Matthew G. Knepley

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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

Professor, Computer Science and Engineering, University at Buffalo, 2024–*Present*

Associate Professor, Computer Science and Engineering, University at Buffalo, 2017–2024

Visiting Researcher, Department of Earth Science and Engineering, Imperial College London, 2018–2020

Adjunct Professor, Computational and Applied Mathematics, Rice University, 2018–2022

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, 2017–2018

Director, Intel Parallel Computing Center, Rice University, 2016–2022

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	$23,506,744	$5,759,993
Internal Sources	$80,000	$20,000
Total Funded Research	$23,586,744	$5,779,993

Understanding the grant information below:

The total amount to PI Knepley is given.

Current Funding

Computational Infrastructure for Geodynamics
Sponsor: NSF, Subcontract through UC Davis (2022–2027)
Subcontract PI: Matthew Knepley
Award Amount: $125,000

Scalable algorithms for the Vlasov-Poisson-Landau system
Sponsor: DOE, Subcontract through Lawrence Berkeley National Laboratory (2022–2023)
Subcontract PI: Matthew Knepley
Award Amount: $150,000

Capturing Dynamic Compound Flooding Events in E3SM
Sponsor: DOE Basic Energy Research (2022–2027)
UB PI: Matthew Knepley
Award Amount: $746,870

Multiscale acceleration: Powering future discoveries in High Energy Physics
Sponsor: DOE High Energy Physics (2022–2027)
UB PI: Matthew Knepley
Award Amount: $750,000

Extending PETSc's Composable Solvers
Sponsor: DOE Applied Math Research (2022–2025)
UB PI: Matthew Knepley
Award Amount: $327,000

PSAAPIII CHREST Center
Sponsor: DOE (2020–2025)

UB co-PI: Matthew Knepley (UB PIs: DesJardin, Salac, Chen, Chandola, Swihart)
Award Amount: $1,176,579 (UB Total: $8,530,000)

Multiphase Fluid-Structure Interaction Software Infrastructure to Enable Applications in Medicine, Biology, and Engineering
Sponsor: NSF, SI2 Framework (2020–2025)
UB PI: Matthew Knepley
Award Amount: $504,431

Previous Funding

Development of Terrestrial Dynamical Cores for the ACME to Simulate Water Cycle
Sponsor: DOE Basic Energy Research (2021–2022)
UB PI: Matthew Knepley
Award Amount: $100,000

Explaining Mass Loss in the Antarctic Ice Sheet through Integrated Systems Modeling
Sponsor: UB Blue Sky Fund (2022)
UB co-PI: Matthew Knepley (UB PIs: Jadamec, Csatho, Lowry)
Award Amount: $10,000 (UB Total: $30,000)

CHREST: Grant in aid of research
Sponsor: SUNY (2019)
UB co-PI: Matthew Knepley (UB PIs: DesJardin, Salac, Chen, Chandola, Swihart)
Award Amount: $10,000 (UB Total: $50,000)

ECP–WDMApp
Sponsor: DOE, Subcontract through Princeton Plasma Physics Laboratory (2020–2022)
Subcontract PI: Matthew Knepley
Award Amount: $112,333

Scalable Infrastructure for Enabling Multiscale and Multiphysics Applications in Fluid Dynamics, Solid Mechanics, and Fluid-Structure Interaction
Sponsor: NSF, SI2-SSI (2015–2020)
UB PI: Matthew Knepley
Award Amount: $262,655

Computational Infrastructure for Geodynamics
Sponsor: NSF, Subcontract through UC Davis (2016–2021)
Subcontract PI: Matthew Knepley
Award Amount: $585,000

Development of Terrestrial Dynamical Cores for the ACME to Simulate Water Cycle
Sponsor: DOE Basic Energy Research (2018–2021)
UB PI: Matthew Knepley
Award Amount: $160,000

Extending PETSc's Composable Hierarchically Nested Linear Solvers
Sponsor: DOE Applied Math Research (2018–2021)
UB PI: Matthew Knepley
Award Amount: $247,000

Support for SCREAM and EPSI
Sponsor: DOE Fusion Energy Sciences SciDAC, Subcontract through Lawrence Berkeley National Laboratory (2018–2020)
Subcontract PI: Matthew Knepley
Award Amount: $100,000

