

Dr. Patrick Diehl

Curriculum Vitæ

Education

2017 PhD, Applied mathematics, University of Bonn, Germany.

2012 Diploma, Computer Science, University of Stuttgart, Germany.

Awards and Honors

2019 IEEE SCIVIS Contest 2019, First Prize, Visual Analysis of Structure Formation in Cosmic Evolution, Video, Poster, and Short paper

Grant history

Current Research (chronological order; most recent one first)

1. Grant #524125 (Hartmut Kaiser)

Name of Funding Organization: Pacific Northwest National Laboratory

Amount Awarded: \$50,000

Period of Grant Award: June 25 - Oct 31 2020

Title of Project: High Performance Data Analytics (HPDA) Scalable Second-

Order Optimization (SSO)

Role on Project: Co-PI

Journal editor

06/20-current **Topic editor**, Computational fracture mechanics, Applied mathematics, C++, asynchronous and task-based programming, The Journal of Open Source Software.

Research experience

10/18–current **Research scientist**, *Center for Computation & Technology*, Louisiana State University, Baton Rouge, LA, USA.

- o Treatment of local boundary conditions in non-local models
- o Review of peridynamic and phase-field models
- o Comparison of phase-field and peridynamic models against experimental data
- o Applying machine learning techniques for auto tuning HPC applications (with Gabriel Laberge)
- 02/17–09/18 **Postdoctoral fellow**, *Laboratory of Multiscale Mechanics*, Polytechnique Montréal, QC, Canada.
 - o Benchmark peridynamic simulations against experimental data for composite materials
 - o Extracting constitutive mechanical parameters in linear elasticity using the virtual fields method within the ordinary state-based peridynamic framework (with Rolland Delorme)
 - o Hybrid image processing approach for crack area detection and tracking using local Digital Image Correlation results (with Ilyass Tabiai)
- 04/13–01/17 **Research Assistant**, *Institute for Numerical Simulation*, University Bonn, Bonn, Germany.
 - o Modeling and simulation of crack and fractures in solids using peridynamic
- 07/12–03/13 **Research Assistant**, *Institute for Simulation of large Systems*, University Stuttgart, Stuttgart, Germany.

Visiting positions

2015 **Guest Research Assistant**, *Center for Computation and Technology*, Louisiana State University.

Research Interests

Computational engineering

- o Peridynamics theory for the application in solids, like glassy or composite materials,
- o Validation and verification of simulations against experimental data,
- o Assembly of experimental data for comparison with simulations,
- o Application of machine learning to experiments and simulations.

High Performance Computing

- o The C++ Standard Library for Parallelism and Concurrency (HPX),
- o Asynchronous many task systems and there application in computational engineering.

Open science

- o Open Source Software for scientific applications,
- o Open data for sharing raw experimental results.

Teaching experience

Instructor

o Parallel computational mathematics (Math 4997), Louisiana State University, 2019.2020

Teaching assistant

- o Einführung in die Numerische Mathematik (Introduction to numerical mathematics), University of Bonn, 2015
- o Algorithmische Mathematik (Mathematical algorithms), University of Bonn, 2013/2014
- o Wissenschaftliches Rechnen 2 (Scientific Computing 2), University of Bonn, 2013

Certificates

Certificate

Baden- Certificate for successful completion of the program in higher education pedagogy Württemberg by the center for educational development of the state of Baden-Württemberg.

Academic-related Professional and Public Service

10/17-09/18 ASSEP Labor relations officers for postdoctoral fellows

03/20-current Liaison for the Louisiana district of the SIAM Texas-Louisiana Section **Duties:**

- o Making sure that people at universities, research institutions and industry in your district know about our activities and getting their suggestions on what we can do better
- o Serving on the organizing committee for the annual meeting

Organization of Conferences, Workshops and Symposia

Symposia

- o Modeling and Simulation for Complex Material Behavior, 14th U.S. National Congress on Computational Mechanics, Link.
- o Peridynamic Theory and Multiscale Methods for Complex Material Behavior, 14th World Congress on Computational Mechanics (WCCM XIV).
- o Peridynamic Theory and Multiscale Methods for Complex Material Behavior, 16th National Congress on Computational Mechanics.

