



# Dr. Patrick Diehl

## *Curriculum Vitæ*

### Research experience

- Oct 2025–current **Research scientist**, *Computing and Artificial Intelligence (CAI-1)*, Los Alamos National Laboratory, Los Alamos, NM, USA
- May 2022–current **Adjunct faculty**, *Department of Physics & Astronomy*, Louisiana State University, Baton Rouge, LA, USA
- Jun 2024–Sep 2025 **Research scientist**, *Applied Computer Science (CCS-7)*, Los Alamos National Laboratory, Los Alamos, NM, USA
- Oct 2018–Jun 2024 **Research scientist**, *Center for Computation & Technology*, Louisiana State University, Baton Rouge, LA, USA
- Feb 2017–Sep 2018 **Postdoctoral fellow**, *Laboratory of Multiscale Mechanics*, Polytechnique Montréal, QC, Canada
- Apr 2013–Jan 2017 **Research Assistant**, *Institute for Numerical Simulations*, University of Bonn, Bonn, Germany
- Jul 2012–Mar 2013 **Research Assistant**, *Institute for Simulation of large Systems*, University of Stuttgart, Stuttgart, Germany
- Oct 2007–Jun 2012 **Student**, *Computer Science (Major software engineering)*, University Stuttgart, Stuttgart, Germany

### Visiting positions

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

### Education

- January 2017 **PhD**, *Applied mathematics*, University of Bonn, Germany
- August 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

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## Editorial duties

- 06/20–current **Topic editor**, *Computational fracture mechanics, Applied mathematics, C++, asynchronous and task-based programming*, The Journal of Open Source Software
- 2025 **Topical issue editor**, *Recent advances in Asynchronous Many Task Runtime Systems*, SN Computer Science
- 2025 **Guest editor**, *Research Software Engineering – Code, Practices, and People*, Future Generation Computer Systems
- 2024 **Guest editor**, *Research Software Engineering – Software-Enabled Discovery and Beyond*, Future Generation Computer Systems
- 2023 **Topical issue editor**, *Applications and Frameworks using the Asynchronous Many Task Paradigm*, SN Computer Science
- 2022 **Guest editor**, *Special issue: Science Gateways: Accelerating Research and Education*, Computing in Science & Engineering
- 2021 **Guest editor**, *Special issue: Peridynamics and its Current Progress*, Computer Modeling in Engineering & Sciences (CMES)

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## 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.
- Efficient, performance portable, and scalable High-Performance Parallel Programming using Modern C++.

### Open science

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

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## Teaching experience

### Instructor

- Research Technologies and Methods (MEDP 7098), Department of Physics & Astronomy, Louisiana State University, Taught: 2022
- Parallel computational mathematics (M 4997), Department of Mathematics, Louisiana State University, Taught: 2019, 2020, and 2021

### 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

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## 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.

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## Advising and related student services

### Co-supervised theses

- University of Stuttgart:
  - 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 (LSU, 2020) and C. He (2023)
- Honors project: J. Trepper (LSU, 2020)

### Google Summer of Code

- University of Bonn: A. Nigam (2016)
- Polytechnique Montreal: M. Seshadri (2017), G. Laberge and J. Golinowski (2018)

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- Louisiana State University: P. Gadika (2020)

#### Google Season of Docs

- Louisiana State University: R. Stobaugh (2019)

#### NSF REU

- Louisiana State University: A. Edwards (2021), E. Downing (2022), and N. Tabb (2023).

### Academic-related Professional and Public Service

- 08/25–current Chair of the USACM Technical Thrust Area (TTA) on Large Scale Structural Systems and Optimal Design (Large-Scale)
- 08/23–07/25 Vice Chair of the USACM Technical Thrust Area (TTA) on Large Scale Structural Systems and Optimal Design (Large-Scale)
- 01/213–current Mentor for the USACM Student Chapter
- 07/21–07/23 Member-at-Large of the USACM Technical Thrust Area (TTA) on Large Scale Structural Systems and Optimal Design (Large-Scale)
- 03/20–12/23 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
- 10/17–09/18 ASSEP Labor relations officers for postdoctoral fellows

### Organization of Conferences, Workshops, and Symposia

#### Committee

- Programming Frameworks, Technical Papers, Member
- ChapelCon '25, Program Committee
- AI track of 54th International Conference on Parallel Processing, Program Committee
- 2nd Annual Conference of the US Research Software Engineer Association, Publication chair
- SC25 Reproducibility Challenge, Committee member
- 1st Annual Conference of the US Research Software Engineer Association, Special Issue Editor

- Science Gateways Conference 2023, Program committee member
- The First International Workshop on Democratizing High-Performance Computing (D-HPC 2023), Program committee member
- Science Gateways Conference 2022, Publication chair
- The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC) 21, AD/AE Appendices
- Science Gateways Conference 2021, Program committee member
- The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC) 21, Virtual logistics

