

Dr. Patrick Diehl

Curriculum Vitæ

	Research experience
06/24-current	Research scientist, Applied Computer Science (CCS-7), Los Alamos National Laboratory, Los Alamos, NM, USA
05/22-current	Adjunct faculty , <i>Department of Physics & Astronomy</i> , Louisiana State University, Baton Rouge, LA, USA
10/18-06/24	Research scientist, Center for Computation & Technology, Louisiana State University, Baton Rouge, LA, USA
02/17-09/18	Postdoctoral fellow , <i>Laboratory of Multiscale Mechanics</i> , Polytechnique Montréal, QC, Canada
07/12-03/13	Research Assistant , <i>Institute for Simulation of large Systems</i> , University Stuttgart, Stuttgart, Germany
10/07-06/12	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
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 For-
	mation in Cosmic Evolution, Video, Poster, and Short paper

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

Research Interests

Computational engineering

- 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

- 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.

Teaching experience

Instructor

Research Technologies and Methods (MEDP 7098), Department of Physics
 & Astronomy, Louisiana State University, Taught: 2022

O Parallel computational mathematics (M 4997), Department of Mathematics, Louisiana State University, Taught: 2019, 2020, and 2021

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.

Advising and related student services

Co-supervised theses

- O 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

- O Master thesis: M. Reeser (LSU, 2020) and C. He (2023)
- O Honors project: J. Trepper (LSU, 2020)

Google Summer of Code

- O University of Bonn: A. Nigam (2016)
- O Polytechnique Montreal: M. Seshadri (2017), G. Laberge and J. Golinowski (2018)
- O Louisiana State University: P. Gadika (2020)

Google Season of Docs

O Louisiana State University: R. Stobaugh (2019)

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NSF REU

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

Academic-related Professional and Public Service

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

- 1st Annual Conference of the US Research Software Engineer Association, Special Issue Editor
- O 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
- O 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.

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

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- 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
- 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

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 (AmeriMech)
- 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
- O Workshop on Experimental and Computational Fracture Mechanics, Link.
- Asynchronous Many-Task systems for Exascale 2024 held in conjunction with Euro-Par 2024, 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

 Al 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.
- O Large-Scale TTA Early-Career Colloquium, USACM. Link
- O Large-Scale TTA Industrial Colloquium, USACM. Link
- O 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

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

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

Allocations

Current Allocations (chronological order; most recent one first)

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

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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)

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

Publications

Preprints

S. Shiber, O. D. 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 WD-WD mergers and the origin of RCB stars. *arXiv preprint arXiv:2404.06864*, 2024, 2404.06864.

- P. K. Jha, P. Diehl, and R. Lipton. Nodal finite element approximation of peridynamics. *arXiv preprint arXiv:2403.05501*, 2024, 2403.05501.
- P. Diehl, N. Nader, S. Brandt, and H. Kaiser. Evaluating Al-generated code for C++, Fortran, Go, Java, Julia, Matlab, Python, R, and Rust. *arXiv* preprint arXiv:2405.13101, 2024, 2405.13101.

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.
- 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.
- 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.
- D. Blanco Heras, G. Pallis, H. Herodotou, D. Balouek, P. Diehl, T. Cojean, K. Fürlinger, M. H. Kirbey, M. Nardelli, P. Di Sanzo, and e. Zeinalipour, Demetris, editors. *Euro-Par 2023 International Workshops, Limassol, Cypress, 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. Fürlinger, M. H. Kirbey, M. Nardelli, P. Di Sanzo, and e. Zeinalipour, Demetris, editors. *Euro-Par 2023 International Workshops, Limassol, Cypress, 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.

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

- 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.
- 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. Celker, 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. Celker, 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. Nlmech: 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. Pfl"uger, D. C. Eder, A. Koniges, and K. Huck. Performance Measurements within Asynchronous Task-based Runtime Systems: A Double White Dwarf Merger as an Application. *Computing in Science & Engineering*, 2021.
- P. Diehl, G. Daiß, D. Marcello, K. Huck, S. Shiber, H. Kaiser, J. Frank, G. C. Clayton, and D. Pflüger. Octo-Tiger's New Hydro Module and Performance Using HPX+ CUDA on ORNL's Summit. In *2021 IEEE International Conference on Cluster Computing (CLUSTER)*, pages 204–214. IEEE, 2021.
- 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.
- 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.