Workshops

- o Workshop on Experimental and Computational Fracture Mechanics: Validating peridynamics and phase field models for fracture prediction and experimental design, Link. Sponsored by
 - US Association for Computational Mechanics,
 - Center for Computation & Technology at Louisiana State University,
 - Oak Ridge National Laboratory,
 - Society for Experimental Mechanics,
 - U.S. National Committee on Theoretical and Applied Mechanics (AmeriMech)

Panel

TBAA: Task-Based Algorithms and Applications, Moderator, "International Conference for High Performance Computing, Networking, Storage and Analysis (SC)" 2020.

Meetings

o 3rd Annual Meeting of the SIAM Texas-Louisiana Section, October 16 - 18, 2020.Link.

Conference and Workshop Grants

2020 AmeriMech symposium: Experimental and Computational Fracture Mechanics: Validating peridynamics and phase field models for fracture prediction and experimental design (\$4000)

Advising and related student services

Co-supervised theses

- o Pfander, David: Eine künstliche Intelligenz für das Kartenspiel Tichu, Studienarbeit Nr. 2398, 2013.
- o Kanis, Sebastian: GPU-based Numerical Integration in the Partition of Unity Method, Diplomarbeit Nr. 3405, 2013.

Graduate Committee Member

o Master thesis: Maxwell Reeser

Publications

Journal articles

Michael Bußler, Patrick Diehl, Dirk Pflüger, Steffen Frey, Filip Sadlo, Thomas Ertl, and Marc Alexander Schweitzer. Visualization of Fracture Progression in Peridynamics. *Computer & Graphics*, 67:45–57, 2017.

Gregor Daiß, Parsa Amini, John Biddiscombe, Patrick Diehl, Juhan Frank, Kevin Huck, Hartmut Kaiser, Dominic Marcello, David Pfander, and Dirk Pfüger. From piz daint to the stars: Simulation of stellar mergers using high-level abstractions. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '19, pages 62:1–62:37, New York, NY, USA, 2019. ACM.

Rolland Delorme, Patrick Diehl, Ilyass Tabiai, Louis Laberge Lebel, and Martin Lévesque. Extracting constitutive mechanical parameters in linear elasticity using the virtual fields method within the ordinary state-based peridynamic framework. *Journal of Peridynamics and Nonlocal Modeling*, Jan 2020.

Patrick Diehl, Fabian Franzelin, Dirk Pflüger, and Georg C. Ganzenmüller. Bondbased peridynamics: a quantitative study of Mode I crack opening. *International Journal of Fracture*, 2(201):157–170, 2016.

Patrick Diehl, Serge Prudhomme, and Martin Lévesque. A review of benchmark experiments for the validation of peridynamics models. *Journal of Peridynamics and Nonlocal Modeling*, 1(1):14–35, 2019.

Patrick Diehl, Ilyass Tabiai, Felix W. Baumann, Daniel Therriault, and Martin Levesque. Long term availability of raw experimental data in experimental fracture mechanics. *Engineering Fracture Mechanics*, 197:21–26, 2018.

Ilyass Tabiai, Gleb Tkachev, Patrick Diehl, Steffen Frey, Thomas Ertl, Daniel Therriault, and Martin Lévesque. Hybrid image processing approach for autonomous crack area detection and tracking using local digital image correlation results applied to single-fiber interfacial debonding. *Engineering Fracture Mechanics*, 216, 2019.