#### 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, 2020
- Peridynamic Theory and Multiscale Methods for Complex Material Behavior, 15th World Congress on Computational Mechanics (WCCM XV).
- Recent Developments in Peridynamics Modeling, 19th U.S. National Congress on Theoretical and Applied Mechanics.
- Peridynamic Theory and Multiscale Methods for Complex Material Behavior, 9th GACM Colloquium on Computational Mechanics
- Theoretical and Computational Aspects of Nonlocal Operator, 7th Annual Meeting of SIAM Central States Section
- Nonlocal Models in Mathematics and Computation, 5th Annual Meeting of the SIAM Texas-Louisiana Section, 2022
- Recent Developments in Peridynamics Modeling, 17th U.S. National Congress on Computational Mechanics, 2023
- Nonlocal Modeling, Analysis, and Computation, 10th International Congress on Industrial and Applied Mathematics, 2023
- Computational and analytical advances in nonlocal modeling, 16th World Congress on Computational Mechanics, 2024

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- Recent developments in peridynamics modeling, 16th World Congress on Computational Mechanics, 2024
- Computational and Analytical Advances in Nonlocal Modeling, SIAM Conference on Mathematical Aspects of Materials Science, 2024
- Peridynamic Theory and Multiscale Methods for Complex Material Behavior, 18th National Congress on Computational Mechanics, 2025

Mathematisches  
Forschungsinstitut  
Oberwolfach

- Fracture as an Emergent Phenomenon, 7 January - 12 January 2024 (Co-Organizers: Anna Pandofi, Robert Lipton, and Thomas Wick)

#### 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 (Amer-iMech)
- Asynchronous Many-Task systems for Exascale 2021 held in conjunction with Euro-Par 2021, Link
- Asynchronous Many-Task systems for Exascale 2022 held in conjunction with Euro-Par 2022, Link
- Workshop on Workshop on Asynchronous Many-Task Systems and Applications 2023, Link Sponsored by
  - Tactical Computing Lab,
  - Center for Computation & Technology at Louisiana State University,
  - HPE Enterprise
- Asynchronous Many-Task systems for Exascale 2023 held in conjunction with Euro-Par 2023, Link
- Workshop on Workshop on Asynchronous Many-Task Systems and Applications 2024, Link
- Workshop on Experimental and Computational Fracture Mechanics, Link.

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- Asynchronous Many-Task systems for Exascale 2024 held in conjunction with Euro-Par 2024, [Link](#)
- Workshop on Workshop on Asynchronous Many-Task Systems and Applications 2024, [Link](#)
- Workshop on Asynchronous Many-Task Systems and Applications 2025, [Link](#)
- Workshop on Asynchronous Many-Task Systems and Applications 2026, [Link](#)

#### Panel

- D-HPC Workshop Panel : S4PST: Stewardship of Programming Systems and Tools, Panelist, International Conference for High Performance Computing, Networking, Storage and Analysis (SC)" 2023
- Joint USACM Large-Scale TTA – EMI Computational Mechanics Committee Career Path Panel, Organizer, Engineering Mechanics Institute Conference 2023
- Joint USACM Large-Scale TTA – EMI Computational Mechanics Committee Career Path Panel, Speaker, Engineering Mechanics Institute Conference 2022
- TBAA: Task-Based Algorithms and Applications, Moderator, "International Conference for High Performance Computing, Networking, Storage and Analysis (SC)" 2020. [Link](#)
- AI Ethics/Algorithmic Justice, Organizer, Colloquium on Artificial Intelligence Research and Optimization, Louisiana State University.

#### Meeting

- 3rd Annual Meeting of the SIAM Texas-Louisiana Section, October 16 - 18, 2020. [Link](#).
- 4th Annual Meeting of the SIAM Texas-Louisiana Section, November, 5 - 7, 2021 [Link](#).
- 5th Annual Meeting of the SIAM Texas-Louisiana Section, November, 4 - 6, 2022 [Link](#).
- 6th Annual Meeting of the SIAM Texas-Louisiana Section, November, 3 - 5, 2023 [Link](#).

#### Colloquium

- Colloquium on Artificial Intelligence Research and Optimization, Louisiana State University. [Link](#).