Extending the Practicality and Scalability of LibMesh-Based Unstructured, Adaptive Finite Element Computations
Sponsor: NSF SI2-SSE (2017–2020)
UB PI: Matthew Knepley
Award Amount: $350,065

Extending PETSc with Adaptive Mesh Refinement and Optimal Solvers, Applied to PFLOTRAN, and Optimized for Modern Intel Processors
Sponsor: Intel, Parallel Computing Center (2015–2017)
Rice PI: Matthew Knepley
Award Amount: $400,000

Extending PETSc's Composable Hierarchically Nested Linear Solvers
Sponsor: DOE Applied Math Research (2015–2018)
Rice PI: Matthew Knepley
Award Amount: $240,000

SPIKE — An Implementation of a Recursive Divide-and-Conquer Parallel Strategy for Solving Large Systems of Linear Equations
Sponsor: NSF, SI2-SSE (2012–2015)
UC PI: Matthew Knepley
Award Amount: $117,710

Extending PETSc's Composable Hierarchically Nested Linear Solvers
Sponsor: DOE Applied Math Research (2012–2015)
UB PI: Matthew Knepley
Award Amount: $240,000

Nonlinear Algorithms to Circumvent the Memory Bandwidth Limitations of Implicit PDE Simulations
Sponsor: DOE, Math-CS Institute (2009–2014)
UC PI: Matthew Knepley
Award Amount: $550,000

Mechanical Transformation of Knowledge to Libraries
Sponsor: NSF STCI (2009–2011)
UC PI: Matthew Knepley
Award Amount: $90,000

Towards Optimal Petascale Simulations
Sponsor: DOE Advanced Scientific Computing Research, Subcontract through Argonne National Laboratory (2001–2011)
Subcontract PI: Matthew Knepley
Award Amount: $1,200,000

Computational Infrastructure for Geodynamics
Sponsor: NSF, Subcontract through UC Davis (2010–2015)
Subcontract PI: Matthew Knepley
Award Amount: $650,000

Computational Infrastructure for Geodynamics
Sponsor: NSF, Subcontract through UC Davis (2005–2010)
Subcontract PI: Matthew Knepley
Award Amount: $650,000

Classical Density Functional Theory of Fluids: Ions at a Dielectric Interface
Sponsor: Army Research Office, W911NF-09-1-0488, Subcontract through Rush University Medical Center (2010–2012)

Subcontract PI: Matthew Knepley
Award Amount: $45,000

Unstructured Mesh Management for Fluid Simulation
Sponsor: DOE Reactor Core Modeling, Subcontract through Idaho National Laboratory (2005–2007)
Subcontract PI: Matthew Knepley
Award Amount: $210,000

Research Areas

Scalable linear and nonlinear solvers for multiphysics problems

Finite element and boundary element discretizations for nonlinear problems

Scientific library development for high performance computing

Geophysical modeling in crustal deformation, subsurface flow, and mantle convection

Modeling of combustion in hybrid rocket engines

Efficient solvers and preconditioners for GPUs and accelerators

Bioelectrostatics and molecular modeling for ion channels

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. He is a principal author of the PETSc libraries, one of the most widely used scientific libraries in the world. 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 Ansys Fluent, FIDAP 8.5, 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 more than 13,000 citations according to Google Scholar with an H-index of 36, and more than 41,000 reads on ResearchGate.

Four of his most noteworthy contributions are highlighted here. **1** 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 quantum chromodynamics, bioelectrostatic calculations, crustal deformation, fracture mechanics, rocket engine combustion, and airfoil simulation. **2** Development of a scalable preconditioning strategy based upon patch solves. This block, multilevel preconditioner has been used for quasi-static crustal deformation problems with complex fault rheologies on large parallel machines, and also to produce a Reynolds number-independent preconditioner for incompressible flow. It is generally applicable to the saddle-point problems. **3** 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 accurate thermodynamics of these molecular mixtures. This strategy has recently been employed to model protein-ligand binding, and

favorably compared with experimental results. **4** 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 $\mathcal{O}(N \log N)$, for the entire simulation, and applied the code to ryanodine receptor transport.

Publications

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

Book Chapters

[7] Dave A. May and Matthew G. Knepley. Numerical modeling of subduction. In João C. Duarte, editor, *Dynamics of Plate Tectonics and Mantle Convection*, pages 539–571. 2023.

