yaolin Shi, editors, *GPU Solutions to Multi-scale Problems in Science and Engineering*, Lecture Notes in Earth System Sciences, pages 321–333. Springer Berlin Heidelberg, 2013.
- [12] Matthew G. Knepley and David A. Yuen. Why scientists and engineers need GPUs today. In David A. Yuen, Long Wang, Xuebin Chi, Lennart Johnsson, Wei Ge, and Yaolin Shi, editors, *GPU Solutions to Multi-scale Problems in Science and Engineering*, Lecture Notes in Earth System Sciences, pages 131–140. Springer Berlin Heidelberg, 2013.
- [11] Jed Brown, Matthew G. Knepley, David A. May, Lois C. McInnes, and Barry F. Smith. Composable linear solvers for multiphysics. In *Proceedings of the 11th International Symposium on Parallel and Distributed Computing (ISPDC 2012)*, pages 55–62. IEEE Computer Society, 2012.
- [10] Amal Alghamdi, Aron Ahmadi, David I. Ketcheson, Matthew G. Knepley, Kyle T. Mandli, and Lisandro Dalcin. PetClaw: A scalable parallel nonlinear wave propagation solver for Python. In *Proceedings of SpringSim 2011*. ACM, 2011.
- [9] Blaise Bourdin, Matthew G. Knepley, and C. Maurini. Numerical simulation of reservoir stimulation - a variational approach. In *Proceedings of the 37th Stanford Geothermal Workshop*, Stanford, CA, 2010. <http://www.geothermal-energy.org/pdf/IGAstandard/SGW/2011/bourdin.pdf>.
- [8] Blaise Bourdin, Matthew G. Knepley, and C. Maurini. Secondary thermal cracks in EGS: a variational approach. In *Proceedings of the 34th Annual Meeting of the Geothermal Resources Council*, Sacramento, CA, 2010. [https://www.math.lsu.edu/~bourdin/Biography\\_assets/Bourdin-Knepley-Maurini-2010.pdf](https://www.math.lsu.edu/~bourdin/Biography_assets/Bourdin-Knepley-Maurini-2010.pdf).
- [7] Felipe A Cruz, Lorena A. Barba, and Matthew G. Knepley. Fast multipole method for particle interactions: an open source parallel library component. In Tromeur-Dervout et. al., editor, *Proceedings of ParCFD2008*. Elsevier, 2008.

- [6] Charles A. Williams, Carl Gable, Bradford H. Hager, Brendan Meade, Brad Aagaard, and Matthew G. Knepley. Modeling of multiple earthquake cycles in southern california using the SCEC community fault model. In *Proceedings of Geosciences '08*, Wellington, NZ, November 2008.
- [5] Matthew G. Knepley, Vivek Sarin, and Ahmed H. Sameh. Multilevel preconditioning for parallel CFD. In *International Conference On Preconditioning Techniques For Large Sparse Matrix Problems In Industrial Applications*, Minneapolis, MN, June 1999.
- [4] Matthew Knepley, Ahmed H. Sameh, and Vivek Sarin. Design of large scale parallel simulations. In *Proceedings of Parallel CFD'99*. Elsevier, 1999.
- [3] Matthew Knepley and Vivek Sarin. Algorithm development for large scale computing. In *Proceedings of the SIAM Workshop on Object Oriented Methods for Inter-operable Scientific and Engineering Computing*. SIAM, 1999. <http://books.google.com/books?id=2Da5OcnjPSgC&lpg=PA58&ots=TJCK64BUeg&dq=Bill%20Gropp%20Science%20Engineering%20Object%20Oriented&pg=PA138#v=onepage&q&f=false>.
- [2] Matthew Knepley and Denis Vanderstraeten. Parallel building blocks for finite element simulations: Application to solid-liquid mixture flows. In *Proceedings of Parallel CFD'97*, pages 281–287. Elsevier, 1998.
- [1] Matthew Knepley, Ahmed H. Sameh, and Vivek Sarin. Parallel simulation of particulate flows. In *Solving Irregularly Structured Problems in Parallel*, volume 1457 of *Lecture Notes in Computer Science*, pages 226–237, 1998.

#### Other Conference Papers and Technical Reports

- [25] Matthew G. Knepley, Jed Brown, Lois Curfman McInnes, Barry Smith, Karl Rupp, and Mark Adams. Exascale computing without threads. 2015. Whitepaper for the DOE High Performance Computing Operational Review (HPCOR) on Scientific Software Architecture for Portability and Performance.
- [24] Matthew G. Knepley, Jed Brown, Lois Curfman McInnes, Barry Smith, Karl Rupp, and Mark Adams. Overview of the PETSc library. 2015. Whitepaper for the DOE High Performance Computing Operational Review (HPCOR) on Scientific Software Architecture for Portability and Performance.
- [23] Karl Rupp, Satish Balay, Jed Brown, Matthew G. Knepley, Lois Curfman McInnes, and Barry F. Smith. On the evolution of user support topics in computational science and engineering software. *ArXiv e-prints*, 2015. Whitepaper for Computational Science & Engineering Software Sustainability and Productivity Challenges.
- [22] Barry Smith, Lois Curfman McInnes, Emil Constantinescu, Mark Adams, Satish Balay, Jed Brown, Matthew Knepley, and Hong Zhang. PETSc's software strategy for the design space of composable extreme-scale solvers. Preprint ANL/MCS-P2059-0312, Argonne National Laboratory, 2012. DOE Exascale Research Conference, April 16-18, 2012, Portland, OR.
- [21] **Peter R. Brune**, Matthew G. Knepley, Barry F. Smith, and Xuemin Tu. Composing scalable nonlinear algebraic solvers. Preprint ANL/MCS-P2010-0112, Argonne National Laboratory, 2013.
- [20] L. Ridgway Scott, Jed Brown, George W. Bergantz, Dan Cooley, Clint Dawson, Maarten de Hoop, Donald Estep, Natasha Flyer, Efi Foufoula-Georgiou, Michael Ghil, Matthew G. Knepley, Randall J. LeVeque, Lek-Heng Lim, Serge Prudhomme, Adrian Sandu, Frederik J. Simons, Philip B. Stark, Michael Stein, Seth Stein, Toshiro Tanimoto, Daniel Tartakovsky, Jonathan Weare, Robert Weiss, Grady B. Wright, and Dave Yuen. Fostering interactions between the geosciences and mathematics, statistics, and computer science. Technical Report 2012-02, University of Chicago, 2012.