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- Large-Scale TTA Early-Career Colloquium, USACM. [Link](#)
- Large-Scale TTA Industrial Colloquium, USACM. [Link](#)
- Applied Computer Science Invited Speaker Series, LANL. [Link](#)

#### Short course

- SC16-001 Advanced Parallel Programming in C++, 16th U.S. National Congress on Computational Mechanics
- Advanced Parallel Programming in C++, 15th World Congress on Computational Mechanics
- SC17-002 Advanced Parallel Programming in C++, 17th U.S. National Congress on Computational Mechanics

#### Mentoring events

- 18th U.S. National Congress on Computational Mechanics, 2025
- 17th U.S. National Congress on Computational Mechanics, 2023
- 6th Annual Meeting of the SIAM Texas-Louisiana Section, 2023
- 15th World Congress on Computational Mechanics, 2022
- 5th Annual Meeting of the SIAM Texas-Louisiana Section, 2022

### 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)

### Travel Awards

- 2023 SIAM Travel Award - 10th International Congress on Industrial and Applied Mathematics (ICIAM) (\$1750)

### Grant history

Current Research (chronological order; most recent one first)

#### 1. Grant #4000211901 (Hartmut Kaiser)

Name of Funding Organization: UT-Battelle, LLC

Amount Awarded: \$9,999

Period of Grant Award: July 15 2022 - April 30 2024

Title of Project: S4PST, Sustainability for Node Level Programming Systems and Tools

Role on Project: Senior Personal

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Completed Research (chronological order; most recent one first)

1. Grant #2229751 (Rod Tohid)

Name of Funding Organization: National Science Foundation

Amount Awarded: \$300,000

Period of Grant Award: Sept 15 2022 - Oct 31 2023

Title of Project: POSE: Phase I: Constellation: A Pathway to Establish the STE||AR Open-Source Organization

Role on Project: Co-PI

2. 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

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## Allocations

Current Allocations (chronological order; most recent one first)

1. Project xpress (Alice Koniges)

Title of Project: HPX and OpenMP

Amount awarded: CPU node hours 4300 and GPU node hours 1700

Cluster: Perlmutter @ NERSC

Role on Project: Senior personal

Completed Allocations (chronological order; most recent one first)

1. Project hp210311 (Patrick Diehl)

Title of Project: Porting Octo-Tiger, an astrophysics program simulating the evolution of star systems based on the fast multipole method on adaptive Octrees

Type: Test-bed

Amount awarded: 21k node hours

Cluster: Fugaku @ RIKEN Center for Computational Science, Japan

Role on Project: PI

2. Project PaDi032321F (Patrick Diehl)

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Title of Project: Porting Octo-Tiger, an astrophysics program simulating the evolution of star systems based on the fast multipole method on adaptive Octrees

Type: Test-bed

Amount awarded: 10k node hours

Cluster: Ookami @ Stonybrook University, USA

Role on Project: PI

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## Publications

### Preprints

A. Mhatre, N. Nader, P. Diehl, and D. Gupta. LLM-GUARD: Large Language Model-Based Detection and Repair of Bugs and Security Vulnerabilities in C++ and Python. *arXiv preprint arXiv:2508.16419*, 2025, arXiv:2508.16419.

S. Gupta, K. Kamalakkannan, M. Moraru, G. Shipman, and P. Diehl. From Legacy Fortran to Portable Kokkos: An Autonomous Agentic AI Workflow. *arXiv preprint arXiv:2509.12443*, 2025, arXiv:2509.12443.

P. Diehl, Y. W. Li, C. Junghans, J. K. Holmen, E. MacCarthy, S. Parete-Koon, Y. H. He, R. Hartman-Baker, C. Lively, K. Gott, L. Gupta, K. Streu, Y. Ghadar, P. Kinsley, J. Herriman, E. W. Draeger, V. Eijkhout, and S. Mehringer. Shaping the future workforce: Challenges and lessons learned in HPC education from national labs and computing centers. *EdArXiv preprint edarxiv.org/sua4v\_v1*, 2025.

S. R. Brandt, M. Morris, P. Diehl, C. Bowen, J. Tucker, L. Bristol, and G. G. R. III. Locking Down Science Gateways. *arXiv preprint arXiv:2509.18548*, 2025, arXiv:2509.18548.

### Books

P. Diehl, S. R. Brandt, and H. Kaiser. *Parallel C++ – Efficient and Scalable High-Performance Parallel Programming Using HPX*, volume 1. Springer Cham, 2024.

### Edited books

J. Singer, Y. Elkhatib, D. B. Heras, P. Diehl, N. Brown, and A. Ilic, editors. *Euro-Par 2022 International Workshops, Glasgow, UK, August 22–26, 2022, Revised Selected Papers*, volume 13835 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2022.

P. Diehl, P. Thoman, H. Kaiser, and L. Kale, editors. *Asynchronous Many-Task Systems and Applications*, volume 13861 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2023.

P. Diehl, J. Schuchart, P. Valero-Lara, and G. Bosilca, editors. *Asynchronous Many-Task Systems and Applications*, volume 14626 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2024.

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P. Diehl and S. Gesing, editors. *Editorial: Research Software Engineering – Software-Enabled Discovery and Beyond*, Future Generation Computer Systems. Elsevier, 2025.

P. Diehl and R. F. da Silva, editors. *Science Gateways: Accelerating Research and Education—Part I*, volume 25 of *Computing in Science & Engineering*, Los Alamitos, CA, USA, 2023. IEEE.