Series- and conference contributions

- A. Strack, C. Taylor, P. Diehl, and D. Pflüger. Experiences Porting Shared and Distributed Applications to Asynchronous Tasks: A Multidimensional FFT Case-Study. In P. Diehl, J. Schuchart, P. Valero-Lara, and G. Bosilca, editors, *Asynchronous Many-Task Systems and Applications*, pages 111–122, Cham, 2024. Springer Nature Switzerland.
- P. Diehl, M. Morris, S. R. Brandt, N. Gupta, and H. Kaiser. Benchmarking the Parallel 1D Heat Equation Solver in Chapel, Charm++, C++, HPX, Go, Julia, Python, Rust, Swift, and Java. In D. Blanco Heras, G. Pallis, H. Herodotou, D. Balouek, P. Diehl, T. Cojean, K. Fürlinger, M. H. Kirbey, M. Nardelli, P. Di Sanzo, and D. Zeinalipour, editors, *Euro-Par 2023: Parallel Processing Workshops*, volume 14352 of Lecture Notes in Computer Science (LNCS), pages 120–131, Cham, 2024. Springer Nature Switzerland.
- P. Diehl, S. R. Brandt, G. Daiß, and H. Kaiser. HPX with Spack and Singularity Containers: Evaluating Overheads for HPX/Kokkos Using an Astrophysics Application. In P. Diehl, J. Schuchart, P. Valero-Lara, and G. Bosilca, editors, *Asynchronous Many-Task Systems and Applications*, pages 173–184, Cham, 2024. Springer Nature Switzerland.
- N. Wu, I. Gonidelis, S. Liu, Z. Fink, N. Gupta, K. Mohammadiporshokooh, P. Diehl, H. Kaiser, and L. V. Kale. Quantifying Overheads in Charm++ and HPX Using Task Bench. In J. Singer, Y. Elkhatib, D. Blanco Heras, P. Diehl, N. Brown, and A. Ilic, editors, *Euro-Par 2022: Parallel Processing Workshops*, pages 5–16, Cham, 2023. Springer Nature Switzerland.
- P. Diehl, G. Daiss, S. Brandt, A. Kheirkhahan, H. Kaiser, C. Taylor, and J. Leidel. Evaluating HPX and Kokkos on RISC-V Using an Astrophysics Application Octo-Tiger. In *Proceedings of the SC '23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, SC-W '23, page 1533–1542, New York, NY, USA, 2023. Association for Computing Machinery.

- P. Diehl, G. Dais, K. Huck, D. Marcello, S. Shiber, H. Kaiser, and D. Pfluger. Simulating Stellar Merger using HPX/Kokkos on A64FX on Supercomputer Fugaku. In *2023 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*, pages 682–691, Los Alamitos, CA, USA, may 2023. IEEE Computer Society.
- P. Diehl, S. R. Brandt, and H. Kaiser. Shared Memory Parallelism in Modern C++ and HPX. In P. Diehl, P. Thoman, H. Kaiser, and L. Kale, editors, *Asynchronous Many-Task Systems and Applications*, pages 27–38, Cham, 2023. Springer Nature Switzerland.
- G. Daiß, P. Diehl, H. Kaiser, and D. Pflüger. Stellar Mergers with HPX-Kokkos and SYCL: Methods of Using an Asynchronous Many-Task Runtime System with SYCL. In *Proceedings of the 2023 International Workshop on OpenCL*, IWOCL '23, New York, NY, USA, 2023. Association for Computing Machinery.
- G. Daiß, S. Singanaboina, P. Diehl, H. Kaiser, and D. Pflüger. From Merging Frameworks to Merging Stars: Experiences using HPX, Kokkos and SIMD Types. In *2022 IEEE/ACM 7th International Workshop on Extreme Scale Programming Models and Middleware (ESPM2)*, pages 10–19, Los Alamitos, CA, USA, nov 2022. IEEE Computer Society.
- G. Daiß, P. Diehl, D. Marcello, A. Kheirkhahan, H. Kaiser, and D. Pflüger. From Task-Based GPU Work Aggregation to Stellar Mergers: Turning Fine-Grained CPU Tasks into Portable GPU Kernels. In 2022 IEEE/ACM International Workshop on Performance, Portability and Productivity in HPC (P3HPC), pages 89–99, Los Alamitos, CA, USA, nov 2022. IEEE Computer Society.
- P. Gadikar, P. Diehl, and P. K. Jha. Load balancing for distributed nonlocal models within asynchronous many-task systems. In *2021 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*, pages 669–678, Los Alamitos, CA, USA, Jun 2021. IEEE Computer Society.
- 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.
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Invited talks and Presentations

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

<u>Posters</u>

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- P. Diehl. Numerical verification of the bond-based peridynamic softening model against classical theory. Nonlocal Models in Mathematics, Compution, 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.

Thesis

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

Open source software

- NLMech Implementation of finite element and finite difference approximation of Nonlocal models Joss 10.21105/joss.03020
- O HPX C++ standard library for parallelism and concurrency [055] 10.21105/joss.02352
- $\,\circ\,$ Octo-Tiger GPU-accelerated astrophysics code to simulate the merging of stars

Raw experimental data

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Professional Organizations

- Society for Industrial and Applied Mathematics (SIAM)
- o U.S. Association for Computational Mechanics (USACM)
- O 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, and Concurrency and Computation: Practice and Experience.

References

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