- [19] **Peter R. Brune**, Matthew G. Knepley, and L. Ridgway Scott. Exponential grids in high-dimensional space. Technical Report TR-2011-07, University of Chicago, December 2011. <http://www.cs.uchicago.edu/research/publications/techreports/TR-2011-07>.
- [18] David I. Ketcheson, Aron Ahmadi, and Matthew G. Knepley. Conference review: High performance computing and hybrid programming concepts for hyperbolic pde codes. *SIAM News*, 44(7), September 2011. <http://www.siam.org/pdf/news/1912.pdf>.
- [17] Liang Zheng, Taras Gerya, Matthew G. Knepley, David A. Yuen, Huai Zhang, and Yaolin Shi. Implementation of a multigrid solver on GPU for Stokes equations with strongly variable viscosity based on Matlab and CUDA. Research Report UMSI 2011/33, University of Minnesota Supercomputing Institute, March 2011. <http://static.msi.umn.edu/rreports/2011/33.pdf>.
- [16] Satish Balay, Shrirang Abhyankar, Mark F. Adams, Jed Brown, Peter Brune, Kris Buschelman, Lisandro Dalcin, Alp Dener, Victor Eijkhout, William D. Gropp, Dmitry Karpeyev, Dinesh Kaushik, Matthew G. Knepley, Dave A. May, Lois Curfman McInnes, Richard Tran Mills, Todd Munson, Karl Rupp, Patrick Sanan, Barry F. Smith, Stefano Zampini, Hong Zhang, and Hong Zhang. PETSc users manual. Technical Report ANL-95/11 - Revision 3.15, Argonne National Laboratory, 2021.
- [15] Charles A. Williams, Brad Aagaard, and Matthew G. Knepley. PyLith: A finite-element code for modeling quasi-static and dynamic crustal deformation. In *Eos Transactions of the AGU*. American Geophysical Union, 2011. Fall Meeting Supplemental, Abstract D114A-08.
- [14] Liang Zheng, Taras Gerya, David A. Yuen, Matthew G. Knepley, Huai Zhang, and Yaolin Shi. GPU implementation of Stokes equation with strongly variable coefficients. In *Eos Transactions of the AGU*. American Geophysical Union, 2010. Fall Meeting Supplemental, Abstract IN41A-1350.
- [13] Robert C. Kirby, Matthew G. Knepley, and L. Ridgway Scott. Languages and compilers for variational forms. Technical Report TR-2010-09, University of Chicago, October 2010. <http://www.cs.uchicago.edu/research/publications/techreports/TR-2010-09>.
- [12] Robert C. Kirby, Matthew G. Knepley, and L. Ridgway Scott. Evaluation of the action of finite element operators. Technical Report TR-2010-08, University of Chicago, October 2010. <http://www.cs.uchicago.edu/research/publications/techreports/TR-2010-08>.
- [11] M. G. Knepley, D. A. Karpeev, R. S. Eisenberg, and D. Gillespie. Energetics of Calcium Selectivity: A Three-Dimensional Classical Density Functional Theory Approach. *Biophysical Journal*, 96:661, feb 2009.
- [10] Dave A. May, Matthew G. Knepley, and Michael Gurnis. CitcomSX: Robust preconditioning in CitcomS via PETSc. In *Eos Transactions of the AGU*. American Geophysical Union, 2009. Fall Meeting Supplemental, Abstract P31A-A1241.
- [9] David A. Yuen, Matthew G. Knepley, Gordon Erlebacher, and Grady B. Wright. The coming role of GPU in computational geodynamics. In *Eos Transactions of the AGU*. American Geophysical Union, 2009. Fall Meeting Supplemental, Abstract D122A-05.
- [8] Brad Aagaard, Charles A. Williams, and Matthew G. Knepley. PyLith: A finite-element code for modeling quasi-static and dynamic crustal deformation. In *Eos Transactions of the AGU*, volume 89. American Geophysical Union, 2007. Fall Meeting Supplemental, Abstract T41A-1925.
- [7] Charles A. Williams, Brad Aagaard, and Matthew G. Knepley. PyLith: A finite-element code for modeling quasi-static and dynamic crustal deformation. In *Eos Transactions of the AGU*, volume 88. American Geophysical Union, 2007. Fall Meeting Supplemental, Abstract T21B-1798.
- [6] C. Zhang, M. G. Knepley, D. A. Yuen, and Y. Shi. Two new approaches in solving the nonlinear shallow water equations for tsunamis. Preprint ANL/MCS-P1459-0907, ANL, September 2007.