P. Diehl and R. da Silva, editors. *Science Gateways: Accelerating Research and Education—Part II*, volume 25 of *Computing in Science & Engineering*, Los Alamitos, CA, USA, 2023. IEEE.

P. Diehl, Q. Cao, T. Herault, and G. Bosilca, editors. *Asynchronous Many-Task Systems and Applications*, volume 15690 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2025.

R. Chaves, D. B. Heras, A. Ilic, D. Unat, R. M. Badia, A. Bracciali, P. Diehl, A. Dubey, O. Sangyoon, S. L. Scott, and L. Ricci, editors. *Euro-Par 2021: Parallel Processing Workshops (Euro-Par 2021 International Workshops, Lisbon, Portugal, August 30-31, 2021, Revised Selected Papers)*, volume 13098 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2021.

S. Caino-Lores, D. Zeinalipour, T. D. Doudali, D. E. Singh, G. E. M. Garzón, L. Sousa, D. Andrade, T. Cucinotta, D. D'Ambrosio, P. Diehl, M. F. Dolz, A. Jukan, R. Montella, M. Nardelli, M. Garcia-Gasulla, and S. Neuwirth, editors. *Euro-Par 2024: Parallel Processing Workshops (Volume 2)*, volume 15386 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2025.

S. Caino-Lores, D. Zeinalipour, T. D. Doudali, D. E. Singh, G. E. M. Garzón, L. Sousa, D. Andrade, T. Cucinotta, D. D'Ambrosio, P. Diehl, M. F. Dolz, A. Jukan, R. Montella, M. Nardelli, M. Garcia-Gasulla, and S. Neuwirth, editors. *Euro-Par 2024: Parallel Processing Workshops (Volume 1)*, volume 15385 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2025.

D. Blanco Heras, G. Pallis, H. Herodotou, D. Balouek, P. Diehl, T. Cojean, K. Furlinger, M. H. Kirbey, M. Nardelli, P. Di Sanzo, and e. Zeinalipour, Demetris, editors. *Euro-Par 2023 International Workshops, Limassol, Cyprus, 28 August – 1 September, 2023 Revised Selected Papers*, volume 14351 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2024.

D. Blanco Heras, G. Pallis, H. Herodotou, D. Balouek, P. Diehl, T. Cojean, K. Furlinger, M. H. Kirbey, M. Nardelli, P. Di Sanzo, and e. Zeinalipour, Demetris, editors. *Euro-Par 2023 International Workshops, Limassol, Cyprus, 28 August – 1 September, 2023 Revised Selected Papers*, volume 14352 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2024.

#### Reviews and Surveys

P. Diehl, R. Lipton, T. Wick, and M. Tyagi. A comparative review of peridynamics and phase-field models for engineering fracture mechanics. *Computational Mechanics*, Feb 2022.

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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.

#### Journal Papers

P. K. Jha, P. Diehl, and R. Lipton. Nodal finite element approximation of peridynamics. *Computer Methods in Applied Mechanics and Engineering*, 434, 2025.

J. Frank, A. Straub, S. Shiber, P. Amini, D. C. Marcello, P. Diehl, T. Ertl, F. Sadlo, and S. Frey. Visualizing the mass transfer flow in direct-impact accretion. *Monthly Notices of the Royal Astronomical Society*, 543(4):4003–4019, 10 2025.

P. Diehl, C. Soneson, R. C. Kurchin, R. Mounce, and D. S. Katz. The Journal of Open Source Software (JOSS): Bringing Open-Source Software Practices to the Scholarly Publishing Community for Authors, Reviewers, Editors, and Publishers. *Journal of Librarianship and Scholarly Communication*, 12, 2 2025.

P. Diehl, N. Nader, M. Moraru, and S. R. Brandt. LLM Benchmarking with LLaMA2: Evaluating Code Development Performance Across Multiple Programming Languages. *Journal of Machine Learning for Modeling and Computing*, 6(3):95–129, 2025.

P. Diehl, E. Downing, A. Edwards, and S. Prudhomme. Coupling Approaches with Non-matching Grids for Classical Linear Elasticity and Bond-based Peridynamic Models in 1D. *Journal of Peridynamics and Nonlocal Modeling*, 7(2), 2025.

G. Daiß, P. Diehl, J. Yan, J. K. Holmen, R. Gayatri, C. Junghans, A. Straub, J. R. Hammond, D. Marcello, M. Tsuji, D. Pflüger, and H. Kaiser. Asynchronous-many-task systems: Challenges and opportunities - Scaling an AMR astrophysics code on exascale machines using Kokkos and HPX. *The International Journal of High Performance Computing Applications*, 2025.