[6] Satish Balay, Jed Brown, Matthew G. Knepley, Lois McInnes, and Barry Smith. Providing mixed language and legacy support within a library. In J. Carver, editor, *Software Engineering for Science*. 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, 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

[56] **Darsh K. Nathawani** and Matthew G. Knepley. A one-dimensional mathematical model for shear-induced droplet formation in co-flowing fluids. *Theoretical and Computational Fluid Dynamics*, 2024.

[55] David A. Ham, Vaclav Hapla, Matthew G. Knepley, Lawrence Mitchell, and Koki Sagiyama. Efficient n-to-m checkpointing algorithm for finite element simulations. *SIAM Journal on Scientific Computing*, 2024. Under review.

[54] **Daniel S. Finn**, Matthew G. Knepley, **Joseph V. Pusztay**, and Mark F. Adams. A numerical study of Landau damping with PETSc-PIC. *Communications in Applied Mathematics and Computational Science*, 18(1):135–152, 2023.

[53] **Robert L. Walker**, Matthew G. Knepley, Brad T. Aagaard, and Charles A. Williams. Multiphysics modeling in PyLith: Poroelasticity. *Geophysical Journal International*, 235(3):2442–2475, 2023.

[52] **Aman Timalsina** and Matthew G. Knepley. Tetrahedralization of a hexahedral mesh. In *SIAM International Meshing Roundtable Workshop 2023*, 2023.

[51] **Darsh K. Nathawani** and Matthew G. Knepley. Droplet formation simulation using mixed finite elements. *Physics of Fluids*, 34:064105, 2022.

[50] **Joseph V. Pusztay**, Matthew G. Knepley, and Mark F. Adams. Conservative projection between FEM and particle bases. *SIAM Journal on Scientific Computing*, 44(4):C310–C319, 2022.

[49] Junchao Zhang, Jed Brown, Satish Balay, Jacob Faibussowitsch, Matthew Knepley, Oana Marin, Richard Tran Mills, Todd Munson, Barry F. Smith, and Stefano Zampini. The PetscSF scalable communication layer. *IEEE Transactions on Parallel and Distributed Systems*, 33(4):842–853, 2022.

[48] Mark Adams, Satish Balay, Jed Brown, Victor Eijkhout, Jacob Faibussowitsch, Fande Kong, Matthew Knepley, Scott Kruger, Oana Marin, Richard Mills, Todd Munson, Patrick Sanan, Barry Smith, Hong Zhang, Hong Zhang, and Junchao Zhang. The community is the infrastructure: A short discussion of the PETSc user community. *Computing in Science and Engineering*, 24(03):6–15, May 2022.

[47] Gabriele Morra, Ebru Bozdag, Matthew G. Knepley, Ludovic Räss, and Velimir Vesselinov. A tectonic shift in analytics and computing is coming. *Eos*, 102, Jun 2021.

[46] 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*, 87(2):905870229, 2021.

[45] **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.

[44] Patrick E Farrell, Matthew G Knepley, Lawrence Mitchell, and Florian Wechsung. PCPATCH: software for the topological construction of multigrid relaxation methods. *ACM Transaction on Mathematical Software*, 47(3):1–22, 2021.

[43] 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*, 43(2):C127–C153, 2021.

[42] **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*, 8:100089, 2020.

[41] **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*, 28(3):161–174, 2019.

[40] 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.

[39] 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.

[38] 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*, 36(4):513–548, 2019.

[37] **Maurice S. Fabien**, Matthew G. Knepley, and Béatrice M. Rivieré. A hybridizable discontinuous galerkin method for two-phase flow in heterogeneous porous media. *International Journal for Numerical Methods in Engineering*, 116(3):161–177, 2018.

[36] **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.

[35] **Justin Chang**, Kalyana B. Nakshatrala, Matthew G. Knepley, and Lennart Johnsson. A performance spectrum for parallel computational frameworks that solve PDEs. *Concurency: Practice and Experience*, 30(11), 2017.

[34] 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.

[33] **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.

[32] 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. PMCID: PMC5336475.

[31] 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*, (6):2897–2914, 2017.

[30] 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.

[29] 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.

[28] **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.

