

Preprints

- [1] 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.
- [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, 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. Herрман, 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.
- [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.

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. Ilıc, 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.
- [8] 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.
- [9] 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.
- [10] 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.
- [11] 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, Cypress, 28 August – 1 September, 2023 Revised Selected Papers*, volume 14351 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2024.
- [12] 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, Cypress, 28 August – 1 September, 2023 Revised Selected Papers*, volume 14352 of *Lecture Notes in Computer Science (LNCS)*. Springer, 2024.

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.
- [3] 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.
- [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.
- [5] 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.
- [6] 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.
- [7] 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.
- [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.
- [9] 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.
- [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.
- [16] P. Diehl and S. Prudhomme. Coupling approaches for classical linear elasticity and bond-based peridynamic models. *Journal of Peridynamics and Nonlocal Modeling*, Mar 2022.
- [17] 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.
- [18] 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.
- [19] 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.
- [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.
- [21] P. K. Jha and P. Diehl. Nlmech: Implementation of finite difference/meshfree discretization of nonlocal fracture models. *Journal of Open Source Software*, 6(65):3020, 2021.
- [22] 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. Performance Measurements within Asynchronous Task-based Runtime Systems: A Double White Dwarf Merger as an Application. *Computing in Science & Engineering*, 2021.
- [23] P. Diehl, G. Daïß, 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.
- [24] 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.
- [25] 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.

- [26] 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.
- [27] 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.
- [28] 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.
- [29] G. Daiß, P. Amini, J. Biddiscombe, P. Diehl, J. Frank, K. Huck, H. Kaiser, D. Marcello, D. Pfander, and D. Pflüger. 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.
- [30] 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.
- [31] 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.
- [32] 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

- [1] N. Nader, P. Diehl, S. Brandt, and H. Kaiser. LLM & HPC: Benchmarking DeepSeek's Performance in High-Performance Computing Tasks. In S. Neuwirth, A. K. Paul, T. Weinzierl, and E. C. Carson, editors, *High Performance Computing*, pages 626–638, Cham, 2026. Springer Nature Switzerland.
- [2] 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.
- [3] 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.

- [4] A. Barai, K. Kamalakkannan, P. 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. In *Proceedings of the SC '25 Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC Workshops '25, page 1712–1722, New York, NY, USA, 2025. Association for Computing Machinery.
- [5] 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.
- [6] P. Diehl, P. Syskakis, G. Dais, S. R. Brandt, A. Kheirkhahan, S. Y. Singanaboina, D. Marcello, C. Taylor, J. Leidel, and H. Kaiser. Preparing for HPC on RISC-V: Examining Vectorization and Distributed Performance of an Astrophysics Application with HPX and Kokkos. In *SC24-W: Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis*, pages 1656–1665, Los Alamitos, CA, USA, Nov. 2024. IEEE Computer Society.
- [7] 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. Furlinger, 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.
- [8] 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.
- [9] N. Wu, I. Gonidelis, S. Liu, Z. Fink, N. Gupta, K. Mohammadiporshokoooh, 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.
- [10] 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.
- [11] P. Diehl, G. Dais, K. Huck, D. Marcello, S. Shiber, H. Kaiser, and D. Pflüger. 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.

- [12] 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.
- [13] 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*, IWOCCL '23, New York, NY, USA, 2023. Association for Computing Machinery.
- [14] 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.
- [15] 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.
- [16] 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.
- [17] 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.
- [18] 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.
- [19] 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*, IWOCCL'19, pages 13:1–13:10, New York, NY, USA, 2019. ACM.
- [20] 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.
- [21] R. Tohid, B. Wagle, S. Shirzad, P. Diehl, A. Serio, A. Kheirkhahan, P. Amini, K. Williams, K. Isaacs, K. Huck, S. Brandt, and H. Kaiser. Asynchronous Execution of Python Code on Task-Based Runtime Systems. In *2018 IEEE/ACM 4th International Workshop on Extreme Scale Programming Models and Middleware (ESPM2)*, pages 37–45, Nov 2018.

- [22] P. Diehl, M. Seshadri, T. Heller, and H. Kaiser. Integration of CUDA Processing within the C++ Library for Parallelism and Concurrency (HPX). In *2018 IEEE/ACM 4th International Workshop on Extreme Scale Programming Models and Middleware (ESPM2)*, pages 19–28, Nov 2018.
- [23] T. Heller, P. Diehl, Z. Byerly, J. Biddiscombe, and H. Kaiser. HPX – An open source C++ Standard Library for Parallelism and Concurrency. In *Proceedings of OpenSuCo 2017, Denver, Colorado USA, November 2017 (OpenSuCo 17)*, page 5, 2017.
- [24] P. Diehl, M. Bußler, D. Pflüger, S. Frey, T. Ertl, F. Sadlo, and M. A. Schweitzer. Extraction of Fragments and Waves After Impact Damage in Particle-Based Simulations. In M. Griebel and M. A. Schweitzer, editors, *Meshfree Methods for Partial Differential Equations VIII*, pages 17–34, Cham, 2017. Springer International Publishing.
- [25] T. Heller, H. Kaiser, P. Diehl, D. Fey, and M. A. Schweitzer. Closing the Performance Gap with Modern C++. In M. Tauber, B. Mohr, and J. M. Kunkel, editors, *High Performance Computing: ISC High Performance 2016 International Workshops, ExaComm, E-MuCoCoS, HPC-IODC, IXPUG, IWOPH, P³MA, VHPC, WOPSSS, Frankfurt, Germany, June 19–23, 2016, Revised Selected Papers*, volume 9945 of *Lecture Notes in Computer Science*, pages 18–31. Springer International Publishing, 2016.
- [26] P. Diehl and M. A. Schweitzer. Simulation of wave propagation and impact damage in brittle materials using peridynamics. In M. Mehl, M. Bischoff, and M. Schäfer, editors, *Recent Trends in Computational Engineering – CE2014*, volume 105 of *Lecture Notes in Computational Science and Engineering*, pages 251–265. Springer, 2015.
- [27] F. Franzelin, P. Diehl, and D. Pflüger. Non-intrusive Uncertainty Quantification with Sparse Grids for Multivariate Peridynamic Simulations. In M. Griebel and M. A. Schweitzer, editors, *Meshfree Methods for Partial Differential Equations VII*, volume 100 of *Lecture Notes in Computational Science and Engineering*, pages 115–143. Springer International Publishing, 2014.
- [28] P. Diehl and M. A. Schweitzer. Efficient neighbor search for particle methods on GPUs. In M. Griebel and M. A. Schweitzer, editors, *Meshfree Methods for Partial Differential Equations VII*, volume 100 of *Lecture Notes in Computational Science and Engineering*, pages 81–95. Springer, 2014.

Short papers

- [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.
- [3] 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.

- [4] K. Schatz, C. Müller, P. Gralka, M. Heinemann, A. Straub, C. Schulz, M. Braun, T. Rau, M. Becher, P. Diehl, et al. Visual Analysis of Structure Formation in Cosmic Evolution. In *2019 IEEE Scientific Visualization Conference (SciVis)*, pages 33–41. IEEE, 2019.

Technical reports

- [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.
- [4] I. P. Demeshko, P. Diehl, B. Adelstein-Lelbach, R. Buch, H. Kaiser, L. S. Kale, Z. Khatami, A. Koniges, and S. Shirzad. TBAA20: Task-Based Algorithms and Applications. Technical Report LA-UR-21-20928, Los Alamos National Laboratory, 2021.
- [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. Mehlinger. 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, 19.06-22.06 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.