

Daniel Nichols

Sidney Fernbach Postdoctoral Fellow, Lawrence Livermore National Laboratory

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Interested in leveraging AI to advance scientific computing.

Research and Professional Experience

- 2025–present **Sidney Fernbach Postdoctoral Fellow**, Lawrence Livermore National Laboratory
- 2020–2025 **Graduate Research Assistant**, University of Maryland, College Park
- Summers **Research Assistant**, Lawrence Livermore National Laboratory
- 2022–2024
- 2018–2020 **Undergraduate Research Assistant**, Innovative Computing Laboratory and Joint Institute for Computer Science, Knoxville
- Summer 2019 **Research Assistant**, Joint Institute for Computer Science REU, Knoxville

Education

- 2020–2025 **Ph.D., Computer Science**, University of Maryland, College Park, USA
Advisor: Abhinav Bhatele
Thesis: On Learning Parallel Code and System Behaviors Across Modalities
- 2017–2020 **B.S., Computer Science**, University of Tennessee, Knoxville, USA

Awards and Honors

- 2025 Sidney Fernbach Fellow at LLNL
- 2024 ACM-IEEE CS George Michael Memorial HPC Fellowship
- 2024 HPDC '24 Student Travel Grant
- 2024 ICPP IPDPS '24 Student Travel Grant
- 2023 Outstanding Graduate Assistant; *top 2% of graduate assistants university wide*
- 2021 GRFP Honorable Mention
- 2020 Dean's Fellowship, University of Maryland
- 2020 Summa Cum Laude, University of Tennessee
- 2017–2020 Dean's List, University of Tennessee
- 2017–2020 UT Volunteer Scholarship
- 2019 Herbert & Lillian Duggan Scholarship
- 2019 Harlan D. Mills Scholarship
- 2018 Edgar Wyman Mccall Scholarship
- 2017 Frederick T. Bonham Scholarship
- 2017 Henry, Robert, & Velma Scholarship

Professional Service

AI4Dev '25 Invited Panelist
SCI '25 Technical Program Committee
AI4Dev '25 Workshop Technical Program Committee
ICPP '25 Technical Program Committee
SC '25 Technical Program Committee
SC '25 Tutorials Committee
ISC '25 LLM4HPC Workshop Co-Organizer
SC '24 BoF Organizer and Session Leader: Towards integrating llms in hpc software
IEEE Cluster Conference 2022, Web Co-Chair
IEEE TPDS Reviewer (x3)
Reviews for HPDC, SC, IPDPS

Software Projects

Personal Projects

Slurm Dashboard	VSCode extension for interacting with the slurm workload manager
Performance Profile Viewer	VSCode extension for viewing and analyzing performance profiles
CSScholar	Computer science publication data dashboard
Research Projects	
ParEval	Parallel code generation benchmark for LLMs
MagmaDNN	High performance deep learning framework

Teaching Experience

- 2025 Systems for Machine Learning, UMD CMSC828G (designed and taught grad course)
2021–2024 CUDA Lectures for UMD Intro to Parallel Computing
2019 Teaching Assistant for UTK Data Structures and Algorithms

Publications, Talks, & Reports

Publications

- [1] Aman Chaturvedi*, **Daniel Nichols*** (* contributed equally), Siddharth Singh, and Abhinav Bhatele. Hpc-coder-v2: Studying code llms across low-resource parallel languages. In *ISC High Performance 2025 Research Paper Proceedings (40th International Conference)*, Jun 2025. **29% Acceptance Rate.**
- [2] Keita Teranishi, Harshitha Menon, William F. Godoy, Prasanna Balaprakash, David Bau, Tal Ben-Nun, Abhinav Bhatele, Franz Franchetti, Michael Franusich, Todd Gamblin, Giorgis Georgakoudis, Tom Goldstein, Arjun Guha, Steven E. Hahn, Costin Iancu, Zheming Jin, Terry Jones, Tze Meng Low, Het Mankad, Narasinga Rao Miniskar, Mohammad Alaul Haque Monil, **Daniel Nichols**, Konstantinos Parasyris,