[27] 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.

[26] **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.

[25] 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.

[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. Ahmadia, 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 Petropolous. Closed strings with low harmonics and kinks. *Physical Review D*, 48(6), 1993.

Peer-Reviewed Conference Papers

[30] Georgios Georgalis, **Darsh K. Nathawani**, Matthew G. Knepley, and Abani Patra. Uncertainty quantification of shear-induced paraffin droplet pinch-off in hybrid rocket motors. In *AIAA SciTech 2024*, 2023. Accepted.

[29] **Darsh K. Nathawani** and Matthew G. Knepley. Simulating paraffin wax droplets using mixed finite element method. In Christoph Brehm and Shishir Pandya, editors, *Proceeedings of the International Conference on Computational Fluid Dynamics 11 (ICCFD11)*, number 4103, 2022.

[28] **Aman Timalsina** and Matthew G. Knepley. Tetrahedralization of a hexahedral mesh. In *SIAM International Meshing Roundtable Workshop 2023*, 2023.

[27] **Joseph G. Wallwork**, Matthew G. Knepley, Nicolas Barral, and Matthew D. Piggott. Parallel metric-based mesh adaptation in PETSc using ParMmg. In Trevor Robinson, editor, *SIAM International Meshing Roundtable Workshop 2022*, pages 1–5, Seattle, WA, January 2022.

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Other Conference Papers and Technical Reports

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[28] **Thomas S. Klotz**, Jaydeep Bardhan, and Matthew G. Knepley. Efficient evaluation of ellipsoidal harmonics for potential modeling. *arXiv e-prints*, 2018. http://arxiv.org/abs/1708.06028.

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Software Toolkits

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

8000+ scientific publications have cited PETSc, including combustion, brain surgery, subsurface flow, fusion, and cardiology.

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

Used at all DOE laboratories and NSF/EU Supercomputing Centers, Boeing, Shell, GM, Dassault

Designer and developer of the parallel unstructured grid component

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

200+ 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

Technical Presentations

Plenary and Keynote Presentations

Keynote Address, Southern Ontario Numerical Analysis Day, Waterloo, CA May 2023

Keynote Address, Domain Decomposition, Newfoundland, CA Jul 2018

Keynote Address, Computational and Data-Enabled Science and Engineering Days, Univ. at 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, Györ, 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

Dept. of Civil and Environmental Engineering Seminar, Louisiana State University, Baton Rouge, LA, April 2023

SIAM CSE, Amsterdam, February 2023

Finger Lakes Regional HPC Symposium, Rochester, NY, October 2022

ICCFD 2022, Maui, HI, July 2022

Parallel CFD 2022, Alba, Italy, Online, May 2022

Appel Group Seminar, Princeton University, Online, March 2022

ETHZ Institut für Geophysik Seminar, Online, June 2021

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, Minisymposterium, 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 April 2016

Ken Kennedy Institute Seminar, Houston, TX March 2016

Melt in the Mantle 2016, Cambridge UK February 2016

SPPEXA 2016, Munich DE January 2016

ASME IMECE 2015, Houston TX November 2015

Composing Nonlinear Solvers, ICERM, Providence RI September 2015

ME & IE Seminar, Northeastern University, Boston, MA March 2015

SIAM CS&E, Salt Lake City, UT March 2015

CAAM Seminar, Rice University, Houston, TX February 2015

Numerical Analysis Seminar, Texas A&M University, College Station, TX January 2015

Numerical Analysis Seminar, Texas A&M University, College Station, TX December 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

Composble 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 Reseach, Norway, August 2011

Conference on Simulation and Optimization, Győr, Hungary, June 2011

HPC^3 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 Colloquim, 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, Colordao 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

PyLith Tutorial, Crustal Deformation Conference, Golden, CO, June 2022

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, September 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, Györ, 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 Francsico, 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 Research Associates

Joseph Pusztay, University at Buffalo, 2023–*present*

Robert Walker, University at Buffalo, 2019–*present*

Justin Chang, University at Buffalo, 2018–2019

Justin Chang, Rice University, 2017

Tobin Isaac, University of Chicago and Rice University, 2015–2017

Graduate Students

Phd Students Advised

Mosaddeq Hossain, University at Buffalo Ph.D., supervisor since 9/23

Albert Cowie, University at Buffalo Ph.D., supervisor since 9/17

Vivek Bhavsar, Geology, University at Buffalo Ph.D., 2024, co-supervisor
Thesis: .