- [5] Matthew G. Knepley and Dmitry A. Karpeev. Mesh algorithms for PDE with Sieve I: Mesh distribution. Technical Report ANL/MCS-P1455-0907, Argonne National Laboratory, February 2007. [ftp://info.mcs.anl.gov/pub/tech\\_reports/reports/P1455.pdf](ftp://info.mcs.anl.gov/pub/tech_reports/reports/P1455.pdf).
- [4] Charles A. Williams, Brad Aagaard, and Matthew G. Knepley. Development of software for studying earthquakes across multiple spatial and temporal scales by coupling quasi-static and dynamic simulations. In *Eos Transactions of the AGU*, volume 86. American Geophysical Union, 2005. Fall Meeting Supplemental, Abstract S53A-1072.
- [3] Matthew G. Knepley and Dmitry A. Karpeev. Flexible representation of computational meshes. Technical Report ANL/MCS-P1295-1005, Argonne National Laboratory, October 2005. [ftp://info.mcs.anl.gov/pub/tech\\_reports/reports/P1295.pdf](ftp://info.mcs.anl.gov/pub/tech_reports/reports/P1295.pdf).
- [2] Robert C. Kirby, Matthew G. Knepley, and L. Ridgway Scott. Optimal evaluation of finite element matrices. Technical Report TR-2004-04, University of Chicago, May 2004. <http://www.cs.uchicago.edu/research/publications/techreports/TR-2004-04>.
- [1] Andrew Cleary and Matthew G. Knepley. Solvers as operators. Technical Report UCRL-ID-135342, Lawrence Livermore National Laboratory, 1999.

## Software Toolkits

Developer of the Portable, Extensible, Toolkit for Scientific Computation (**PETSc**) for PDE simulation

700+ scientific publications have used PETSc, including combustion, brain surgery, subsurface flow, fusion, and cardiology. See <http://www.mcs.anl.gov/petsc/petsc-as/publications>

30+ community scientific simulators are built on PETSc, ranging from micromagnetics to geosciences

300,000 processes have been used efficiently on the IBM BG/P

500 billion unknowns used in the simulation of neutron transport

3+ teraflops realized on groundwater reactive flow using PFLOTRAN

Used at all DOE laboratories and Supercomputing Centers, Boeing, Shell, GM

Designer and developer of the parallel unstructured grid component

Co-Creator of **PyLith** code for large, parallel seismic and post-seismic simulation

30+ scientific publications have used PyLith

Capable of simulating both dynamic and quasi-static problems in parallel

Can use both simplicial and tensor elements in 1D, 2D, and 3D

Fully documented and supported, [http://geodynamics.org/cig/software/pylith/pylith\\_manual-1.6.2.pdf](http://geodynamics.org/cig/software/pylith/pylith_manual-1.6.2.pdf)

## Technical Presentations

### *Plenary and Keynote Presentations*

Keynote Address, Domain Decomposition, Newfoundland, CA Jul 2018

Keynote Address, Computational and Data-Enabled Science and Engineering Days, Univ. of Buffalo, Buffalo NY, April 2017

High Performance Python Libraries, Keynote for PyHPC Workshop, SC 14, New Orleans, LA Nov 2014

Keynote Address, GPU-SMP GPU Solutions to Multiscale Problems, Shenzhen, China June 2012

Keynote Address, GPU-SMP GPU Solutions to Multiscale Problems, Lanzhou, China July 2011  
Lindbergh Lecture, Department of Mechanical Engineering, UW Madison, April 2011  
NSF PASI Institute, Valparaiso, Chile, January 2011  
Plenary, Parallel and Accelerated Computing, Széchenyi István University, Győr, Hungary, October 2010  
International Workshop on Modern Computational Geoscience Frontiers, GUCAS, Beijing, July 2009  
AuScope Inaugural Conference, Monash University, Victoria, Australia, February 2008  
Special Semester on Biological Computing, University of Linz, Linz, Austria, October 2007

*Invited Presentations*

SIAM CSE, Online, February 2021  
Applied and Computational Mathematics Virtual Seminar, Univ. of Edinburgh, Edinburgh UK, November 2020  
SIAM PP, Seattle, WA, February 2020  
Firedrake 2020, Seattle, WA, February 2020  
Firedrake 2019, Durham UK, September 2019  
Seminar, Department of Engineering Science, University of Auckland, Auckland NZ, July 2019  
AMS Sectional Meeting, Honolulu, HI, March 2019  
SIAM CSE, Spokane, WA, February 2019  
AGU Fall Meeting, Washington D.C., December 2018  
AGU: Data Science, Machine Learning, and Jupyter, Washington D.C., December 2018  
MCS Seminar, ANL, Chicago, IL, September 2018  
SIAM Life Sciences, Minneapolis, MN, July 2018  
SIAM PP, Tokyo, JP, March 2018  
DOE Scientific Machine Learning, Bethesda, MD January 2018  
Scientific and Statistical Computing Seminar, Department of Statistics, Univ. of Chicago, Chicago IL, May 2017  
Scientific Computing Seminar, Department of Mathematics, Univ. of Houston, Houston TX, April 2017  
ICL Earth Sciences Seminar, London UK, March 2017  
SIAM CS&E, Minisymposium, Atlanta GA, March 2017  
Rice Laboratory for Space and Astrophysical Plasmas Seminar, Houston TX, October 2016  
ICL Earth Sciences Seminar, London UK, October 2016  
UNC Mathematics Seminar, Chapel Hill NC, September 2016  
MIT AeroAstro Seminar, Boston MA, May 2016  
SIAM PP, Paris, FR Apr 2016  
Ken Kennedy Institute Seminar, Houston, TX Mar 2016  
Melt in the Mantle 2016, Cambridge UK Feb 2016  
SPPEXA 2016, Munich DE Jan 2016