S. Shiber, O. De Marco, P. M. Motl, B. Munson, D. C. Marcello, J. Frank, P. Diehl, G. C. Clayton, B. N. Skinner, H. Kaiser, G. Daiß, D. Pflüger, and J. E. Staff. Hydrodynamic simulations of white dwarf-white dwarf mergers and the origin of R Coronae Borealis stars. *Monthly Notices of the Royal Astronomical Society*, 10 2024.

N. Nader, P. Diehl, M. D’Elia, C. Glusa, and S. Prudhomme. ML-based identification of the interface regions for coupling local and nonlocal models. *Journal of Machine Learning for Modeling and Computing*, 2024.

P. Diehl, G. Daiß, K. Huck, D. Marcello, S. Shiber, H. Kaiser, and D. Pflüger. Simulating stellar merger using HPX/Kokkos on A64FX on Supercomputer Fugaku. *The Journal of Supercomputing*, April 2024.

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P. Diehl, S. R. Brandt, and H. Kaiser. Shared Memory Parallelism in Modern C++ and HPX. *SN Computer Science*, 5(5):459, April 2024.

M. Birner, P. Diehl, R. Lipton, and M. A. Schweitzer. A multiscale fracture model using peridynamic enrichment of finite elements within an adaptive partition of unity: Experimental validation. *Mechanics Research Communications*, April 2024.

B. Aksoylu, F. Celiker, and P. Diehl. Construction of Nonlocal Governing Operators with Local Boundary Conditions on a General Interval. *Journal of Peridynamics and Nonlocal Modeling*, 2024.

B. Aksoylu, F. Celiker, and P. Diehl. Analysis and Implementation of Nonlocal Governing Operators with Local Boundary Conditions on a General Interval. *Journal of Peridynamics and Nonlocal Modeling*, 2024.

D. J. Littlewood, M. L. Parks, J. T. Foster, J. A. Mitchell, and P. Diehl. The Peridigm Meshfree Peridynamics Code. *Journal of Peridynamics and Nonlocal Modeling*, May 2023.

D. Bhattacharya, R. Lipton, and P. Diehl. Quasistatic fracture evolution using a nonlocal cohesive model. *International Journal of Fracture*, Jun 2023.

P. Diehl and S. Prudhomme. Coupling approaches for classical linear elasticity and bond-based peridynamic models. *Journal of Peridynamics and Nonlocal Modeling*, Mar 2022.

P. Diehl and R. Lipton. Quasistatic fracture using nonlinear-nonlocal elastostatics with explicit tangent stiffness matrix. *International Journal for Numerical Methods in Engineering*, May 2022.

P. Diehl and S. R. Brandt. Interactive C++ code development using C++ Explorer and GitHub classroom for educational purposes. *Concurrency and Computation: Practice and Experience*, 2022.

M. Birner, P. Diehl, R. Lipton, and M. A. Schweitzer. A fracture multiscale model for peridynamic enrichment within the partition of unity method. *Advances in Engineering Software*, 176, Nov 2022.

D. C. Marcello, S. Shiber, O. De 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. *Monthly Notices of the Royal Astronomical Society*, 2021.

P. K. Jha and P. Diehl. NImech: Implementation of finite difference/mesh-free discretization of nonlocal fracture models. *Journal of Open Source Software*, 6(65):3020, 2021.

P. Diehl, D. Marcello, P. Armini, H. Kaiser, S. Shiber, G. C. Clayton, J. Frank, G. Daiss, D. Pflüger, D. C. Eder, A. Koniges, and K. Huck.

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#### Series- and conference contributions

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Los Alamos National Laboratory – Los Alamos, NM 87545, USA

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in patrickdiehl • [diehlpk](#) • [0000-0003-3922-8419](#)

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#### Short papers

S. R. Brandt and P. Diehl. Locking Down Science Gateways. In *Proceedings of Gateways 2024*. Science Gateways Community Institute (SGCI), 2024.

D. Bhattacharya, P. Diehl, and R. P. Lipton. Peridynamics for Quasistatic Fracture Modeling. volume 12: Mechanics of Solids, Structures, and Fluids; Micro- and Nano- Systems Engineering and Packaging of *ASME International Mechanical Engineering Congress and Exposition*, 11 2021.

P. Diehl and S. R. Brandt. Interactive C++ code development using C++ Explorer and GitHub Classroom for educational purposes. In *Proceedings of Gateways 2020*. 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.

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## Technical reports

P. Diehl, R. Lipton, A. Pandolfi, and T. Wick. Fracture as an emergent phenomenon. Technical Report Report No. 1/2024, Reporter: Nicole Buczkowski, Mathematisches Forschungsinstitut Oberwolfach, 2024.

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P. Diehl. Porting Octo-Tiger, an astrophysics program simulating the evolution of star systems based on the fast multipole method on adaptive Octrees. Technical report, HPCI User Report, 2022.