Daniel Finn, University at Buffalo Ph.D., 2023
Thesis: *Structure-Preserving Particle-In-Cell Methods for the Vlasov-Poisson-Landau System.*

Darsh Kiritbhai Nathawani, University at Buffalo Ph.D., 2023
Thesis: *Droplet Formation: One-dimensional Mathematical Model and Computations*

Abhishek Mishra, University at Buffalo Ph.D., 2022, with Prof. David Salac
Thesis: *Enabling computational methods for discretization of partial differential equation models using stencil composition.* Engineer at AMD.

Brandon Denton, University at Buffalo Ph.D. 2022,
Thesis: *Geometry Aware Mesh Topologies.* Sr. Design Engineer at ArcField.

Joseph Pusztay, University at Buffalo Ph.D. 2022,
Thesis: *A Particle Basis Vlasov-Poisson-Landau Solver for Plasma Simulation in PETSc.* Postdoc at University at Buffalo.

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.* Asst. Prof. at University of Wisconsin.

Thomas Klotz, Rice University Ph.D. 2019,
Thesis: *Numerical Analysis of Nonlinear Boundary Integral Equations Arising in Molecular Biology.*

Research Scientist at Smiths Detection.

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

Andrew Gmerek, University at Buffalo 2022, *Temporal Convergence of Crustal Deformation Solvers*

Aman Timalsina, University at Buffalo 2022, *Automated Mesh Transformations*

Rachel Bakowski, University at Buffalo 2022, *Data Assimilation for Subduction Dynamics*

Thomas Kowalski, University at Buffalo 2022, *Immersive Visualization for Earth Science*

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, *Probablistic Performance Modeling*

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

Phd Committees

Feng-Mao Tsai, Phd, Computer Science, University at Buffalo 2026

Isys Johnson, Phd, Computer Science, University at Buffalo 2026

Darshana Balakrishnan, Phd, Computer Science, University at Buffalo 2023

Vivek Bhavsar, Phd, Computation and Data-Enabled Science and Engineering, University at Buffalo 2023

Amol Salunkhe, Phd, Computation and Data-Enabled Science and Engineering, University at Buffalo 2023

Boris Boutkov, Phd, Computation and Data-Enabled Science and Engineering, University at Buffalo 2019

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

Bailey Valint, MS, Geology, University at Buffalo 2023

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 (2020–2022)

Associate Editor, Cogent Geoscience, Taylor & Francis (2015–2019)

International Committees and Visiting positions

Member, Committee on Gene Golub SIAM Summer School, (2023–2026)

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, Györ, 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 Uniersity, 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, PETSc 2023, Chicago, IL, website (June 2023)

Program Committee, PyLith Hackathon 2023, Golden, CO, (June 2023)

Program Committee, CDM 2022, Golden, CO, website (June 2022)

Co-Chair for Algorithms Track, IPCC 2022, Chicago, IL, website (August 2021)

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, Switerland, 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^3 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

Graduate Course *High Performance Computing II* CSE 548 Spring 2022–2023

Graduate Course *High Performance Computing I* CSE 547 Fall 2020, Fall 2021

Undergraduate/Graduate Course *Linear Algebra and Quantum Algorithms* CSE 410 Fall 2018, CSE 410/510 Fall 2019, CSE 439 Fall 2020, CSE 499 Fall 2021, CSE 439 Fall 2022

Undergraduate Course *Discrete Structures* CSE 191 Spring 2018, CSE 191 Spring 2019–2023

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 Graduate Program Assessment Committee (2021–2022)

Member, UB CSE Ad Hoc Tenure Committee (2022)

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

Member, UB CSE Faculty Search Committee (2019–2022)

Member, UB CSE Graduate Admissions Committee (2017–2022)

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 Ahmadia (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)

College Service

PHYS Faculty Search Committee (2023)

Graduation Marshall (2023)

SEAS IAD Director Search Committee (2019)

CDSE Days Committee (2018, 2019)

CDSE Admissions Committee (2018, 2019, 2022)

MATH Faculty Search Committee (2018)

Last updated: 2024-04-24