ASME IMECE 2015, Houston TX Nov 2015  
Composing Nonlinear Solvers, ICERM, Providence RI Sept 2015  
ME & IE Seminar, Northeastern University, Boston, MA Mar 2015  
SIAM CS&E, Salt Lake City, UT Mar 2015  
CAAM Seminar, Rice University, Houston, TX Feb 2015  
Numerical Analysis Seminar, Texas A&M University, College Station, TX Jan 2015  
Numerical Analysis Seminar, Texas A&M University, College Station, TX Dec 2014  
Nonlinear Preconditioning in PETSc, ICERM, Providence RI July 2014  
Scalable Nonlinear Solvers for Geophysical Problems, SIAM Annual Meeting, Chicago IL July 2014  
Nonlinear Preconditioning in PETSc, PMAA 14, Lugano CH July 2014  
PETSc Solvers for Crustal Deformation, Stanford University, Palo Alto CA June 2014  
Composable Solvers in PETSc, CACDS Seminar, University of Houston, Houston TX June 2014  
Nonlinear Preconditioning in PETSc, Oxford University, Oxford UK March 2014  
Nonlinear Preconditioning in PETSc, Imperial College, London UK March 2014  
Runtime Configurability in PETSc, SIAM PP, Portland OR February 2014  
Algorithms for Exascale Computational Mesoscience, ExaMath13 Workshop, Wash. D.C. August 2013  
Finite Element Integration using CUDA and OpenCL, GPU-SMP 13, Changchun, China July 2013  
The Process of Computational Science, Maison de la Simulation, Orsay, France June 2013  
Nested and Hierarchical Solvers in PETSc, SIAM CS&E, Boston, February 2013  
APAM Colloquium, Columbia University, New York February 2013  
Mathematics Colloquium, Széchenyi István University, Győr, Hungary November 2012  
School of Mathematical Sciences Colloquium, Monash University, VIC Australia October 2012  
Bridging the Gap Between the Geosciences and Mathematics, Statistics, and Computer Science, Princeton, NJ October 2012  
ACTS Workshop, Berkeley, CA August 2012  
SIAM Annual Meeting, Minneapolis, MN July 2012  
CIG Crustal Deformation Modeling workshop, Golden, CO June 2012  
Specialized Topics Workshop, Center for Biomedical Computing, Simula Research, Norway, August 2011  
Conference on Simulation and Optimization, Győr, Hungary, June 2011  
HPC<sup>3</sup> Workshop, KAUST, March 2011  
Advanced Algorithms on GPUs, SIAM CS&E, Reno, March 2011  
IMA Workshop on High Performance Computing and Emerging Architectures, January 2011  
AGU: Large-Scale Geosciences Applications using GPU and Multicore Architectures, December 2010  
Conference in Honor of Prof. Ahmed Sameh, Purdue University, October 2010  
39th SPEEDUP Workshop on High Performance Computing, ETH Zurich, September 2010  
Geophysical Fluid Dynamics Seminar, Department of Earth Sciences, ETH Zurich, September 2010  
Automated and Distributed Computing Seminar, Simula Res. Lab., Oslo Norway, August 2010

Int. Workshop of GPU Solutions to Multiscale Problems in Sci. and Eng., Harbin China, July 2010  
ESCO 2nd European Seminar on Coupled Problems, Pilsen Czech Republic, July 2010  
KAUST Applied Math & Computer Science Seminar, Saudi Arabia, March 2010  
Tufts Mathematics Department Seminar, Medford, MA, February 2010  
AGU Fall Meeting, San Francisco, CA, December 2009  
Sharing Data and Code in Computational Science, New Haven, CT, November 2009  
NSF-NAIS Intelligent Software Workshop, Edinburgh, Scotland, October 2009  
Department of Mathematics Colloquium, LSU, Baton Rouge, September 2009  
International Workshop on Geodynamical Phenomena, Suzdal, Russia, August 2009  
HPC Group, SSC, Shanghai, July 2009  
Path to Petascale (GPU Meeting), UIUC, IL, March 2009  
SIAM CS&E, Miami, FL, March 2009  
ICES Seminar, Austin, TX, August 2008  
SIAM Annual Meeting, San Diego, CA, July 2008  
Advancing Num. Mod. of Mantle Convection and Lithospheric Dynamics, UC Davis, CA, July 2008  
Num. Mod. of Crustal Deformation and Earthquake Faulting, Colorado School of Mines, CO, June 2008  
Sandia CSRI Workshop on Next-Generation Scalable Applications, Albuquerque, NM, June 2008  
Workshop on Automating the Development of Sci. Comp. Software, LSU, Baton Rouge, LA, March 2008  
Role of Symbolic, Numeric and Algebraic Comp. in CDI, NSF, Washington D.C., October 2007  
Adaptive Mesh Refinement Workshop, UC Boulder, Boulder, CO, October 2007  
Seminar, University of Duisberg-Essen, Essen, Germany, October 2007  
VLAB Seminar, University of Minnesota, Minneapolis, MN, August 2007  
Biomedical Flows Workshop, Simula Research, Oslo, Norway, June 2007  
Seminar, Supercomputing Institute, University of Minnesota, Minneapolis, MN, December 2006  
Seminar, Simula Research, Oslo, Norway, November 2006  
FEniCS 06, TU Delft, Delft, Netherlands, November 2006  
Multiphysics Simulation, INL, Idaho Falls, ID, September 2006  
Magma Dynamics Workshop, Columbia University, New York, NY, August 2006  
SIAM Annual Meeting, Boston, MA, July 2006  
Fault Systems Workshop, Colorado School of Mines, Golden, CO, June 2006  
Compressible Convection Workshop, Purdue University, West Lafayette, IN, March 2006  
CIG Science Steering Committee Meeting, Pasadena, CA, November 2005  
FEniCS 05, TTI, Chicago, IL, October 2005  
CIG Meeting, Monash University, Melbourne, Australia, October 2005  
Seminar, Indiana University, Bloomington, IN, September 2005  
Short-Term Crustal Dynamics Workshop, LANL, Los Alamos, NM, July 2005