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## Invited talks and Presentations

P. Diehl. Evaluating AI-generated code for C++, Fortran, Go, Java, Julia, Matlab, Python, R, and Rust. Workshop on Asynchronous Many-Task Systems and Applications 2025, 19.02-21.02 2025, St. Louis, USA.

A. Barai, K. Kamalakkannan, Patrick Diehl, M. Moraru, J. Dominguez-Trujillo, H. Pritchard, N. Santhi, F. Fatollahi-Fard, and G. Shipman. Bridging Simulation and Silicon: A Study of RISC-V Hardware and FireSim Simulation. Third International workshop on RISC-V for HPC held in conjunction with the International Conference on High Performance Computing, Network, Storage, and Analysis 2025, 17.11 2025, St. Louis, US.

D. S. Katz, P. Diehl, and W. Gearty. Joss: A journal for open source software that is an open source software project. US Research Software Engineering Conference 2025 (USRSE'25), 6.10-08.10 2025, Philadelphia, USA.

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P. Diehl. Asynchronous-Many-Task Systems: Challenges and Opportunities – Scaling an AMR Astrophysics Code on Exascale machines using Kokkos and HPX. Algorithms For Multiphysics Models In The Post-Moore’s Law Era, 02.06-13.06 2025, Los Alamos, USA.

P. Diehl. Asynchronous-Many-Task Systems: Challenges and Opportunities – Scaling an AMR Astrophysics Code on Exascale machines using Kokkos and HPX. Salishan Conference on High Speed Computing, 22.04-25.04 2025, Lincoln Beach, USA.

Patrick Diehl, Y. W. Li, C. Junghans, J. K. Holmen, E. MacCarthy, S. Parete-Koon, Y. H. He, R. Hartman-Baker, C. Lively, K. Gott, L. Gupta, K. Streu, Y. Ghadar, P. Kinsley, J. Herriman, E. W. Draeger, V. Eijkhout, and S. Mehringer. Shaping the future workforce: Challenges and lessons learned in HPC education from national labs and computing centers. 12th SC Workshop on best Practices for HPC Training and Education held in conjunction with the International Conference on High Performance Computing, Network, Storage, and Analysis 2025, 17.11 2025, St. Louis US.

P. Diehl. The Journal of Open Source Software: Developing a Software Review Community. Computer Science Seminar Series at Argonne National Laboratory, 12.11 2024, Virtual event.

P. Diehl. Kokkos Pitch. US-RSE Community Call, 12.09 2024, Virtual event.

P. Diehl. Is RISC-V ready for HPC workloads? (random access talk). Salishan Conference on High Speed Computing, 22.04-25.04 2024, Lincoln Beach, USA.

P. Diehl. HPX with Spack and Singularity Containers: Evaluating Overheads for HPX/Kokkos using an astrophysics application. Workshop on Asynchronous Many-Task Systems and Applications 2024, 14.02-16.02 2024, Knoxville, US.

P. Diehl. Evaluating HPX and Kokkos on RISC-V using an Astrophysics Application Octo-Tiger. 21th Annual Workshop on Charm++ and Its Application, 25.04-26.04 2024, Champaign, USA.

P. Diehl. Preparing for HPC on RISC-V: Examining Vectorization and Distributed Performance of an Astrophysics Application with HPX and Kokkos. International workshop on RISC-V for HPC held in conjunction with the International Conference on High Performance Computing, Network, Storage, and Analysis 2024, 18.11 2024, Atlanta, US.

P. Diehl. Evaluating AI-generated code for C++, Fortran, Go, Java, Julia, Matlab, Python, R, and Rust. Asynchronous Many-Task systems for Exascale (AMTE24) held in conjunction with 30th International European

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20/27

Conference on Parallel and Distributed Computing (EuroPar24), 26.08-30.08 2024, Madrid, Spain.

P. Diehl. JOSS and FLOSS for science: Examples for promoting open source software and science communication. SIGDIUS Seminars, 14.06 2023, Virtual event.

P. Diehl. Simulating Stellar Merger using HPX/Kokkos on A64FX on Supercomputer Fugaku. The 24th IEEE International Workshop on Parallel and Distributed Scientific and Engineering Computing (PDSEC 2023), 15.05-19.05 2023, St. Petersburg, USA.

P. Diehl. Evaluating HPX and Kokkos on RISC-V using an Astrophysics Application Octo-Tiger. Second International workshop on RISC-V for HPC held in conjunction with the International Conference on High Performance Computing, Network, Storage, and Analysis 2023, 13.11 2023, Denver, US.

P. Diehl. Recent developments in HPX and Octo-Tiger. Physics & Astronomy Colloquium, 23.1 2023, Baton Rouge, USA.

P. Diehl. AI-based identification of coupling regions for local and non-local one-dimensional coupling approaches. 17th U. S. National Congress on Computational Mechanics (USNCCM), 23.07-27.07 2023, Albuquerque, US.

