

Preprints

- [1] N. Nader, P. Diehl, S. R. Brandt, and H. Kaiser. LLM & HPC: Benchmarking DeepSeek's Performance in High-Performance Computing Tasks. *arXiv preprint arXiv:2504.03665*, 2025, 2504.03665.
- [2] 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.
- [3] 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.
- [4] 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.
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Books

- [1] 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

- [1] 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.
- [2] 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.
- [3] 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.
- [4] P. Diehl and S. Gesing, editors. *Editorial: Research Software Engineering – Software-Enabled Discovery and Beyond*, Future Generation Computer Systems. Elsevier, 2025.
- [5] 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.

- [6] 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.
- [7] 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.
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- [11] D. Blanco Heras, G. Pallis, H. Herodotou, D. Balouek, P. Diehl, T. Cojean, K. Fürlinger, M. H. Kirby, 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.
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Reviews and Surveys

- [1] 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.
- [2] 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

- [1] P. K. Jha, P. Diehl, and R. Lipton. Nodal finite element approximation of peridynamics. *Computer Methods in Applied Mechanics and Engineering*, 434, 2025.
- [2] 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.
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- [4] 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.
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- [8] 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.
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- [10] P. Diehl, S. R. Brandt, and H. Kaiser. Shared Memory Parallelism in Modern C++ and HPX. *SN Computer Science*, 5(5):459, April 2024.
- [11] 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.
- [12] 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.

- [13] 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.
- [14] 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.
- [15] D. Bhattacharya, R. Lipton, and P. Diehl. Quasistatic fracture evolution using a nonlocal cohesive model. *International Journal of Fracture*, Jun 2023.
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- [20] 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.
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Series- and conference contributions

- [1] S. Atre, C. Taylor, P. Diehl, and H. Kaiser. Closing a source complexity gap between chapel and hpx. In P. Diehl, Q. Cao, T. Herault, and G. Bosilca, editors, *Asynchronous Many-Task Systems and Applications*, pages 31–43, Cham, 2026. Springer Nature Switzerland.
- [2] P. Diehl, N. Nader, S. Brandt, and H. Kaiser. Evaluating AI-Generated Code for C++, Fortran, Go, Java, Julia, Matlab, Python, R, and Rust. In 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*, pages 243–254, Cham, 2025. Springer Nature Switzerland.

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Short papers

- [1] S. R. Brandt and P. Diehl. Locking Down Science Gateways. In *Proceedings of Gateways 2024*. Science Gateways Community Institute (SGCI), 2024.
- [2] 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.
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Technical reports

- [1] 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.
- [2] P. Diehl, G. Daiss, K. Huck, D. Marcello, S. Shiber, H. Kaiser, J. Frank, G. C. Clayton, and D. Pflueger. Distributed, combined CPU and GPU profiling within HPX using APEX. *arXiv preprint arXiv:2210.06437*, 2022.
- [3] 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

- [1] 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.
- [2] 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.
- [3] 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.
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- [5] 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.
- [6] P. Diehl. Kokkos Pitch. US-RSE Community Call, 12.09 2024, Virtual event.
- [7] 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.
- [8] 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.
- [9] 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.
- [10] 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.
- [11] 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 Conference on Parallel and Distributed Computing (EuroPar24), 26.08-30.08 2024, Madrid, Spain.
- [12] P. Diehl. JOSS and FLOSS for science: Examples for promoting open source software and science communication. SIGDIUS Seminars, 14.06 2023, Virtual event.
- [13] 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.
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- [15] P. Diehl. Recent developments in HPX and Octo-Tiger. Physics & Astronomy Colloquium, 23.1 2023, Baton Rouge, USA.
- [16] 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.
- [17] 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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- [19] 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.
- [20] 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.
- [21] 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.
- [22] 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.
- [23] 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.
- [24] P. Diehl. Recent developments in HPX and Octo-Tiger. ISTI Seminar Series, 1.11 2022, Los Alamos, USA.
- [25] P. Diehl. A tale of two approaches for coupling nonlocal and local models. Continuum Mechanics Seminar (CMS), 10.11 2022, Lincoln, USA.
- [26] P. Diehl. Quantifying Overheads in Charm++ and HPX using Task Bench. Asynchronous Many-Task systems for Exascale (AMTE) 2022, 23.08 2022, Glasgow, UK.
- [27] 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.
- [28] P. Diehl. Quantifying Overheads in Charm++ and HPX using Task Bench. The Charm++ Workshop 2022, 19.10-20.10 2022, College Park , USA.
- [29] 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.
- [30] 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, 19.06-224.06 2022, Austin, USA.
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- [32] 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.
- [33] 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.
- [34] 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.
- [35] 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.
- [36] 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.
- [37] 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.
- [38] 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.
- [39] 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.
- [40] 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.
- [41] 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.
- [42] P. Diehl. An overview for coupling finite elements with peridynamics. International Congress on Industrial and Applied Mathematics, 15.07-19.07 2019, Valencia, Spain.
- [43] 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.
- [44] 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.

- [45] 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.
- [46] P. Diehl. A Review for Benchmark Experiments against Peridynamic Models. Nonlocal Methods in Fracture, 15.01-16.01 2018, Austin, USA.
- [47] 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.
- [48] P. Diehl. Modeling and Simulation of crack and fractures with peridynamics in brittle materials. HIM Junior Seminar, 08.02. 2017, Bonn, Germany.
- [49] P. Diehl. Experimental Validation of Elastic State Based Peridynamic for PMMA and epoxy materials. 14th U.S. National Congress on Computational Mechanics (US-NCCM14), 17.07-20.07 2017, Montreal, Canada.
- [50] P. Diehl. Visualization of Fragments, Stress and Fracture Progression in Peridynamics. Isogeometric Analysis and Meshfree Methods, 10.10-12.10 2016, San Diego, USA.
- [51] P. Diehl. Numerical Validation of the bond-based Softening Model. SIAM Mathematical Aspects of Material Science 2016, 07.05-12.05 2016, Philadelphia, US.
- [52] 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.
- [53] 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.
- [54] 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.
- [55] 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.
- [56] 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.
- [57] 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.
- [58] 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.

- [59] 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.
- [60] 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.
- [61] 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.
- [62] 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

- [1] 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.
- [2] 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.
- [3] 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.

Theses

- [1] P. Diehl. *Modelling and Simulation of cracks and fractures with peridynamics in brittle materials*. Doktorarbeit, University of Bonn, 2017.
- [2] P. Diehl. Implementierung eines Peridynamik-Verfahrens auf GPU. Diplomarbeit, Institute of Parallel and Distributed Systems, University of Stuttgart, 2012.

Raw experimental data

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