

Curriculum Vitae

ANDREAS KLOECKNER

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Education

- 2005 – 2010 Ph.D. in Applied Mathematics
Division of Applied Mathematics, Brown University, Providence, RI
High-Performance High-Order Simulation of Wave and Plasma Phenomena
Advisor: Jan Hesthaven
- 2005 Diplom degree in Applied Mathematics (Technomathematik)
Institut für Angewandte Mathematik, Universität Karlsruhe, Germany
On the Computation of Maximally Localized Wannier Functions
Advisor: Willy Dörfler
- 2001 – 2002 Exchange Student, Department of Mathematics
University of North Carolina at Charlotte, Charlotte, NC
- 2000 Vordiplom in Computer Science, Universität Karlsruhe, Germany

Research

The unifying theme of my research interest is the efficient numerical simulation of wave phenomena. I have worked towards this goal by pursuing a broad range of topics:

Efficient Building Blocks for Integral Equation Methods. Together with Alexander Barnett and Leslie Greengard, I have recently publicized details of a novel, fast, and general scheme to compute Nyström discretizations of layer potential operators for the Helmholtz and Laplace PDEs at a high order of accuracy, termed ‘Quadrature by Expansion’ (QBX). This work holds tremendous promise as a tool for building PDE solvers capable of attacking current engineering problems at scale. My current work aimed at delivering on this promise includes methods for precise error control, automatic adaptivity, and integration with fast algorithms and computational tools.

Tools for Scientific Programming. The advent of massive on-chip parallelism is in the process of turning commonly accepted cost metrics in numerical analysis on their heads. This phenomenon includes, but is not limited to, GPU hardware. Increasingly, proof-of-concept implementations (e.g. in MATLAB) risk being unaware of the drivers of computational cost, and, consequently, are prone to producing methods that are not scalable on actual hardware. Making current computer architectures accessible to numerical analysts is a question of tools and abstractions. I am pursuing a long-term program to develop such a set of languages and tools fundamentally based on the notion of run-time code generation, presenting an alternative point of view to commonly accepted software construction practice.

Numerical Methods for Hyperbolic PDEs. Using time-explicit discontinuous Galerkin (“DG”) methods as a starting point, I am investigating problems arising in applications, such as those arising in computational electromagnetics, as well numerical subjects, such as detection and mitigation methods for Gibbs phenomena encountered in shock-laden flows. I have further developed a number of multi-rate time integration methods to be used in conjunction with DG.

Research Presentations

- 10/2012 GPUs and Python*(Invited speaker and panelist). PyData NYC—Conference on big data with Python. New York, NY.
- 10/2012 Quadrature by expansion*. Applied Mathematics Seminar. Carolina Center for Interdisciplinary Applied Mathematics, University of North Carolina. Chapel Hill, NC.
- 9/2012 Transformational Programming for time- and frequency-domain EM simulation*(Invited plenary talk). SCEE2012—Scientific Computing in Electrical Engineering. ETH Zurich. Zurich, Switzerland.
- 5/2012 Easy, Effective, Efficient: GPU Programming in Python with PyOpenCL and PyCUDA*. HPC & GPU Supercomputing Group of New York City. New York, NY.
- 4/2012 POP Quadrature: Painless high-order-accurate layer potentials*. Applied & Computational Mathematics Seminar. Dartmouth Co. Hanover, NH.
- 3/2012 Loo.py: A Loop Generation Tool for CPUs and GPUs*. Oil and Gas High Performance Computing Workshop. Rice University. Houston, TX.
- 2/2012 Tools and Methods for DG on Modern Computer Architectures*. Oberwolfach workshop “Theory and Applications of Discontinuous Galerkin Methods”. Mathematisches Forschungsinstitut Oberwolfach. Oberwolfach, Germany.
- 2/2012 High-order DG Wave Propagation on GPUs: Infrastructure and Implementation. Minisymposium 13, organized by Takahiro Katagiri, Toshiyuki Imamura, and Keita Teranishi. SIAM Conference on Parallel Processing for Scientific Computing. Savannah, GA.
- 1/2012 Loo.py—a polyhedral code generator for CPUs and GPUs*(lightning talk, invited attendee). Synchronization-reducing and Communication-reducing Algorithms and Programming Models for Large-scale Simulations. Institute for Computational and Experimental Research in Mathematics (ICERM), Brown University. Providence, RI.
- 11/2011 Run-time Code Generation for Heterogeneous Computing: Methods and Applications in High-Order PDE Solvers*. Red Raider Minisymposium. Texas Tech University. Lubbock, TX.
- 10/2011 Discontinuous Galerkin, Python, and GPUs: a case study*. Workshop ‘Programming of Heterogeneous Systems in Physics’. Universität Jena. Jena, Germany.
- 9/2011 Easy, Effective, Efficient: GPU Programming in Python with PyOpenCL and PyCUDA*. HPC & GPU Supercomputing Group of New York City. New York, NY.
- 8/2011 Run Time Code Generation for Heterogeneous Computing: Methods and Applications in High-Order PDE solvers*. Workshop on CBC Key Topics. Center for for Biomedical Computing, Simula Research Laboratory. Lysaker, Norway.