P. Diehl. A Fracture Multiscale Model for Peridynamic enrichment within the Partition of Unity Method: Experimental validation. XVII International Conference on Computational Plasticity, Fundamentals, and Applications (COMPLAS 23), 05.09-07.09 2023, Barcelona, Spain.

P. Diehl. AI-based identification of coupling regions for local and non-local one-dimensional coupling approaches. 10th International Congress on Industrial and Applied Mathematics (ICIAM), 20.08-25.08 2023, Tokyo, Japan.

P. Diehl. Benchmarking the Parallel 1D Heat Equation Solver in Chapel, Charm++, C++, HPX, Go, Julia, Python, Rust, Swift, and Java. Asynchronous Many-Task systems for Exascale (AMTE23) held in conjunction with 29th International European Conference on Parallel and Distributed Computing (EuroPar23), 28.08-01.09 2023, Limassol, Cyprus.

P. Diehl and G. Daiß. Porting our astrophysics application to Arm64FX and adding Arm64FX support using Kokkos. Ookami user group meeting, 10.02 2022, Virtual event.

P. Diehl and S. Brandt. Interactive C++ code development using C++ Explorer and GitHub Classroom for educational purposes. emBO++ Embedded C++ and C conference, 25.03-23.03 2022, Virtual event.

P. Diehl. Quasistatic Fracture using Nonlinear-Nonlocal Elastostatics with an Explicit Tangent Stiffness Matrix for arbitrary Poisson ratios. 15th.

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World Congress on Computational Mechanics (WCCM XV), 31.07-05.08 2022, Virtual event.

P. Diehl. A Fracture Multiscale Model for Peridynamic enrichment within the Partition of Unity Method. SIAM Annual Meeting (AN22), 11.07-15.07 2022, Pittsburgh, USA.

P. Diehl. Recent developments in HPX and Octo-Tiger. ISTI Seminar Series, 1.11 2022, Los Alamos, USA.

P. Diehl. A tale of two approaches for coupling nonlocal and local models. Continuum Mechanics Seminar (CMS), 10.11 2022, Lincoln, USA.

P. Diehl. Quantifying Overheads in Charm++ and HPX using Task Bench. Asynchronous Many-Task systems for Exascale (AMTE) 2022, 23.08 2022, Glasgow, UK.

P. Diehl and S. Prudhomme. Challenges for coupling approaches for classical linear elasticity and bond-based peridynamic models for non-uniform meshes and damage . Society of Engineering Science Annual Technical Meeting (SES2022), 16.10-19.10 2022, College Station, USA.

P. Diehl. Quantifying Overheads in Charm++ and HPX using Task Bench. The Charm++ Workshop 2022, 19.10-20.10 2022, College Park , USA.

P. Diehl. A Fracture Multiscale Model for Peridynamic enrichment within the Partition of Unity Method. Engineering Mechanics Institute Conference, 01.06-03.06 2022, Baltimore, USA.

P. Diehl and S. Prudhomme. On the coupling of classical and non-local models for applications in computational mechanics. 19th U.S. National Congress on Theoretical and Applied Mechanics, 19.06-22.06 2022, Austin, USA.

P. Diehl. Recent developments in HPX and Octo-Tiger. 19th Annual Workshop on Charm++ and Its Application, 18.10-19.10. 2021, Virtual event.

P. Diehl. Quasistatic Fracture using Nonlinear-Nonlocal Elastostatics with an Analytic Tangent Stiffness Matrix. 16th U.S. National Congress on Computational Mechanics (USNCCM16), 25.07-29.07 2021, Virtual event.

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. An asynchronous and task-based implementation of peridynamics utilizing HPX—the C++ standard library for parallelism and concurrency. Nonlocal code event, 02.12 2021, Virtual event.

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P. Diehl. A comparative review of peridynamics and phase-field models for engineering fracture mechanics. Engineering Mechanics Institute Conference, 26.05-28.05 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.

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*Los Alamos National Laboratory – Los Alamos, NM 87545, USA*

☎ +1 (505) 500 9948 • ✉ [diehlpk@lanl.gov](mailto:diehlpk@lanl.gov) • 🌐 [www.diehlpk.de](http://www.diehlpk.de)  
in [patrickdiehl](#) • 🌐 [diehlpk](#) • 🆔 0000-0003-3922-8419

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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.

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*Los Alamos National Laboratory – Los Alamos, NM 87545, USA*

☎ +1 (505) 500 9948 • ✉ [diehlpk@lanl.gov](mailto:diehlpk@lanl.gov) • 🌐 [www.diehlpk.de](http://www.diehlpk.de)  
in [patrickdiehl](#) • 🌐 [diehlpk](#) • 🆔 0000-0003-3922-8419



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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.

