Tyler H. Chang – CV

Mathematics and Computer Science Division, Argonne National Laboratory

@ tchang@anl.gov 9700 S. Cass Ave, Bldg. 240, Lemont, IL 60439



RESEARCH INTERESTS

Blackbox optimization, scientific machine learning, approximation theory, computational geometry, and scientific software



EDUCATION

Ph.D., May 2020, Computer Science, Virginia Polytechnic Institute & State University (Virginia Tech)

- Advisor: Layne Watson
- Dissertation: Mathematical Software for Multiobjective Optimization Problems

B.S., May 2016, Computer Science & Mathematics (double-major), Virginia Wesleyan University

• Summa cum laude; 2x ACM ICPC site champion; 8x Dean's list; 4x all-ODAC (conference) for varsity tennis



RESEARCH EXPERIENCE

Postdoctoral appointee: Argonne National Laboratory, MCS Division Jun 2020 - Present.

- Supervisor: Stefan Wild
- Designed and implemented a Python framework for building and deploying multiobjective optimization solvers
- Deployed solvers for particle accelerator design, autonomous material discovery, and neural-network architecture search
- Applied for grants, supervised interns, authored scientific papers, and represented Argonne at internat'l conferences

Aug 2016 - May 2020. Cunningham fellow: Virginia Tech, Dept. of Computer Science

- Designed parallel algorithms and software for predicive modeling, blackbox optimization, and computational geometry
- Applied solvers to model and tune HPC systems to control performance variability
- Published papers in academic journals and conferences

Jun 2019 - Dec 2019. SCGSR awardee: Argonne National Laboratory, MCS Division

Conducting research in multiobjective optimization software via DOE SCGSR program (see awards)

Feb 2016 - Aug 2016. Research assistant: Old Dominion University, Dept. of Computer Science

• Aided in parallelizing NASA's FUN3D CFD kernel on NVIDIA GPUs using CUDA and MPI

Dec 2015 - Jan 2016. Intern: US Army Research Labs, Computational Science Division Intern: US Army Research Labs, Computational Science Division May 2015 - Aug 2015.

Accelerating software for real-time optimal control (summer) & using AR technology for info viz (winter)

Dec 2014 - Jan 2015. Intern: US Army Research Labs, Guidance Technology Branch May 2014 - Aug 2014. Intern: US Army Research Labs, Guidance Technology Branch

• Using OpenCV for real-time sensing (summer) & developing software for embedded systems (winter)



AWARDS

2021.	Nominee for Outstanding Dissertation Award: Virginia Tech, Graduate School
2019.	Davenport Leadership Fellowship: Virginia Tech, College of Engineering
2018.	SCGSR Award: DOE Office of Science, Graduate Student Research (SCGSR) Program
2018.	Pratt Fellowship: Virginia Tech, College of Engineering
2017.	Pratt Fellowship: Virginia Tech, College of Engineering
2016.	Cunningham Doctoral Fellowship: Virginia Tech, Graduate School
2016.	Davenport Leadership Fellowship: Virginia Tech, College of Engineering
2016.	Outstanding Student in Computer Science & Mathematics: Virginia Wesleyan University



Publicly Available Software

4. 2023. ParMOO: Python library for parallel multiobjective simulation optimization. Release: 0.3.0

Devs: T. H. Chang (lead), S. M. Wild, and H. Dickinson¹ Primary Prog. Lang: Python 3

git: https://github.com/parmoo/parmoo

3. 2022. VTMOP: Solver for blackbox multiobjective optimization problems.

Devs: T. H. Chang (sole) Primary Prog. Lang: Fortran 2008

git: https://github.com/vtopt/VTMOP

2. 2020. **DelaunaySparse**: Interpolation via a sparse subset of the Delaunay triangulation.

Devs: T. H. Chang (lead) and T. C. H. Lux Primary Prog. Lang: Fortran 2003

git: https://github.com/vtopt/DelaunaySparse

1. 2019. QAML: Quantum annealing math library.

Devs: T. C. H. Lux (lead), T. H. Chang, and S. S. Tipirneni Primary Prog. Lang: Python 3

git: https://github.com/tchlux/qaml



PUBLICATIONS

Publications In-Press

1. M. Garg², **T. H. Chang**, and K. Raghavan. SF-SFD: Stochastic optimization of Fourier coefficients for space-filling designs. To appear in 2023 Winter Simulation Conference (WSC 2023). Preprint: https://arxiv.org/abs/2305.12043.

Publications Under Review

- 2. G. Chen, **T. H. Chang**, J. Power, and C. Jing. An integrated multi-physics optimization framework for particle accelerator design. Submitted to 2023 Winter Simulation Conference, Aug 2023.
- 1. **T. H. Chang** and S. M. Wild. Designing a framework for solving multiobjective simulation optimization problems. Submitted to INFORMS Journal on Computing, Jul 2023. Preprint: https://arxiv.org/abs/2304.06881.