*Invited.

- 8/2011 Run-time Code Generation for Heterogeneous Computing: Methods and Applications in High-Order PDE Solvers*. Workshop ‘GPU Computing Today and Tomorrow’. GPU Lab, Department for Informatics and Mathematical Modelling, Technical University of Denmark. Lyngby, Denmark.
- 6/2011 Generalized Debye Sources: Computational Aspects on Arbitrary Surfaces*. Frontiers in Applied and Computational Mathematics. New Jersey Institute of Technology. Newark, NJ.
- 5/2011 Discontinuous Galerkin, Python, and GPUs: the ‘hedge’ solver package*. Advances and Challenges in Computational General Relativity. Brown University. Providence, RI.
- 3/2011 High-order DG Wave Propagation on GPUs: Infrastructure, Implementation, Method Improvements*. Scientific Computing and Numerics (SCAN) Seminar. Cornell University. Ithaca, NY.
- 3/2011 Easy, Effective, Efficient: GPU Programming in Python with PyOpenCL and PyCUDA*. Research Seminar. D.E. Shaw Research. New York, NY.
- 3/2011 High-order DG Wave Propagation on GPUs: Infrastructure, Implementation, Method Improvements*. Mechanical Engineering Department, City College of New York. New York, NY.
- 3/2011 Shock Capturing in a Time-Explicit Discontinuous Galerkin Method on the GPU. Minisymposium 116. SIAM Conference on Computational Science and Engineering 2011. Reno, NV.
- 3/2011 Paper to GPU: Optimizing and Executing Discontinuous Galerkin Operators in Python. Minisymposium 62. SIAM Conference on Computational Science and Engineering 2011. Reno, NV.
- 3/2011 High-Order Discontinuous Galerkin Methods by GPU Metaprogramming. Minisymposium 1. SIAM Conference on Computational Science and Engineering 2011. Reno, NV.
- 2/2011 High-order DG Wave Propagation on GPUs: Infrastructure, Implementation, Method Improvements*. Math Department Seminar. UMass Dartmouth. Dartmouth, MA.
- 1/2011 High-order DG Wave Propagation on GPUs: Infrastructure, Implementation, Method Improvements*. Workshop “High Performance Computing and Emerging Architectures”. Institute for Mathematics and Its Applications, University of Minnesota. Minneapolis, MN.
- 12/2010 Machine-adapted Methods: High-order DG Wave Propagation on GPUs*. Imaging and Computing Seminar. Mathematics Department, MIT. Boston, MA.
- 11/2010 Machine-adapted Methods: High-order DG Wave Propagation on GPUs. Numerical Analysis and Scientific Computing Seminar. Courant Institute, NYU. New York, NY.
- 10/2010 PyCUDA: Even Simpler GPU Programming with Python. Nvidia GPU Technology Conference. San Jose, CA.
- 7/2010 High-Order Discontinuous Galerkin Methods by GPU Metaprogramming*. 2010 International Workshop of GPU Solutions to Multiscale Problems in Science and Engineering. Harbin, China.

