

# 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.

- 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

Baden-Württemberg Certificate for successful completion of the program in higher education Certificate 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:** 

- 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.
- o Nonlocal Models in Mathematics and Computation, 3rd Annual Meeting of the SIAM Texas-Louisiana Section, October 16 18, 2020

### 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

o 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: M. Reeser
- o 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<sup>3</sup> 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 structure 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**

### Invited talks and Presentations

- 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

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, Theoretical and Applied Fracture Mechanics.

### 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
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- o Dr. Mayank Tagi, Craft & Hawkins Department of Petroleum Engineering, Louisiana State University, USA, E-Mail: mtyagi@lsu.edu
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