Peer-Reviewed Journal Articles

- 10. 2023. T. C. H. Lux, L. T. Watson, **T. H. Chang**, and W. I. Thacker. Algorithm 1031: MQSI—Monotone quintic spline interpolation. *ACM Transactions on Mathematical Software* 49(1), Article 6, 17 pages. **doi:** 10.1145/3570157
- 9. 2023. **T. H. Chang** and S. M. Wild. ParMOO: a Python library for parallel multiobjective simulation optimization. *Journal of Open Source Software* 8(82), Article 4468, 5 pages. **doi:** 10.21105/joss.04468
- 8. 2023. N. Neveu, **T. H. Chang**, P. Franz, S. Hudson, and J. Larson. Comparison of multiobjective optimization methods for the LCLS-II photoinjector. *Computer Physics Communication* 283, Article 108566, 10 pages. **doi:** 10.1016/j.cpc.2022.108566
- 7. 2023. Y. Wang, L. Xu, Y. Hong, R. Pan, **T. H. Chang**, T. C. H. Lux, J. Bernard, L. T. Watson, and K. W. Cameron. Design strategies and approximation methods for high-performance computing variability management. *Journal of Quality Technology* 55(1), pp. 88–103. **doi:** 10.1080/00224065.2022.2035285
- 6. 2022. **T. H. Chang**, L. T. Watson, J. Larson, N. Neveu, W. I. Thacker, S. Deshpande, and T. C. H. Lux. Algorithm 1028: VTMOP: Solver for blackbox multiobjective optimization problems. *ACM Transactions on Mathematical Software* 48(3), Article 36, 34 pages. **doi:** 10.1145/3529258
- 5. 2021. L. Xu, T. C. H. Lux, **T. H. Chang**, B. Li, Y. Hong, L. T. Watson, A. R. Butt, D. Yao, and K. W. Cameron. Prediction of high-performance computing input/output variability and its application to optimization for system configurations. *Quality Engineering* 33(2), pp. 318–334. **doi:** 10.1080/08982112.2020.1866203
- 4. 2021. T. C. H. Lux, L. T. Watson, **T. H. Chang**, J. Bernard, B. Li, L. Xu, G. Back, A. R. Butt, K. W. Cameron, and Y. Hong. Interpolation of sparse high-dimensional data. *Numerical Algorithms* 88(1), pp. 281–313. doi: 10.1007/s11075-020-01040-2
- 3. 2020. **T. H. Chang**, L. T. Watson, T. C. H. Lux, A. R. Butt, K. W. Cameron, and Y. Hong. Algorithm 1012: DELAUNAYSPARSE: Interpolation via a sparse subset of the Delaunay triangulation in medium to high dimensions. *ACM Transactions on Mathematical Software* 46(4), Article 38, 20 pages. **doi:** 10.1145/3422818
- 2. 2020. L. Xu, Y. Wang, T. C. H. Lux, **T. H. Chang**, J. Bernard, B. Li, Y. Hong, K. W. Cameron, and L. T. Watson. Modeling I/O performance variability in high-performance computing systems using mixture distributions. *Journal of Parallel and Distributed Computing* 139, pp. 87–98. **doi:** 10.1016/j.jpdc.2020.01.005
- 1. 2019. **T. H. Chang**, T. C. H. Lux, and S. S. Tipirneni. Least-squares solutions to polynomial systems of equations with quantum annealing. *Quantum Information Processing* 18(12), Article 374, 17 pages. **doi:** 10.1007/s11128-019-2489-x