Proceedings

- P. Diehl and M. A. Schweitzer. Efficient neighbor search for particle methods on GPUs. In M. Griebel and M. A. Schweitzer, editors, *Meshfree Methods for Partial Differential Equations VII*, volume 100 of *Lecture Notes in Computational Science and Engineering*, pages 81–95. Springer, 2014.
- P. Diehl and M. A. Schweitzer. Simulation of wave propagation and impact damage in brittle materials using peridynamics. In Miriam Mehl, Manfred Bischoff, and Michael Schäfer, editors, *Recent Trends in Computational Engineering CE2014*, volume 105 of *Lecture Notes in Computational Science and Engineering*, pages 251–265. Springer, 2015.
- P. Diehl, M. Seshadri, T. Heller, and H. Kaiser. Integration of cuda processing within the c++ library for parallelism and concurrency (hpx). In 2018 IEEE/ACM 4th International Workshop on Extreme Scale Programming Models and Middleware (ESPM2), pages 19–28, Nov 2018.

Patrick Diehl, Michael Bußler, Dirk Pflüger, Steffen Frey, Thomas Ertl, Filip Sadlo, and Marc Alexander Schweitzer. *Extraction of Fragments and Waves After Impact Damage in Particle-Based Simulations*, pages 17–34. Springer International Publishing, Cham, 2017.

F. Franzelin, P. Diehl, and D. Pflüger. Non-intrusive uncertainty quantification with sparse grids for multivariate peridynamic simulations. In M. Griebel and M. A. Schweitzer, editors, *Meshfree Methods for Partial Differential Equations VII*, volume 100 of *Lecture Notes in Computational Science and Engineering*, pages 115–143. Springer International Publishing, 2014.

Thomas Heller, Patrick Diehl, Zachary Byerly, John Biddiscombe, and Hartmut Kaiser. HPX – An open source C++ Standard Library for Parallelism and Concurrency. In *Proceedings of OpenSuCo 2017, Denver, Colorado USA, November 2017 (OpenSuCo 17)*, page 5, 2017.

Thomas Heller, Hartmut Kaiser, Patrick Diehl, Dietmar Fey, and Marc Alexander Schweitzer. Closing the Performance Gap with Modern C++. In Michaela Taufer, Bernd Mohr, and Julian M. Kunkel, editors, *High Performance Computing: ISC High Performance 2016 International Workshops, ExaComm, E-MuCoCoS, HPC-IODC, IXPUG, IWOPH, P³MA, VHPC, WOPSSS, Frankfurt, Germany, June 19–23, 2016, Revised Selected Papers*, volume 9945 of *Lecture Notes in Computer Science*, pages 18–31. Springer International Publishing, 2016.

G. Laberge, S. Shirzad, P. Diehl, H. Kaiser, S. Prudhomme, and A. S. Lemoine. Scheduling optimization of parallel linear algebra algorithms using supervised learning. In 2019 IEEE/ACM Workshop on Machine Learning in High Performance Computing Environments (MLHPC), pages 31–43, Nov 2019.

Karsten Schatz, Christoph Müller, Patrick Gralka, Moritz Heinemann, Alexander Straub, Christoph Schulz, Matthias Braun, Tobias Rau, Michael Becher, Patrick Diehl, et al. Visual analysis of structure formation in cosmic evolution. In *2019 IEEE Scientific Visualization Conference (SciVis)*, pages 33–41. IEEE, 2019.

R. Tohid, B. Wagle, S. Shirzad, P. Diehl, A. Serio, A. Kheirkhahan, P. Amini, K. Williams, K. Isaacs, K. Huck, S. Brandt, and H. Kaiser. Asynchronous execution of python code on task-based runtime systems. In 2018 IEEE/ACM 4th International Workshop on Extreme Scale Programming Models and Middleware (ESPM2), pages 37–45, Nov 2018.

Tianyi Zhang, Shahrzad Shirzad, Patrick Diehl, R. Tohid, Weile Wei, and Hartmut Kaiser. An introduction to hpxmp: A modern openmp implementation leveraging hpx, an asynchronous many-task system. In *Proceedings of the International Workshop on OpenCL*, IWOCL'19, pages 13:1–13:10, New York, NY, USA, 2019. ACM.

Technical reports

Patrick Diehl, Robert Lipton, and Marc Alexander Schweitzer. Numerical verification of a bond-based softening peridynamic model for small displacements: Deducing material parameters from classical linear theory. Technical report, Institut für Numerische Simulation, 2016.