- Swaroop Pophale, Pedro Valero-Lara, Jeffrey S. Vetter, Samuel Williams, and Aaron Young. Leveraging ai for productive and trustworthy HPC software: Challenges and research directions. In *Proceedings of the First International Workshop on Foundational Large Language Models Advances for HPC (LLM4HPC 2025)*, LLM4HPC '25, June 2025. LLM4HPC 2025, co-located with ISC High Performance 2025.
- [3] Joshua H. Davis, **Daniel Nichols**, Ishan Khillan, and Abhinav Bhatele. Pareval-repo: A benchmark suite for evaluating llms with repository-level hpc translation tasks. In *Proceedings of the 54th International Conference on Parallel Processing*, ICPP '25, New York, NY, USA, 2025. Association for Computing Machinery.
 - [4] Aakash Raj Dhakal, Tanzima Z. Islam, Arunavo Dey, Tapasya Patki, **Daniel Nichols**, Abhinav Bhatele, and Jae-Seung Yeom. xamm: “attention” to details improve cross-platform prediction accuracy. In *2025 IEEE 25th International Symposium on Cluster, Cloud and Internet Computing (CCGrid)*, 2025.
 - [5] Srivishnu Pyda, **Daniel Nichols**, and Abhinav Bhatele. The shortcomings of code llms in modeling code properties. In *Proceedings of the 2025 IEEE/ACM International Workshop on Large Language Models for Code (LLM4Code 2025)*, LLM4Code '25, pages 193–199, 2025.
 - [6] **Daniel Nichols**, Harshitha Menon, Todd Gamblin, and Abhinav Bhatele. A probabilistic approach to selecting build configurations in package managers. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '24, New York, NY, USA, November 2024. Association for Computing Machinery. **22.7% Acceptance Rate**.
 - [7] **Daniel Nichols**, Joshua H. Davis, Zhaojun Xie, Arjun Rajaram, and Abhinav Bhatele. Can large language models write parallel code? In *Proceedings of the 33rd International Symposium on High-Performance Parallel and Distributed Computing*, HPDC '24, New York, NY, USA, June 2024. Association for Computing Machinery. **17% Acceptance Rate**.
 - [8] **Daniel Nichols**, Alexander Movsesyan, Jae-Seung Yeom, Abhik Sarkar, Daniel Milroy, Tapasya Patki, and Abhinav Bhatele. Predicting cross-architecture performance of parallel programs. In *Proceedings of the IEEE International Parallel & Distributed Processing Symposium*, IPDPS '24. IEEE Computer Society, May 2024. **16.6% First-Round Acceptance Rate, 26.1% Overall Acceptance Rate**.
 - [9] Harshita Menon*, **Daniel Nichols*** (* contributed equally), Abhinav Bhatele, and Todd Gamblin. Learning to predict and improve build successes in package ecosystems. In *International Conference on Mining Software Repositories*, MSR '24, April 2024. **26.3% Acceptance Rate**.
 - [10] **Daniel Nichols**, Aniruddha Marathe, Harshitha Menon, Todd Gamblin, and Abhinav Bhatele. Hpc-coder: Modeling parallel programs using large language models. In *ISC High Performance 2024 Research Paper Proceedings (39th International Conference)*, pages 1–12, 2024. **30% Acceptance Rate**.

- [11] Arunavo Dey, Aakash Dhakal, Tanzima Z. Islam, Jae-Seung Yeom, Tapasya Patki, **Daniel Nichols**, Alexander Movsesyan, and Abhinav Bhatele. Relative performance prediction using few-shot learning. In *2024 IEEE 48th Annual Computers, Software, and Applications Conference (COMPSAC)*, pages 1764–1769, 2024.
- [12] Joshua H. Davis, Justin Shafner, **Daniel Nichols**, Nathan Grube, Pino Martin, and Abhinav Bhatele. Porting a computational fluid dynamics code with amr to large-scale gpu platforms. In *Proceedings of the IEEE International Parallel & Distributed Processing Symposium, IPDPS '23*, pages 602–612. IEEE Computer Society, May 2023. **25.7% Acceptance Rate**.
- [13] **Daniel Nichols**, Aniruddha Marathe, Kathleen Shoga, Todd Gamblin, and Abhinav Bhatele. Resource utilization aware job scheduling to mitigate performance variability. In *Proceedings of the IEEE International Parallel & Distributed Processing Symposium, IPDPS '22*, pages 335–345. IEEE Computer Society, May 2022. **9.7% First-Round Acceptance Rate, 25.9% Overall Acceptance Rate**.
- [14] Rick Archibald, Edmond Chow, Eduardo F. D'Azevedo, Jack J. Dongarra, Markus Eisenbach, Rocco Febbo, Florent Lopez, **Daniel Nichols**, Stanimire Tomov, Kwai Wong, and Junqi Yin (Authors Alphabetical). Integrating deep learning in domain sciences at exascale. In *SMC 2020*, volume 1315 of *Communications in Computer and Information Science*. Springer, 2020.
- [15] **Daniel Nichols**, Nathalie-Sofia Tomov, Frank Betancourt, Stanimire Tomov, Kwai Wong, and Jack Dongarra. Magmadnn: Towards high-performance data analytics and machine learning for data-driven scientific computing. In *High Performance Computing*, pages 490–503, Cham, 2019. Springer International Publishing.
- [16] **Daniel Nichols**, Kwai Wong, Stan Tomov, Lucien Ng, Sihan Chen, and Alex Gessinger. Magmadnn: Accelerated deep learning using magma. *PEARC '19*, New York, NY, USA, 2019. ACM.
- [17] Frank Betancourt, Kwai Wong, Efosa Asemota, Quindell Marshall, **Daniel Nichols**, and Stanimire Tomov. opendiel: A parallel workflow engine and data analytics framework. In *Proceedings of the Practice and Experience in Advanced Research Computing on Rise of the Machines (Learning)*, *PEARC '19*, New York, NY, USA, 2019. ACM.