### Posters

S. Gupta, K. Kamalakkannan, M. Moraru, G. Shipman, and P. Diehl. From Legacy Fortran to Portable Kokkos: An Autonomous Agentic AI Workflow. International Conference on High Performance Computing, Network, Storage, and Analysis 2025, 16.11-21.11 2025, St. Louis US.

P. Diehl and D. S. Katz. JOSS – The Journal of Open Source Software. 2nd Annual Conference of the US Research Software Engineer Association, 15.10-17.10 2024, Albuquerque, US.

P. Diehl. Numerical verification of the bond-based peridynamic softening model against classical theory. Nonlocal Models in Mathematics, Computation, Science, and Engineering, 26.11-28.11 2015, Oak Ridge, US.

P. Diehl. Applying Tools and Techniques from Software Engineering in Computational Mechanics. 12th U.S. National Congress on Computational Mechanics (USNCCM12), 21.07-25.07 2013, Raleigh, US.

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## Thesis

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

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## Open source software

- NLMech - Implementation of finite element and finite difference approximation of Nonlocal models [JOSS 10.21105/joss.03020](https://doi.org/10.21105/joss.03020)
- HPX - C++ standard library for parallelism and concurrency [JOSS 10.21105/joss.02352](https://doi.org/10.21105/joss.02352)

- Octo-Tiger - GPU-accelerated astrophysics code to simulate the merging of stars

## 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)
- U.S. Association for Computational Mechanics (USACM)
- Informatik-Forum Stuttgart e. V.
- Association for Computing Machinery (ACM)

## Reviewer

Computational Particle Mechanics, PLOS ONE, 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, Mathematics and Mechanics of Solids, Journal of Engineering Mechanics, Computational Mechanics, Mathematical Reviews, Engineering with Computers, Computer Modeling in Engineering & Sciences (CMES), Journal of Peridynamics and Nonlocal Modeling, Engineering Analysis with Boundary Elements, Computers in Biology and Medicine, and Concurrency and Computation: Practice and Experience.

## References

### Phd advisers

- Dr. Marc Alexander Schweitzer, Institute for Numerical Simulation, University of Bonn, Germany, E-Mail: [schweitzer@ins.uni-bonn.de](mailto:schweitzer@ins.uni-bonn.de)
- Dr. Daniel Peterseim, Numerische Mathematik, University of Augsburg, Germany, E-Mail: [daniel.peterseim@math.uni-augsburg.de](mailto: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](mailto:serge.prudhomme@polymtl.ca)

## Collaborators

- Dr. Robert Lipton, Mathematics of Materials Science, Louisiana State University, USA, E-Mail: [lipton@math.lsu.edu](mailto:lipton@math.lsu.edu)
- Dr. Thomas Ertl, Visualization and Interactive Systems Institute, University of Stuttgart, Germany, E-Mail: [thomas.ertl@vis.uni-stuttgart.de](mailto:thomas.ertl@vis.uni-stuttgart.de)
- Dr. Hartmut Kaiser, Department of Computer Science, Louisiana State University, USA, E-Mail: [hkaiser@cct.lsu.edu](mailto:hkaiser@cct.lsu.edu)
- Dr. Juhan Frank, Department of Physics & Astronomy, Louisiana State University, USA, E-Mail: [frank@rouge.phys.lsu.edu](mailto:frank@rouge.phys.lsu.edu)
- Dr. Steven R. Brandt, Center of Computation & Technology, Louisiana State University, USA, E-Mail: [sbrandt@cct.lsu.edu](mailto:sbrandt@cct.lsu.edu)
- Dr. Ilyass Tabiai, École de Technologie Supérieure, Canada, E-Mail: [ilyass.tabiai@etsmtl.net](mailto:ilyass.tabiai@etsmtl.net)
- Dr. Steffen Frey, University of Groningen, Netherlands, E-Mail: [s.d.frey@rug.nl](mailto: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](mailto:Dirk.Pflueger@ipvs.uni-stuttgart.de)
- Dr. Mayank Tagi, Craft & Hawkins Department of Petroleum Engineering, Louisiana State University, USA, E-Mail: [mtyagi@lsu.edu](mailto:mtyagi@lsu.edu)
- Dr. Geoffrey C. Clayton, Department of Physics and Astronomy, Louisiana State University, USA, E-Mail: [gclayton@fenway.phys.lsu.edu](mailto:gclayton@fenway.phys.lsu.edu)
- Dr. Orsola De Marco, Department of Physics and Astronomy, Macquarie University, Australia, E-Mail: [orsola.demarco@mq.edu.au](mailto:orsola.demarco@mq.edu.au)
- Dr. Thomas Wick, Leibniz Universität Hannover, Institut für Angewandte Mathematik, Germany, E-Mail: [thomas.wick@ifam.uni-hannover.de](mailto:thomas.wick@ifam.uni-hannover.de)

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