Tianyi Zhang, Shahrzad Shirzad, Bibek Wagle, Adrian S. Lemoine, Patrick Diehl, and Hartmut Kaiser. Supporting openmp 5.0 tasks in hpxmp – a study of an openmp implementation within task based runtime systems. Technical report, arXiv, 2020.

Preprints

Patrick Diehl, Prashant K Jha, Hartmut Kaiser, Robert Lipton, and Martin Levesque. Implementation of Peridynamics utilizing HPX—the C++ standard library for parallelism and concurrency. *arXiv preprint arXiv:1806.06917*, 2018.

Invited talks and Presentations

Patrick Diehl. Efficient k-nearest neighbor search on the GPU. Seventh International Workshop Meshfree Methods for Partial Differential Equations, 09.09-11.09 2013, Bonn, Germany.

Patrick Diehl. Coupling CPU and GPU to simulate efficient dynamic cracks and fractures in solids. 12th U.S. National Congress on Computational Mechanics (USNCCM12), 21.07-25.07 2013, Reilagh, US.

Patrick Diehl. Simulation of high-speed velocity impact on ceramic materials using the Peridynamic technique. III International Conference on Particle-Based Methods. Fundamentals and Applications. Particles 2013, 18.09-20.09 2013, Stuttgart, Germany.

Patrick Diehl. Simulation of wave propagation and impact damage in brittle materials using the peridynamics technique. 11th. World Congress on Computational Mechanics (WCCM XI), 20.07-25.07 2014, Barcelona, Spain.

Patrick Diehl. Sensivity study for wave propagation and impact damage in brittle materials using peridynamics. ASME International mechanical Engineering Congress and Exposition, 14.11-20.11 2014, Montreal, Canada.

Patrick Diehl. Efficient particle-based simulation of dynamic cracks and fractures in ceramic material. GPU Technology Conference 2014, 24.03-27.03 2014, San Francisco, US.

Patrick Diehl. Simulation of wave propagation and impact damage in brittle materials using the peridynamics technique. 3rd Workshop on Computational Engineering, 06.10-10.10 2014, Stuttgart, Germany.

Patrick Diehl. A sensitivity study for critical traction in quasi-static peridynamics simulations. 1st. PAN-American Congress on Computational Mechanics, 27.04-30.04 2015, Buenos Aires, Argentina.

Patrick Diehl. A benchmark study for mode I crack opening for brittle materials. 13th US National Congress on Computational Mechanics (USNCCM), 26.07-30.07 2015, San Diego, US.

Patrick Diehl. Energy equivalence for the horizon independent bond-based peridynamic softening model according to classical theory. The Mathematics of Finite Elements and Applications 2016 (MAFELAP), 14.06-17.06 2016, London, UK.

Patrick Diehl. Numerical Validation of the bond-based Softening Model. SIAM Mathematical Aspects of Material Science 2016, 07.05-12.05 2016, Philadelphia, US.

Patrick Diehl. Visualization of Fragments, Stress and Fracture Progression in Peridynamics. Isogeometric Analysis and Meshfree Methods, 10.10-12.10 2016, San Diego, USA.

Patrick Diehl. Modeling ductile materials with bond-based softening peridynamic model. 12th. World Congress on Computational Mechanics (WCCM XII), 24.07-29.07 2016, Seoul, Korea.

Patrick Diehl. Modeling and simulation of crack and fractures with peridynamics in brittle materials. HIM Junior Seminar, 08.02. 2017, Bonn, Germany.

Patrick Diehl. Experimental Validation of Elastic State Based Peridynamic for PMMA and epoxy materials. 14th U.S. National Congress on Computational Mechanics (USNCCM14), 17.07-20.07 2017, Montreal, Canada.

Patrick Diehl. A Review for Benchmark Experiments against Peridynamic Models. Nonlocal Methods in Fracture, 15.01-16.01 2018, Austin, USA.

Patrick Diehl. Integration of CUDA Processing within the C++ library for parallelism and concurrency (HPX). IEEE/ACM 4th International Workshop on Extreme Scale Programming Models and Middleware (ESPM2'18), 12.11-16.11 2018, Dallas, USA.