- 7/2010 Machine-adapted Methods: Shock Detection and Capture in GPU-DG. Minisymposium 1. SIAM Annual Meeting 2010. Pittsburgh, PA.
- 3/2010 High-Order Discontinuous Galerkin Methods by GPU Metaprogramming*. Aerospace Computational Design Laboratory Seminar. Mechanical Engineering, MIT. Boston, MA.
- 1/2010 High-Order Discontinuous Galerkin Methods by GPU Metaprogramming*. Mathematics and Computer Science Division Seminar. Argonne National Laboratory. Chicago, IL.
- 11/2009 GPU metaprogramming using PyCUDA: methods and applications*. GPU@BU project launch workshop. Boston University Center for Computational Science. Boston, MA.
- 10/2009 High-Order Discontinuous Galerkin Methods and Loop Generation by GPU Metaprogramming. Seminar Departement Mathematik. Universität Basel. Basel, Switzerland.
- 10/2009 GPU Metaprogramming using PyCUDA: Methods & Applications*. Nvidia GPU Technology Conference. San Jose, CA.
- 8/2009 GPU Metaprogramming Applied to High-Order DG and Loop Generation*. Frontiers of Geophysical Simulation. Institute for Mathematics Applied to Geosciences. Boulder, CO.
- 7/2009 GPU Computing: Introduction, Scripting, and Time-domain DG*. Advanced Computation Department Seminar. SLAC National Accelerator Laboratory. Menlo Park, CA.
- 5/2009 Scripting for GPUs (feat. Discontinuous Galerkin Time Domain)*. Hess Corporation. Houston, TX.
- 3/2009 High-Productivity Supercomputing: Metaprogramming GPUs. Minisymposium 134. SIAM Conference on Computational Science and Engineering 2009. Miami, FL.
- 3/2009 PyCUDA and PyUblas: Hybrid HPC in Python made easy. Minisymposium 98. SIAM Conference on Computational Science and Engineering 2009. Miami, FL.
- 10/2008 High-Order Unstructured Particle-in-Cell Simulation*. Mathematics Department Seminar. Southern Methodist University. Dallas, TX.
- 10/2008 High-Order Unstructured Particle-in-Cell Simulation*. Computational & Applied Mathematics Department Seminar. Rice University. Houston, TX.
- 7/2008 Methods for High-Order Unstructured Particle-in-Cell Simulation*. Seminar des Instituts für Aerodynamik und Gasdynamik. Uni Stuttgart. Stuttgart, Germany.

Workshops and Guest Lectures

- 4/2012 Guest lecture *Time-Domain Computational Electromagnetics using Discontinuous Galerkin Methods*
Computational Electromagnetics, Courant Institute, NYU, New York, NY

8/2011	<i>Easy, Effective, Efficient: GPU Programming in Python with PyOpenCL and PyCUDA.</i> One-day workshop at Simula Research Laboratory, Lysaker, Norway
8/2011	<i>Easy, Effective, Efficient: GPU Programming in Python with PyOpenCL and PyCUDA.</i> One-day workshop at GPULab, Department for Informatics and Mathematical Modelling, Technical University of Denmark, Lyngby, Denmark
3/2011	<i>Easy, Effective, Efficient: GPU Programming in Python with PyOpenCL and PyCUDA.</i> Guest lecture in CS264, Massively Parallel Computing, Harvard University, Boston, MA
1/2011	Course on <i>GPU programming with PyOpenCL and PyCUDA</i> . (4 lectures and labs) Pan-American Advanced Studies Institute (PASI) “Scientific Computing in the Americas: the challenge of massive parallelism”, Valparaíso, Chile
6/2010	Half-day Tutorial on <i>GPU Computing</i> using <i>PyOpenCL</i> . Conference on Scientific Computing in Python (SciPy 2010), Austin, TX
3/2010	Guest lecture <i>GPU Computing</i> . COMP150-06: Introduction to High Performance Computing: Tools and Algorithms. Tufts University, Boston, MA
2/2010	Guest lecture <i>GPU Computing</i> . APMA2821: Introduction to High Performance Computing: Tools and Algorithms. Brown University, Providence, RI
10/2009	Tutorial: <i>Programming GPUs with PyOpenCL</i> . Bernstein Center for Computational Neuroscience, Freiburg, Germany
5/2009	Day-long lecture: <i>Accelerated Computing</i> HPC Summer Institute, Ken Kennedy Institute for Information Technology, Rice University, Houston, TX

Teaching

See <http://goo.gl/WTure> for current teaching evaluations.