Mantle Convection Workshop, UC Boulder, Boulder, CO, June 2005  
CIG Executive Committee Meeting, Berkeley, CA, May 2005  
Parallel Computing Workshop, University of Houston, Houston, TX, April 2005  
CIG Meeting, Caltech, Pasadena, CA, March 2005  
SIAM CS&E, Orlando, FL, February 2005  
MCS Seminar, ANL, Lemont, IL, October 2004  
CIG Meeting, Monash University, Melbourne, Australia, October 2004  
CRI Seminar, Purdue University, West Lafayette, IN, October 2004  
Domain Specific Languages for PDE Constrained Optimization, ANL, Lemont, IL, August 2004  
Seminar, CMU, Pittsburgh, PA, July 2004  
Climate Simulation Colloquium, University of Chicago, Chicago, IL, June 2004  
Parallel CFD 2004, Gran Canaria, May 2004  
Lecture, Columbia University, New York, NY, February 2004  
CIG Kickoff Meeting, LAX, Los Angeles, CA, January 2004  
CRI Seminar, Purdue University, West Lafayette, IN, February 2003  
Seminar, LBL, Berkeley, CA, August 1999  
Parallel CFD, Williamsburg, VA, May 1999  
Seminar, Lucent, Murray Hill, NJ, May 1999  
SIAM Workshop on OO Meth. for InterOp. Sci. & Eng. Comp., IBM T.J. Watson, NY October 1998  
Conference on Capability Computing, NCSA, Urbana-Champaign, IL, September 1998  
Solving Irregularly Structured Problems in Parallel, LBL, Berkeley, CA August 1998  
Seminar, CERFACS, Toulouse, France, June, 1996

#### *Tutorial Presentations*

Linear and Nonlinear Solvers, PETSc Users Meeting, Atlanta, GA, June 2019  
Using LaTeX, Git, and Make, CDSE Days 2019, Buffalo, NY, April 2019  
PDEs, optimization, and eigenproblems with PETSc/TAO and SLEPc, ECP Annual Meeting, Houston, TX, January 2019  
Introductory PETSc, PETSc Users Meeting, London, UK, June 2018  
Using LaTeX, Git, and Make, CDSE Days, Buffalo, NY, April 2018  
PETSc Tutorial, CDSE Days, SUNY Buffalo, NY, April 2017  
PETSc Tutorial, CEMRACS, CIRM, Luminy, France, July 2016  
PyLith Tutorial, CIG All-Hands Meeting, UC Davis, CA, June 2016  
PETSc Tutorial, Rice Oil & Gas HPC, Houston, TX, March 2016  
SC 14 PyHPC Tutorial, New Orleans, LA, November 2014  
PETSc Tutorial, Imperial College, London, March 2014  
PETSc Tutorial, Minnesota Supercomputing Institute, University of Minnesota, Minneapolis MN, Septem-



ber 2013

Crustal Deformation Modeling Tutorial Week, June 2013

Advanced PETSc Tutorial, Maison de la Simulation, Orsay, France June 2013

PETSc Tutorial, ACTS Workshop, University of California, Berkeley, August 2012

PETSc Tutorial, ICES, University of Texas at Austin, September 2011

PETSc Tutorial, UW Madison, April 2011

NSF PASI Institute, Scientific Computing in the Americas, Valparaíso, Chile, January 2011

Széchenyi István University, Győr, Hungary, October 2010

ACTS Toolkit Workshop, LBL, Berkeley, CA, August 2010

Short Course on Sci. Comp., Graduate Univ., Chinese Academy of Sciences, Beijing, China, July 2010

PETSc Tutorial, T.J. Watson Research Center, NY, October 2009

Short Course on Sci. Comp., Graduate Univ., Chinese Academy of Sciences, Beijing, China, July 2009

PETSc Tutorial, TACC, Austin, TX, May 2009

Short Course on Foundations of Finite Element Computing, Simula Research, Oslo, Norway, August 2008

PETSc Tutorial, TACC, Austin, TX, August 2008

ACTS Toolkit Workshop, LBL, Berkeley, CA, August 2007

PETSc short course, Parallel CFD 07, Antalya, Turkey, May 2007

Summer school, SCAT 2007, UTFSM, Valparaiso, Chile, January 2007

PETSc Tutorial, AMCS 4302, Columbia University, New York, NY, October 2006

ACTS Toolkit Workshop, LBL, Berkeley, CA, August 2006

PETSc Tutorial, SIAM PP, San Francisco, CA, February 2006

ACTS Toolkit Workshop, LBL, Berkeley, CA, August 2005

Parallel Computing Workshop, University of Houston, Houston, TX, April 2005

Week long PETSc short course, INL, Idaho Falls, ID, March 2005

PETSc Tutorial, DD16, Courant Institute, New York, NY, January 2005

ACTS Toolkit Workshop, LBL, Berkeley, CA, August 2004

Week long PETSc short course, Parallel CFD 2004, Gran Canaria, May 2004

#### *Contributed Presentations*

Rice Oil & Gas HPC, Houston, TX, March 2018

Rice Oil & Gas HPC, Houston, TX, March 2017

Rice Oil & Gas HPC, Houston, TX, March 2016

Biophysical Society Annual Meeting, Boston, MA, March 2009

Parallel CFD 08, Lyon, France, May 2008

SIAM PP, Atlanta, GA, March 2008

USNCCM 10, San Francisco, CA, July 2007

Workshop on Scientific Computing, UT Austin, Austin, TX, October 2006

SIAM PP, San Francisco, CA, February 2006  
SciPy 2005, Caltech, Pasadena, CA, September 2005  
USNCCM 8, Austin, TX, July 2005  
SciPy 2004, Caltech, Pasadena, CA, September 2004  
Parallel CFD, Gran Canaria, Spain, May 2004  
SIAM PP, San Francisco, CA, February 2004  
Geoframeworks Workshop, Caltech, Pasadena, CA, October 2003  
SciPy 2003, Caltech, Pasadena, CA, September 2003