Patrick Diehl. Extracting constitutive mechanical parameters in linear elasticity using the virtual fields method within the ordinary state-based peridynamics framework. Optimization days 2018, 07.05-09.05 2018, Montreal, Canada.

Patrick Diehl. A Review for Benchmark Experiments against Peridynamic Models. 13th. World Congress on Computational Mechanics (WCCM XIII), 23.07-27.07 2018, New York City, US.

Patrick Diehl. Extracting constitutive mechanical parameters in linear elasticity using the virtual fields method within the ordinary state-based peridynamics framework. 18th U.S. National Congress for Theoretical and Applied Mechanics, 04.06-09.06 2018, Rosemont, US.

Patrick Diehl. Computational Analysis of Coupling Methods for Classical Continuum Mechanics and Peridynamics Models. 15th U.S. National Congress on Computational Mechanics (USNCCM15), 28.07-01.08 2019, Austin, USA.

Patrick Diehl. Implementation of Peridynamics utilizing HPX–the C++ standard library for parallelism and concurrency. Engineering Mechanics Institute Conference, $18.06-21.06\ 2019$, Pasadena, USA.

Patrick Diehl. An overview for coupling finite elements with peridynamics. International Congress on Industrial and Applied Mathematics, 15.07-19.07 2019, Valencia, Spain.

Patrick Diehl. Long term availability of raw experimental data in experimental fracture mechanics. Scientific Computing Around Louisiana (SCALA), 07.02-08.02. 2020, Baton Rouge, USA.

Patrick Diehl. A review of benchmark experiments for the validation of peridynamics models. Workshop on Experimental and Computational Fracture Mechanics, 26.02-28.02. 2020, Baton Rouge, USA.

Thesis

Patrick Diehl. Implementierung eines Peridynamik-Verfahrens auf GPU. Diplomarbeit, Institute of Parallel and Distributed Systems, University of Stuttgart, 2012.

Patrick Diehl. Modelling and Simulation of cracks and fractures with peridynamics in brittle materials. Doktorarbeit, University of Bonn, 2017.

Raw experimental data

Ilyass Tabiai, Rolland Delorme, Patrick Diehl, Louis Laberge Lebel, and Martin Levesque. PMMA 3 point bending test until failure loaded in displacement, February 2018.

Professional Organizations

- o Society for Industrial and Applied Mathematics (SIAM)
- o Association for Computing Machinery (ACM)
- o Informatik-Forum Stuttgart e. V.

Reviewer

International Journal of Mechanical Sciences, Fatigue & Fracture of Engineering Materials & Structures, Computer Physics Communications, International Journal of Fracture, Parallel Computing, International Journal of High Performance Computing Applications, Computer Methods in Applied Mechanics and Engineering.

References

Phd advisers

- o Dr. Marc Alexander Schweitzer, Institute for Numerical Simulation, University of Bonn, Germany, E-Mail: schweitzer@ins.uni-bonn.de
- o Dr. Daniel Peterseim, Numerische Mathematik, University of Augsburg, Germany, E-Mail: daniel.peterseim@math.uni-augsburg.de

Postdoctoral fellow adviser

o Dr. Serge Prudhomme, Department of Mathematical and Industrial Engineering, Polytechnique Montréal, Canada, E-Mail: serge.prudhomme@polymtl.ca

Collaborators

- o Dr. Robert Lipton, Mathematics of Materials Science, Louisiana State University, USA, E-Mail: lipton@math.lsu.edu
- o Dr. Thomas Ertl, Visualization and Interactive Systems Institute, University of Stuttgart, Germany, E-Mail: thomas.ertl@vis.uni-stuttgart.de
- o Dr. Hartmut Kaiser, Department of Computer Science, Louisiana State University, USA, E-Mail: hkaiser@cct.lsu.edu
- o Dr. Juhan Frank, Department of Physics & Astronomy, Louisiana State University, USA, E-Mail: frank@rouge.phys.lsu.edu
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