

## Preprints

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- [2] 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.
- [3] P. Diehl, N. Nader, and D. Gupta. LLM-HPC++: Evaluating LLM-Generated Modern C++ and MPI+OpenMP Codes for Scalable Mandelbrot Set Computation. *arXiv preprint arXiv:2512.17023*, 2025, arXiv:2512.17023.
- [4] 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.
- [5] 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

- [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.
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- [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.

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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.
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## Journal Papers

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## Series- and conference contributions

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## Short papers

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## Technical reports

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- [5] T. Zhang, S. Shirzad, B. Wagle, A. S. Lemoine, P. Diehl, and H. Kaiser. Supporting OpenMP 5.0 Tasks in hpxMP – A study of an OpenMP implementation within Task Based Runtime Systems. Technical report, arXiv preprint arXiv:2002.07970, 2020.
- [6] P. Diehl, S. Prudhomme, and P. Seleson. Workshop on experimental and computational fracture mechanics 2020. Technical Report ORNL/TM-2020/1714, Oak Ridge National Laboratory, 2020.
- [7] P. Diehl, R. Lipton, and M. A. Schweitzer. Numerical verification of a bond-based softening peridynamic model for small displacements: Deducing material parameters from classical linear theory. Technical report, Institut für Numerische Simulation, 2016.

## 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] 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.
- [3] 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.
- [4] 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.
- [5] 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.
- [6] 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.
- [7] 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.
- [8] P. Diehl. Kokkos Pitch. US-RSE Community Call, 12.09 2024, Virtual event.
- [9] 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.
- [10] 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.
- [11] 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.
- [12] 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.
- [13] 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.

- [14] P. Diehl. JOSS and FLOSS for science: Examples for promoting open source software and science communication. SIGDIUS Seminars, 14.06 2023, Virtual event.
- [15] 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.
- [16] 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.
- [17] P. Diehl. Recent developments in HPX and Octo-Tiger. Physics & Astronomy Colloquium, 23.1 2023, Baton Rouge, USA.
- [18] 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.
- [19] 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.
- [20] 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.
- [21] 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.
- [22] 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.
- [23] 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.
- [24] 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.
- [25] 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.
- [26] P. Diehl. Recent developments in HPX and Octo-Tiger. ISTI Seminar Series, 1.11 2022, Los Alamos, USA.

- [27] P. Diehl. A tale of two approaches for coupling nonlocal and local models. Continuum Mechanics Seminar (CMS), 10.11 2022, Lincoln, USA.
- [28] P. Diehl. Quantifying Overheads in Charm++ and HPX using Task Bench. Asynchronous Many-Task systems for Exascale (AMTE) 2022, 23.08 2022, Glasgow, UK.
- [29] 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.
- [30] P. Diehl. Quantifying Overheads in Charm++ and HPX using Task Bench. The Charm++ Workshop 2022, 19.10-20.10 2022, College Park , USA.
- [31] 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.
- [32] 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.
- [33] P. Diehl. Recent developments in HPX and Octo-Tiger. 19th Annual Workshop on Charm++ and Its Application, 18.10-19.10. 2021, Virtual event.
- [34] 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.
- [35] 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.
- [36] 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.
- [37] 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.
- [38] 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.
- [39] 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.
- [40] 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.

- [41] 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.
- [42] 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.
- [43] 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.
- [44] P. Diehl. An overview for coupling finite elements with peridynamics. International Congress on Industrial and Applied Mathematics, 15.07-19.07 2019, Valencia, Spain.
- [45] 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.
- [46] 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.
- [47] 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.
- [48] P. Diehl. A Review for Benchmark Experiments against Peridynamic Models. Nonlocal Methods in Fracture, 15.01-16.01 2018, Austin, USA.
- [49] 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.
- [50] P. Diehl. Modeling and Simulation of crack and fractures with peridynamics in brittle materials. HIM Junior Seminar, 08.02. 2017, Bonn, Germany.
- [51] P. Diehl. Experimental Validation of Elastic State Based Peridynamic for PMMA and epoxy materials. 14th U.S. National Congress on Computational Mechanics (USNCCM14), 17.07-20.07 2017, Montreal, Canada.
- [52] P. Diehl. Visualization of Fragments, Stress and Fracture Progression in Peridynamics. Isogeometric Analysis and Meshfree Methods, 10.10-12.10 2016, San Diego, USA.
- [53] P. Diehl. Numerical Validation of the bond-based Softening Model. SIAM Mathematical Aspects of Material Science 2016, 07.05-12.05 2016, Philadelphia, US.
- [54] 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.

- [55] 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.
- [56] 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.
- [57] 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.
- [58] 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.
- [59] 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.
- [60] 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.
- [61] 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.
- [62] 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.
- [63] 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.
- [64] 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] 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.
- [2] 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.

- [3] 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.
- [4] 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.