## Postdoctoral Researcher Associates

Robert Walker, University at Buffalo, 2019–*present*  
Justin Chang, Rice University, 2017–2019  
Tobin Isaac, University of Chicago and Rice University, 2015–2017

## Graduate Students

### *Phd Students Advised*

Alexander Stone, University at Buffalo Ph.D., supervisor since 5/20  
Feng-Mao Tsai, University at Buffalo Ph.D., supervisor since 5/20  
Daniel Finn, University at Buffalo Ph.D., supervisor since 9/19  
Darsh Kiritbhai Nathawani, University at Buffalo Ph.D., supervisor since 9/19  
Brandon Denton, University at Buffalo Ph.D., supervisor since 9/19  
Joseph Pusztay, University at Buffalo Ph.D., supervisor since 9/17  
Albert Cowie, University at Buffalo Ph.D., supervisor since 9/17  
Maurice Fabien, Rice University Ph.D. 2019, with Prof. Beatrice Rivere  
Thesis: *Hybridizable Discontinuous Galerkin Methods for Flow and Transport: Applications, Solvers, and High Performance Computing*  
Thomas Klotz, Rice University Ph.D. 2019,  
Thesis: *Numerical Analysis of Nonlinear Boundary Integral Equations Arising in Molecular Biology*  
Andy Terrel, University of Chicago Ph.D. 2010, with Prof. L. Ridgway Scott  
Thesis: *Finite Element Method Automation for Non-Newtonian Fluid Models*. CTO of Fashion Metric, Chairman of the Board of the NumFOCUS foundation.  
Peter Brune, University of Chicago Ph.D. 2011, with Prof. L. Ridgway Scott  
Thesis: *Fast Numerical Methods and Biological Problems*. Software Engineer at Google.

### *Masters Students Advised*

Jonas Actor, Rice University MA, 2018  
*Computation for the Kolmogorov Superposition Theorem*  
Thomas Klotz, Rice University MA, 2017  
*Optimal Integration for Boundary Integral Models*

Jeremy Tillay, Rice University MA, 2017  
*Analysis of Segmental Refinement Multigrid*, Chevron

Hannah Morgan, University of Chicago MA 2015, with Prof. Ridgway Scott  
*Numerical solutions to the KdV equation*. Phd student at University of Chicago.

Eric Buras, Rice University MA 2016,  
*A Multigrid Solver for Graph Laplacian Linear Systems on Power-Law Graphs*. Associate Research Engineer at Aptima, Inc.

#### *Summer Graduate Students Advised*

Hannah Morgan, University of Chicago 2014, with Prof. Ridgway Scott

Sean Laguna, University of Chicago 2014, with Prof. Ridgway Scott

Peter Brune, ANL Givens Fellow 2009

Samuel Daitch, ANL Givens Fellow 2007

Emma Rainey, Krell Institute Computational Science Graduate Fellow 2005

Richard Katz, Krell Institute Computational Science Graduate Fellow 2004

Dmitry Leykekhman, ANL Givens Fellow 2003

Nessy Tania, ANL Givens Fellow 2003

#### *Undergraduate Students Advised*

Alexander Stone, University at Buffalo 2019, *Kolmogorov Superposition Theorem*

Evan Walley, University at Buffalo 2017, *Kolmogorov Superposition Theorem*

David Clark, Rice University 2017, *Plasma Dynamics*

David Clark, Rice University 2016, *Magma Dynamics*

Victor Gonzalez, Rice University 2016, *Magma Dynamics*

Ian Alevy, University of Chicago 2012, *Probabilistic Performance Modeling*

Seth Davidovitz, Rush University Medical Center 2010, *Ion Channel Modeling*

#### *Phd Committees*

Vivek Bhavsar, Phd, Geology, University at Buffalo 2023

Hannah Morgan, Phd, Computer Science, University of Chicago 2019

Kirstie Haynie, Phd, Earth and Atmospheric Sciences, University of Houston 2019

Boris Brimkov, Phd, Computational and Applied Mathematics, Rice University 2017

Xiaodi Deng, Phd, Computational and Applied Mathematics, Rice University 2017

Justin Chang, Phd, Civil Engineering, University of Houston 2017

Caleb Magruder, Phd, Computational and Applied Mathematics, Rice University 2017

Arturo Vargas, Phd, Computational and Applied Mathematics, Rice University 2017

John Riehl, Phd, Computer Science, University of Chicago 2008

### *MS Committees*

Yabin Zhang, MS, Computational and Applied Mathematics, Rice University 2017  
John Gomez, MS, Applied Physics, Rice University 2017  
Bryan Doyle, MS, Computational and Applied Mathematics, Rice University 2017  
Chen Liu, MS, Computational and Applied Mathematics, Rice University 2016  
Rujeko Chinomona, MS, Computational and Applied Mathematics, Rice University 2016  
Frankie Camacho, MS, Computational and Applied Mathematics, Rice University 2016  
Sri Raj Paul, MS, Computer Science, Rice University 2015

### Professional Activities

#### *Editorial Positions*

Associate Editor, SIAM Journal on Scientific Computing, SIAM (2020–Present)  
Associate Editor, Cogent Geoscience, Taylor & Francis (2015–2019)

