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

Completed 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.

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- Treatment of local boundary conditions in non-local models
- Review of peridynamic and phase-field models
- Comparison of phase-field and peridynamic models against experimental data
- 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.

- Benchmark peridynamic simulations against experimental data for composite materials
- Extracting constitutive mechanical parameters in linear elasticity using the virtual fields method within the ordinary state-based peridynamic framework (with Rolland Delorme)
- 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.

- 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

- Peridynamics theory for the application in solids, like glassy or composite materials,
- Validation and verification of simulations against experimental data,
- Assembly of experimental data for comparison with simulations,

- Application of machine learning to experiments and simulations.

High Performance Computing

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

Open science

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

Teaching experience

Instructor

- Parallel computational mathematics (Math 4997), Louisiana State University, 2019,2020

Teaching assistant

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

Certificates

Baden–Württemberg Certificate — Certificate for successful completion of the program in higher education pedagogy 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:

- 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
- Serving on the organizing committee for the annual meeting

Organization of Conferences, Workshops and Symposia

Symposia

- Modeling and Simulation for Complex Material Behavior, 14th U.S. National Congress on Computational Mechanics, Link.
- Peridynamic Theory and Multiscale Methods for Complex Material Behavior, 14th World Congress on Computational Mechanics (WCCM XIV).
- Peridynamic Theory and Multiscale Methods for Complex Material Behavior, 16th National Congress on Computational Mechanics.
- Nonlocal Models in Mathematics and Computation, 3rd Annual Meeting of the SIAM Texas-Louisiana Section, October 16 - 18, 2020

Workshop

- 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. Link

Meeting

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

Colloquium

- Colloquium on Artificial Intelligence Research and Optimization, Spring semester 2021, Louisiana State University. 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

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

Graduate Committee Member

- Master thesis: M. Reeser
- Honors project: J. Trepper

Publications

Journal articles

S. Prudhomme and P. Diehl. On the treatment of boundary conditions for bond-based peridynamic models. *Computer Methods in Applied Mechanics and Engineering*, 372:113391, 2020.

H. Kaiser, P. Diehl, A. S. Lemoine, B. A. Lelbach, P. Amini, A. Berge, J. Biddiscombe, S. R. Brandt, N. Gupta, T. Heller, K. Huck, Z. Khatami, A. Kheirkhahan, A. Reverdell, S. Shirzad, M. Simberg, B. Wagle, W. Wei, and T. Zhang. HPX - The C++ Standard Library for Parallelism and Concurrency. *Journal of Open Source Software*, 5(53):2352, 2020.

P. Diehl, P. K. Jha, H. Kaiser, R. Lipton, and M. Lévesque. An asynchronous and task-based implementation of peridynamics utilizing hpx—the c++ standard library for parallelism and concurrency. *SN Applied Sciences*, 2(12):2144, 2020.

R. Delorme, P. Diehl, I. Tabiai, L. L. Lebel, and M. 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.

I. Tabiai, G. Tkachev, P. Diehl, S. Frey, T. Ertl, D. Therriault, and M. 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.

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

G. Daiß, P. Amini, J. Biddiscombe, P. Diehl, J. Frank, K. Huck, H. Kaiser, D. Marcello, D. Pfander, and D. 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.

P. Diehl, I. Tabiai, F. W. Baumann, D. Therriault, and M. Levesque. Long term availability of raw experimental data in experimental fracture mechanics. *Engineering Fracture Mechanics*, 197:21–26, 2018.

M. Bußler, P. Diehl, D. Pflüger, S. Frey, F. Sadlo, T. Ertl, and M. A. Schweitzer. Visualization of Fracture Progression in Peridynamics. *Computer & Graphics*, 67:45–57, 2017.

P. Diehl, F. Franzelin, D. Pflüger, and G. C. Ganzenmüller. Bond-based peridynamics: a quantitative study of Mode I crack opening. *International Journal of Fracture*, 2(201):157–170, 2016.

Proceedings

B. Hasheminezhad, S. Shirzad, N. Wu, P. Diehl, H. Schulz, and H. Kaiser. Towards a scalable and distributed infrastructure for deep learning applications. In *2020 IEEE/ACM Fourth Workshop on Deep Learning on Supercomputers (DLS)*, pages 20–30, 2020.

N. Gupta, S. R. Brandt, B. Wagle, N. Wu, A. Kheirkhahan, P. Diehl, F. W. Baumann, and H. Kaiser. Deploying a task-based runtime system on raspberry pi clusters. In *2020 IEEE/ACM 5th International Workshop on Extreme Scale Programming Models and Middleware (ESPM2)*, pages 11–20, 2020.

T. Zhang, S. Shirzad, P. Diehl, R. Tohid, W. Wei, and H. 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.

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.

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.

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.

T. Heller, P. Diehl, Z. Byerly, J. Biddiscombe, and H. 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.

P. Diehl, M. Bußler, D. Pflüger, S. Frey, T. Ertl, F. Sadlo, and M. A. Schweitzer. Extraction of fragments and waves after impact damage in particle-based simulations. In M. Griebel and M. A. Schweitzer, editors, *Meshfree Methods for Partial Differential Equations VIII*, pages 17–34, Cham, 2017. Springer International Publishing.