Pre-Prints

- [18] **Daniel Nichols**, Konstantinos Parasyris, Charles Jekel, Abhinav Bhatele, and Harshitha Menon. Integrating performance tools in model reasoning for gpu kernel optimization, 2025. arXiv preprint arXiv:2510.17158.
- [19] **Daniel Nichols**, Konstantinos Parasyris, Harshitha Menon, Brian R. Bartoldson, Giorgis Georgakoudis, Tal Ben-Nun, and Abhinav Bhatele. Modeling code: Is text all you need?, 2025. arXiv preprint arXiv:2507.11467.
- [20] Caetano Melone, **Daniel Nichols**, Konstantinos Parasyris, Todd Gamblin, and Harshitha Menon. Llms as packagers of hpc software, 2025. arXiv preprint arXiv:2511.05626.

- [21] **Daniel Nichols**, Pranav Polasam, Harshitha Menon, Aniruddha Marathe, Todd Gamblin, and Abhinav Bhatele. Performance-aligned llms for generating fast code, 2024. arXiv. cs.DC. 2404.18864.
- [22] Onur Cankur, Aditya Tomar, **Daniel Nichols**, Connor Scully-Allison, Katherine E. Isaacs, and Abhinav Bhatele. Automated programmatic performance analysis of parallel programs, 2024. arXiv. cs.DC. 2401.13150.
- [23] **Daniel Nichols***, Siddharth Singh* (* contributed equally), Shu-Huai Lin, and Abhinav Bhatele. A survey and empirical evaluation of parallel deep learning frameworks, 2022. arXiv. cs.LG. 2111.04949.

Talks & Tutorials

- [24] **Daniel Nichols**. Keynote: Role of ai in hpc software development. ESwML Workshop at EuroSys/ASPLOS 2025, March 2025.
- [25] **Daniel Nichols**. Towards integrating llms in hpc software development. SC24 BoF, Session Leader, November 2024.
- [26] **Daniel Nichols**. Large language models for parallel and hpc code. Talk at PASC 2024 in *Machine Learning Support for the Lifetime of Software* Minisymposia, June 2024.
- [27] Abhinav Bhatele, Siddharth Singh, and **Daniel Nichols**. Distributed training of deep neural networks. ISC High Performance 2024 Tutorials (39th International Conference), May 2024.
- [28] **Daniel Nichols**. Evaluating the capability of large language models for parallel and high performance code generation. The 21st Annual Workshop on Charm++ and Its Applications, 2024.
- [29] **Daniel Nichols**. Probabilistic package builds: Guiding spack's concretizer with predicted build outcomes. PackagingCon, 2023.
- [30] Kwai Wong, Stanimire Tomov, **Daniel Nichols**, Rocco Febbo, and Xianfeng Ma. How to build your own deep neural network framework. Tutorial at PEARC, 2020.

Posters

- [31] Aman Chaturvedi, **Daniel Nichols**, Siddharth Singh, and Abhinav Bhatele. Creating code llms for hpc: It's llms all the way down. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '24, Nov 2024.
- [32] **Daniel Nichols**, Aniruddha Marathe, Harshitha Menon, Todd Gamblin, and Abhinav Bhatele. Modeling parallel programs using large language models. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '23, Nov 2023.

- [33] **Daniel Nichols**, Dilan Gunawardana, Aniruddha Marathe, Todd Gamblin, and Abhinav Bhatele. Noncommittal commits: Predicting performance slowdowns in version control history. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '22, November 2022.
- [34] **Daniel Nichols**, Jae-Seung Yeom, and Abhinav Bhatele. Predicting cross-platform relative performance with deep generative models. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '22, November 2022.
- [35] Joshua Hoke Davis, Justin Shafner, **Daniel Nichols**, Nathan Grube, Pino Martin, and Abhinav Bhatele. Extreme-scale computational fluid dynamics with amr on gpus. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '22, November 2022.