#### *International Committees and Visiting positions*

Member Executive Committee, NSF [Computational Infrastructure for Geodynamics](#), (2011–2014)  
Chair, Computational Science Working Group, NSF [Computational Infrastructure for Geodynamics](#), (2013–2016)  
Guest Researcher, Imperial College London, London, UK (2014, 2015, 2016, 2017)  
Guest Researcher, Princeton Plasma Physics Laboratory, Princeton, NJ (2017)  
Newton Institute Guest, Cambridge University, Cambridge, UK (2016)  
CEMRACS Summer School Instructor, SMAI, Luminy, France (2016)  
Guest Researcher, University of Melbourne, Melbourne, Australia (2015)  
Guest Researcher, Department of Aeronautics and Astronautics, MIT, Boston, MA (2015)  
Guest Researcher, Oxford University, Oxford, UK (2014)  
Guest Researcher, University at Buffalo, Buffalo, NY (2014)  
Guest Researcher, University of Wisconsin, Madison, WI (2013, 2014)  
Guest Researcher, Texas Advanced Supercomputing Center, Austin, TX (2013)  
Guest Researcher, Université Paris Sud, Orsay, France (2013)  
Guest Researcher, Maison de Simulation, Orsay, France (2013)  
Guest Researcher, KAUST, Jeddah, Saudi Arabia (2010, 2011, 2013)  
Guest Researcher, UTFSM, Valpariso, Chile (2011)  
Guest Researcher, Széchenyi István University, Győr, Hungary (2010, 2011, 2012)  
Guest Researcher, ETHZ, Zurich, Switzerland (2010)  
Guest Researcher, Tufts University, Medford, MA (2010)  
Guest Researcher, VPAC, Melbourne, Australia (2010)  
Guest Researcher, GUCAS, Beijing, China (2009, 2010)

Guest Researcher, Caltech, Pasadena, CA (2009, 2010)  
Guest Researcher, IBM T.J. Watson Research Center, White Plains, NY (2009)  
Guest Researcher, Purdue University, West Lafayette, IN (2008, 2012, 2014)  
Guest Researcher, Boston University, Boston, MA (2008, 2009, 2010)  
Guest Researcher, Louisiana State University, Baton Rouge, LA (2008, 2009, 2014)  
Guest Researcher, Monash University, Clayton, Australia (2008, 2010, 2015)  
Guest Researcher, University of Texas Austin, Austin, TX (2008, 2011)  
Guest Researcher, Center for Biomedical Computing, Simula Research, Oslo Norway (2007, 2008, 2009, 2010, 2011)  
Guest Researcher, USGS, Menlo Park, CA (2007, 2009)  
Guest Researcher, TU Delft, Delft, Netherlands (2006)  
Guest Researcher, INL, Idaho Falls, ID (2006)  
Guest Researcher, Columbia University, New York, NY (2006)  
Guest Researcher, RPI, Troy, NY (2006)  
Advisory Computational Scientist, CIG (2004–2010)  
Guest Researcher, University of Minnesota, Minneapolis, MN (1997, 1998, 2009)

#### *Paper Reviews*

Reviewer, ACM Transactions on Mathematical Software  
Reviewer, AMS Mathematics of Computation  
Reviewer, Computer Methods in Applied Mechanics and Engineering  
Reviewer, Concurrency: Practice and Experience  
Reviewer, Journal of Scientific Computing  
Reviewer, Journal of Chemical Physics  
Reviewer, Journal of Computational Physics  
Reviewer, IEEE Transaction on Parallel and Distributed Systems  
Reviewer, IEEE International Parallel & Distributed Processing Symposium (IPDPS)  
Reviewer, International Journal on Computational Science and Engineering  
Reviewer, International Journal on Numerical Methods in Engineering  
Reviewer, Operations Research  
Reviewer, Parallel Computing  
Reviewer, Physics of Earth and Planetary Interiors  
Reviewer, SIAM Journal on Scientific Computing  
Reviewer, SIAM Journal on Numerical Analysis  
Reviewer, Springer-Verlag

#### *Meetings Organized*

Program Committee, CDM 2019, Golden, CO, [website](#) (June 2019)

Program Committee, PETSc 2019, Atlanta, GA, <http://www.mcs.anl.gov/petsc/meetings/2019> (June 2019)

Co-Chair, SIAM [Gene Golub Summer School](#), Aussois, France (July 2019)

Program Committee, SIAM CS&E 2019, Spokane, WA, [website](#) (Mar 2019)

Program Committee, PETSc 2018, London, UK, <http://www.mcs.anl.gov/petsc/meetings/2018> (June 2018)

Program Committee, PETSc 2017, Boulder, CO, <http://www.mcs.anl.gov/petsc/meetings/2017> (June 2017)

Technical Papers Committee for [Supercomputing 2017](#)

Program Committee, CDM 2017, Golden, CO (June 2017)

Program Committee, Scientific Software Days, Austin, TX, <http://scisoftdays.org> (Mar 2017)

Program Committee, IPDPS, Orlando, FL (June 2017)

Program Committee, HPC, Virginia Beach, VA (April 2017)

Program Committee, NSF SI2 PI Meeting, Arlington, VA (February 2017)

Program Chair, PETSc 2016, Vienna, Austria, <http://www.mcs.anl.gov/petsc/meetings/2016> (June 2016)

Program Committee, Scientific Software Days, Austin, TX, <http://scisoftdays.org> (Feb 2016)

Program Committee, PETSc 20, Chicago, IL, <http://www.mcs.anl.gov/petsc/petsc-20.html> (June 2015)

Program Committee, PMAA 14, Lugano, Switzerland, <http://pmaa14.ics.usi.ch> (July 2014)

Technical Papers Committee for [Supercomputing 2014](#)