T. Heller, H. Kaiser, P. Diehl, D. Fey, and M. A. Schweitzer. Closing the Performance Gap with Modern C++. In M. Taufer, B. Mohr, and J. M. Kunkel, editors, *High Performance Computing: ISC High Performance 2016 International Workshops, ExaComm, E-MuCoCoS, HPC-IODC, IXPUG, IWOPH, P^{3}MA, 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.

P. Diehl and M. A. Schweitzer. Simulation of wave propagation and impact damage in brittle materials using peridynamics. In M. Mehl, M. Bischoff, and M. Schäfer, editors, *Recent Trends in Computational Engineering – CE2014*, volume 105 of *Lecture Notes in Computational Science and Engineering*, pages 251–265. Springer, 2015.

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.

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.

Short papers

P. Diehl and S. R. Brandt. Interactive C++ code development using C++Explorer and GitHub Classroom for educational purposes. In *Proceedings of Gateways 2020*, page 5. Science Gateways Community Institute (SGCI), 2020.

K. Schatz, C. Müller, P. Gralka, M. Heinemann, A. Straub, C. Schulz, M. Braun, T. Rau, M. Becher, P. Diehl, et al. Visual analysis of struc-

ture formation in cosmic evolution. In *2019 IEEE Scientific Visualization Conference (SciVis)*, pages 33–41. IEEE, 2019.

Technical reports

T. Zhang, S. Shirzad, B. Wagle, A. S. Lemoine, P. Diehl, and H. Kaiser. Supporting openmp 5.0 tasks in hpxmp – a study of an openmp implementation within task based runtime systems. Technical report, arXiv preprint arXiv:2002.07970, 2020.

S. Silling, T. Wick, K. Ravi-Chandar, J. Guilleminot, J. Dolbow, J. Finberg, P. Diehl, S. Prudhomme, R. Lipton, and P. Seleson. Workshop on experimental and computational fracture mechanics 2020. Technical Report ORNL/TM-2020/1714, Oak Ridge National Laboratory, 2020.

P. Diehl, R. Lipton, and M. A. 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.

Preprints

D. C. Marcello, S. Shiber, O. D. Marco, J. Frank, G. C. Clayton, P. M. Motl, P. Diehl, and H. Kaiser. Octo-tiger: A new, 3d hydrodynamic code for stellar mergers that uses hpx parallelisation. *arXiv preprint arXiv:2101.08226*, 2021.

Invited talks and Presentations

P. Diehl. A comparative review of peridynamics and phase-field models for engineering fracture mechanics. 14th. World Congress on Computational Mechanics (WCCM XIII), 11.01-15.01 2021, Virtual event.

P. Diehl and S. R. Brandt. Deploying a Task-based Runtime System on Raspberry Pi Clusters. IEEE/ACM 4th International Workshop on Extreme Scale Programming Models and Middleware (ESPM2'20), 09.11-19.11 2020, Virtual event.

P. Diehl. On the treatment of boundary conditions for bond-based peridynamic models. 3rd Annual Meeting of the SIAM Texas-Louisiana Section, 16.10-18.10. 2020, Virtual event.

P. 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.

P. 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.

P. 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.

P. 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.

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

P. 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.

P. 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.

P. 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.

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

P. 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.

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

P. 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.

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

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

P. 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.

P. 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.

P. 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.

P. 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.

P. 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.

P. 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.

P. 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.

P. 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.

P. 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.

P. 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.

P. 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.

Thesis

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

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

Raw experimental data

I. Tabiai, R. Delorme, P. Diehl, L. L. Lebel, and M. Levesque. PMMA 3 point bending test until failure loaded in displacement, Feb. 2018.

Professional Organizations

- Society for Industrial and Applied Mathematics (SIAM)
- Association for Computing Machinery (ACM)
- 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, Theoretical and Applied Fracture Mechanics, and Mathematics and Mechanics of Solids.

References

Phd advisers

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

Postdoctoral fellow adviser

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

Collaborators

- Dr. Robert Lipton, Mathematics of Materials Science, Louisiana State University, USA, E-Mail: lipton@math.lsu.edu
- Dr. Thomas Ertl, Visualization and Interactive Systems Institute, University of Stuttgart, Germany, E-Mail: thomas.ertl@vis.uni-stuttgart.de

- Dr. Hartmut Kaiser, Department of Computer Science, Louisiana State University, USA, E-Mail: hkaiser@cct.lsu.edu
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- Dr. Steffen Frey, University of Groningen, Netherlands, E-Mail: s.d.frey@rug.nl
- Dr. Dirk Pflüger, Institute for Parallel and Distributed Systems, University of Stuttgart, Germany, Netherlands, E-Mail: Dirk.Pflueger@ipvs.uni-stuttgart.de
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- Dr. Geoffrey C. Clayton, Department of Physics and Astronomy, Louisiana State University, USA, E-Mail: gclayton@fenway.phys.lsu.edu
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