9/2012 – 12/2012	<i>High Performance Computing</i> (with Marsha Berger) Redeveloped earlier course in a demonstration-based, interactive format. Lecture video available on class web page. [http://bit.ly/hpc12] Courant Institute, NYU, New York, NY
1/2012 – 5/2011	Undergraduate <i>Discrete Mathematics</i> . Courant Institute, NYU, New York, NY
9/2011 – 12/2011	Undergraduate <i>Discrete Mathematics</i> . Courant Institute, NYU, New York, NY
1/2011 – 5/2011	Undergraduate <i>Discrete Mathematics</i> . Courant Institute, NYU, New York, NY
9/2010 – 12/2010	<i>High Performance Computing</i> (with Marsha Berger) Developed course and taught as an early graduate class. Courant Institute, NYU, New York, NY

3/2005 – 7/2005 Recitation leader for *Numerical Analysis for PDEs*
Universität Karlsruhe, Germany (with Vincent Heuveline)

8/2001 – 12/2001 *College Algebra*
University of North Carolina at Charlotte

Experience

9/2010 – Courant Instructor
Courant Institute of Mathematical Sciences, New York University, New York City
Designed and analyzed new numerical methods supporting the use of boundary integral equations in computational electromagnetics and other applications (with Leslie Greengard).

2007 – 2010 Graduate Research Assistant
(Summers) *Division of Applied Mathematics, Brown University, Providence, RI*
Designed efficient, scalable solvers for time-domain electromagnetics. Designed and analyzed new shock detection schemes for high-order discontinuous Galerkin methods. (with Jan Hesthaven and Tim Warburton).

6/2006 – 9/2006 J. Wallace Givens Research Associate
Mathematics and Computer Science Div., Argonne Nat'l Laboratory, Illinois
Designed high-order unstructured electromagnetic simulation methods for particle accelerators (with Paul Fischer, Misun Min, and colleagues at ANL's Advanced Photon Source).

2/2005 – 7/2005 Research Associate (Wissenschaftlicher Mitarbeiter)
Institut für Angewandte Mathematik, Universität Karlsruhe, Germany
Provided a detailed analysis of an optimization procedure aiming to find a maximally localized basis set for an application in photonics (with Willy Dörfler).

5/2002 – 11/2002 Research Intern
DaimlerChrysler Research & Technology, Palo Alto, CA
Worked on driver stress detection, precision GPS, and software infrastructure (with Stefan Schrödl).

Publications

See <http://goo.gl/sjZ2E> for a research impact summary compiled by Google Scholar.

2012 Fast Algorithms for the Evaluation of Layer Potentials using 'Quadrature by Expansion'.
L. Greengard, AK, Z. Gimbutas
(in preparation)

2012 Loopy: Transformation-based code generation for CPUs and GPUs.
AK, T. Warburton
(in preparation)

- 2012 A High-Level, High-Performance Software Architecture for Matrix-Free PDE Solvers.
AK
(in preparation)
- 2012 Quadrature by Expansion: A New Method for the Evaluation of Layer Potentials.
AK, A. Barnett, L. Greengard, M. O’Neil
(submitted) See arxiv:1207.4461.
- 2012 A consistency condition for the vector potential in multiply-connected domains.
C. Epstein, Z. Gimbutas, L. Greengard, AK, M. O’Neil
(submitted) See arxiv:1203.3993
- 2011 Solving Wave Equations on Unstructured Geometries.
AK, T. Warburton, J.S. Hesthaven.
in: GPU Computing Gems “Jade Edition”, Morgan Kaufmann Publishers, Waltham, MA. Available at doi:10.1016/B978-0-12-385963-1.00018-6.
- 2011 GPU Scripting and Code Generation with PyCUDA.
AK, N. Pinto, B. Catanzaro, Y. Lee, P. Ivanov, A. Fasih
in: GPU Computing Gems “Jade Edition”, Morgan Kaufmann Publishers, Waltham, MA. Available at doi:10.1016/B978-0-12-385963-1.00027-7.
- 2011 Viscous Shock Capturing in a Time-Explicit Discontinuous Galerkin Method.
AK, T. Warburton, J.S. Hesthaven.
Mathematical Modelling of Natural Phenomena, Volume 6, Issue 3. Available at doi:10.1051/mmnp/20116303.
- 2011 PyCUDA and PyOpenCL: A Scripting-Based Approach to GPU Run-Time Code Generation.
AK, N. Pinto, Y. Lee, B. Catanzaro, P. Ivanov, and A. Fasih.
Parallel Computing, Volume 38, Issue 3, March 2012, Pages 157—174. Available at doi:10.1016/j.parco.2011.09.001.
- 2009 Nodal Discontinuous Galerkin Methods on Graphics Processors.
AK, T. Warburton, J. Bridge, J.S. Hesthaven.
Journal of Computational Physics, Volume 228, Issue 21, 20 November 2009. available at doi:10.1016/j.jcp.2009.06.041.