Technical Papers Committee for [Supercomputing 2013](#)

Program Committee, CIG [Implementing Solvers in CitcomCU and CitcomS Workshop](#) (September 2013)

Program Committee, GPU-SMP Conference, Changchun, China, <http://gpu-smp2013.csp.escience.cn/dct/page/1> (June 2013)

Program Committee, ICERM Workshop, Brown University, <http://icerm.brown.edu/tw12-1-exascale> (January 2012)

Program Committee, GPU-SMP Conference, Shenzhen, China, <http://gpu-smp2012.csp.escience.cn/dct/page/1> (June 2012)

Program Committee, NSF Pan-American Advanced Studies Institute, *Scientific Computing in the Americas: the challenge of massive parallelism*, Valparaiso, Chile, (2011)

Program Committee, HPC<sup>3</sup> Workshop, KAUST, <https://sites.google.com/site/hpc3atkaust/> (February 2011)

Program Committee, FEniCS Workshop, University of Chicago (March 2005)

#### *Minisymposia Organized*

*Library Development for Manycore Computing*, PETSc 2016, Vienna, Austria 2016

*To Thread or Not To Thread*, SIAM PP, Paris, France 2016

*The Outer Loop*, PETSc 20, Chicago, IL, 2015

## University Service

## Teaching

Undergraduate/Graduate Course *Linear Algebra and Quantum Algorithms* CSE 410 Fall 2018, CSE 410/510 Fall 2019, CSE 439 Fall 2020

Undergraduate Course *Discrete Structures* CSE 191 Spring 2018, CSE 191 Spring 2019–2021

Undergraduate/Graduate Course *Computational Science II* CAAM 520 Spring 2016 (1.70, Rice Mean 1.71), CAAM 520 Spring 2017

Undergraduate/Graduate Course *Computational Science I* CAAM 519 Fall 2015 (2.32, Rice Mean 1.77), CAAM 519 Fall 2016 (1.96, Rice Mean 1.73)

Undergraduate Course *Numerical Analysis*, with Prof. Ahmed H. Sameh, Purdue University (1999)

Guest Lecturer, AMCS 4302, *Parallel Scientific Computing*, Columbia University (2006)

2 Week Short Course on Scientific Computing

Graduate University, Chinese Academy of Sciences, Beijing, China, (2010)

Graduate University, Chinese Academy of Sciences, Beijing, China, (2009)

1 Week Crustal Deformation Modeling Tutorial

NSF CIG [CIG All Hands Conference](#) (2016)

NSF CIG [Crustal Deformation Modeling Conference](#) (2015)

NSF CIG [Crustal Deformation Modeling Conference](#) (2013)

NSF CIG [Crustal Deformation Modeling Conference](#) (2011)

1 Week PETSc Short Course

Maison de la Simulation, Orsay, France (2013)

EuropeAid [Scientific Computing Advanced Training](#), Valparaiso, Chile (2007)

Idaho National Laboratory, Idaho Falls, ID (2005)

Parallel CFD 2004, Gran Canaria (2004)

1 Week GPU Computing Course

NSF Pan-American Advanced Studies Institute, [Scientific Computing in the Americas: the challenge of massive parallelism](#), Valparaiso, Chile, (2011)

8 single day PETSc tutorials, and 9 half day tutorials

1 single day Python HPC tutorial

## Departmental Committees

Member, UB CSE Distinguished Lecturer Committee (2019–2021)

Member, UB CSE Faculty Search Committee (2019–2021)

Member, UB CSE Graduate Admissions Committee (2017–2021)

Member, UB CSE Graduate Curriculum Committee (2017–2018)

Chair, Rice CAAM Faculty Search Committee (2016–2017)

Chair, Rice CAAM Data Science Faculty Search Committee (2016–2017)

Chair, Rice CAAM Computing Committee (2015–2017)  
Member, Rice CAAM Graduate Curriculum Committee (2015–2017)  
Member, Rice CAAM Graduate Committee (2015–2017)  
Member, Rice CAAM Faculty Search Committee (2015–2016)  
Member, Rice CAAM Numerical Analysis Examination Committee (2015–2017)

*Other Departmental Service*

Host for CSE Colloquium speaker: James Brannick (2018)  
Host for CSE Colloquium speaker: Stefan Rosenberger (2017)  
Host for CSE Colloquium speaker: Jack Poulson (2017)  
Host for CAAM Colloquium speaker: Jaydeep P. Bardhan (2017)  
Host for CAAM Colloquium speaker: Blaise Bourdin (2016)  
Host for CAAM Colloquium speaker: Tobin Isaac (2016)  
Host for CAAM Colloquium speaker: Wolfgang Bangreth (2015)  
Host for CAAM Colloquium speaker: Xiao-Chuan Cai (2015)  
Host for CAAM visitor: Florian Potra (2017)  
Host for CAAM visitor: Andy R. Terrel (2016)  
Host for CAAM visitor: Mark Adams (2016)  
Host for CI visitor: Paul Constantine (2014)  
Host for CI visitor: Mark Adams (2014)  
Host for CI visitor: Patrick Farrell (2014)  
Host for CI visitor: Karl Rupp (2014)  
Host for CI visitor: Aron Ahmadi (2010)  
Host for CI visitor: Rio Yokota (2010)  
Host for CI visitor: Liang Zheng (2010)  
Host for CI visitor: Deszo Boda (2008)  
Host for CI visitor: Lorena Barba (2008)  
Host for CI visitor: Blaise Bourdin (2008)  
Host for CI visitor: Felipe Cruz (2007, 2009)  
Host for ANL visitor: Andrei Draganescu (2006)  
Host for ANL visitor: Richard Martineau (2006)

Last updated: 2021-05-15