Conference Proceedings

- 2012 Tools and Methods for Discontinuous Galerkin Solvers on Modern Computer Architectures.
AK, T. Warburton and J.S. Hesthaven
in: Proceedings of the 2012 Oberwolfach Workshop “Theory and Applications of Discontinuous Galerkin Methods” (1208a)

- 2012 High-Order Discontinuous Galerkin Methods by GPU Metaprogramming.
AK, T. Warburton and J.S. Hesthaven
 in: Proceedings of the 2010 Workshop of GPU Solutions to Multiscale Problems in Science and Engineering, Harbin, China. See <http://books.google.com/books?vid=9783642164040>.
- 2011 A Common GPU n -Dimensional Array for Python and C.
F. Bastien, A. Bergeron, AK, P. Vincent and Y. Bengio
 in: Proceedings of the Workshop “Big Learning: Algorithms, Systems, and Tools for Learning at Scale” at NIPS 2011. See <http://www.iro.umontreal.ca/~lisa/publications2/index.php/publications/show/522>
- 2009 Overcoming Performance Bottlenecks in DG-FEM for EM Problems. .
S. Chun, H. Haddar, J.S. Hesthaven, AK, T. Warburton, and L. Wilcox
 in: Proceedings of 9th International Conference on Mathematical and Numerical Aspects of Wave Propagation, Pau, France, June 2009, pp. 80–81

Mentoring

- 6/2012 – 9/2012 Michael Tom, Undergraduate Research Project: *Computation of Harmonic Vector Fields by High-Order Integral Equation Methods*. (Visiting NYU from Harvard University, Boston, MA)
- 4/2009 – 10/2009 Andreas Stock, Master’s Thesis: *Development and Application of a Multirate Multistep AB Method to a Discontinuous Galerkin Method based Particle In Cell Scheme*. (Visiting Brown University from Universität Stuttgart, Germany)
- 4/2009 – 10/2009 Hendrik Riedmann, Project Thesis (“Studienarbeit”): *Efficient Numerical Treatment of the Compressible Navier-Stokes Equations with Nodal Discontinuous Galerkin Methods on Graphics Processors*. (Visiting Brown University from Universität Stuttgart, Germany)

Awards and Achievements

- 2012 NSF US Junior Oberwolfach Fellowship
 Travel grant to attend the Oberwolfach workshop “Theory and Applications of Discontinuous Galerkin Methods”
- 2012 Travel Award for SIAM Conference on Parallel Processing for Scientific Computing (Savannah, GA)
- 2010 David Gottlieb Memorial Award of the Division of Applied Mathematics at Brown University
- 2010 NSF US Junior Oberwolfach Fellowship
 Travel grant to attend the Oberwolfach workshop “Computational Electromagnetism and Acoustics”
- 2009 Brown University Dissertation Fellowship
- 2001 DaimlerChrysler Scholarship Program

Software Packages

Hedge	High-performance hybrid Discontinuous Galerkin solver with CPU, GPU and MPI (for both CPU and GPU) backends
PyOpenCL	Heterogeneous parallel programming and metaprogramming toolkit (more than 70,000 direct downloads since 8/2009.)
PyCUDA	GPU programming in Python (more than 40,000 direct downloads since 6/2008.)
and numerous others	such as PuDB (400k+ direct downloads) CodePy, CGen, MeshPy, PyMetis. See http://mathematician.de/software for a full list. All my software is freely available under the terms of the MIT license.

Service

Reviewer	for Mathematics and Computers in Simulation (Elsevier), Computer Physics Communications (Elsevier), Journal of Scientific Computing (Springer), Journal of Computational Science (Elsevier), Transactions on Mathematical Software (Association for Computing Machinery), International Journal of High Performance Computing Applications (SAGE Publications), GPU Computing Gems (Nvidia/Morgan Kaufmann).
Program Committee Member	for the following conferences/workshops: <ul style="list-style-type: none">• IEEE International Conference on Parallel and Distributed Systems (ICPADS 2012), track “Multicore Computing and Parallel/Distributed Architecture”, Singapore• Innovative Parallel Computing (“InPar”) 2012, San Jose, CA• 4th Workshop on using Emerging Parallel Architectures (WEPA 2012) held at International Conference on Computational Science (ICCS) 2012, Omaha, NE• PyHPC 2011 at Supercomputing ‘11, Seattle, WA
Member	Society for Industrial and Applied Mathematics.

Citizenship

Germany

References

Available upon request.