¹⁼ DOE SULI at Argonne in my supervision

²= NSF MSGI at Argonne in my supervision

Peer-Reviewed Conference Papers

- 13. 2023. **T. H. Chang**, J. R. Elias, S. M. Wild, S. Chaudhuri, and J. A. Libera. A framework for fully autonomous design of materials via multiobjective optimization and active learning: challenges and next steps. *In 11th Intl. Conf. on Learning Representation (ICLR 2023), Workshop on Machine Learning for Materials (ML4Materials*). Kigali, Rwanda. **url:** https://openreview.net/forum?id=8KJS7RPjMqG
- 12. 2020. **T. H. Chang**, J. Larson, and L. T. Watson. Multiobjective optimization of the variability of the high-performance Linpack solver. *In Proc. 2020 Winter Simulation Conference (WSC 2020)*, pp. 3081–3092. Orlando, FL, USA. **doi:** 10.1109/WSC48552.2020.9383875
- 11. 2020. **T. H. Chang**, J. Larson, L. T. Watson, and T. C. H. Lux. Managing computationally expensive blackbox multiobjective optimization problems with libEnsemble. *In Proc. 2020 Spring Simulation Conference (SpringSim '20)*, Article 31, 12 pages. Fairfax, VA, USA. **doi:** 10.22360/springsim.2020.hpc.001
- 10. 2020. T. C. H. Lux, L. T. Watson, **T. H. Chang**, L. Xu, Y. Wang, and Y. Hong. An algorithm for constructing monotone quintic interpolating splines. *In Proc. 2020 Spring Simulation Conference (SpringSim '20)*, Article 33, 12 pages. Fairfax, VA, USA. **doi:** 10.22360/springsim.2020.hpc.003
- 9. 2020. T. C. H. Lux and **T. H. Chang**. Analytic test functions for generalizable evaluation of convex optimization techniques. In Proc. IEEE SoutheastCon 2020, 8 pages. Raleigh, NC, USA. doi: 10.1109/SoutheastCon44009.2020.9368254
- 8. 2020. T. C. H. Lux, L. T. Watson, **T. H. Chang**, L. Xu, Y. Wang, J. Bernard, Y. Hong, and K. W. Cameron. Effective nonparametric distribution modeling for distribution approximation applications. *In Proc. IEEE SoutheastCon 2020*, 6 pages. Raleigh, NC, USA. **doi:** 10.1109/SoutheastCon44009.2020.9368295
- 7. 2018. **T. H. Chang**, L. T. Watson, T. C. H. Lux, S. Raghvendra, B. Li, L. Xu, A. R. Butt, K. W. Cameron, and Y. Hong. Computing the umbrella neighbourhood of a vertex in the Delaunay triangulation and a single Voronoi cell in arbitrary dimension. *In Proc. IEEE SoutheastCon 2018*, 8 pages. St. Petersburg, FL, USA. **doi:** 10.1109/SECON.2018.8479003
- 6. 2018. T. C. H. Lux, L. T. Watson, **T. H. Chang**, J. Bernard, B. Li, X. Yu, L. Xu, G. Back, A. R. Butt, K. W. Cameron, Y. Hong, and D. Yao. Nonparametric distribution models for predicting and managing computational performance variability. *In Proc. IEEE SoutheastCon 2018*, 7 pages. St. Petersburg, FL, USA. **doi:** 10.1109/SECON.2018.8478814
- 5. 2018. **T. H. Chang**, L. T. Watson, T. C. H. Lux, J. Bernard, B. Li, L. Xu, G. Back, A. R. Butt, K. W. Cameron, and Y. Hong. Predicting system performance by interpolation using a high-dimensional Delaunay triangulation. *In Proc. 2018 Spring Simulation Conference (SpringSim '18)*, Article 2, 12 pages. Baltimore, MD, USA. **doi:** 10.22360/springsim.2018.hpc.003
- 4. 2018. T. C. H. Lux, L. T. Watson, **T. H. Chang**, J. Bernard, B. Li, L. Xu, G. Back, A. R. Butt, K. W. Cameron, and Y. Hong. Predictive modeling of I/O characteristics in high performance computing systems. *In Proc. 2018 Spring Simulation Conference (SpringSim '18)*, Article 8, 10 pages. Baltimore, MD, USA. **doi:** 10.22360/springsim.2018.hpc.009
- 3. 2018. **T. H. Chang**, L. T. Watson, T. C. H. Lux, B. Li, L. Xu, A. R. Butt, K. W. Cameron, and Y. Hong. A polynomial time algorithm for multivariate interpolation in arbitrary dimension via the Delaunay triangulation. *In Proc. 2018 ACM Southeast Conference (ACMSE '18)*, Article 12, 8 pages. Richmond, KY, USA. **doi:** 10.1145/3190645.3190680
- 2. 2018. T. C. H. Lux, L. T. Watson, **T. H. Chang**, J. Bernard, B. Li, X. Yu, L. Xu, G. Back, A. R. Butt, K. W. Cameron, D. Yao, and Y. Hong. Novel meshes for multivariate interpolation and approximation. *In Proc. 2018 ACM Southeast Conference (ACMSE '18)*, Article 13, 7 pages. Richmond, KY, USA. **doi:** 10.1145/3190645.3190687
- 1. 2017. C. Raghunath, T. H. Chang, L. T. Watson, M. Jrad, R. K. Kapania, and R. M. Kolonay. Global deterministic and stochastic optimization in a service oriented architecture. *In Proc. 2017 Spring Simulation Conference (SpringSim '17)*, Article 7, 12 pages. Virginia Beach, VA, USA. doi: 10.22360/springsim.2017.hpc.023

Technical Reports and Dissertations

- 4. 2023. **T. H. Chang**, S. M. Wild, and H. Dickinson¹. *ParMOO: Python library for parallel multiobjective simulation optimization*. Technical Report Version 0.3.0. Argonne National Laboratory, Lemont, Illinois, USA. **url:** https://parmoo.readthedocs.io/_/downloads/en/latest/pdf/
- 3. 2020. A. K. Gillette and **T. H. Chang**. *ALGORITHMS: assessing latent space dimension by Delaunay loss*. Technical Report LLNL-CONF-814930. Lawrence Livermore National Laboratory, Livermore, California, USA. **url:** https://www.osti.gov/servlets/purl/1756748
- 2. 2020. T. H. Chang. *Mathematical software for multiobjective optimization problems*. Ph.D. Dissertation. Department of Computer Science, Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, VA, USA. Dept. of Computer Science Nominee for Outstanding Dissertation Award. url: http://hdl.handle.net/10919/98915
- 1. 2016. **T. H. Chang**. *GPU saturation for multiple matrix-vector multiplications*. Bachelor's Thesis. Department of Computer Science, Virginia Wesleyan University, Virginia Beach, VA, USA.



TALKS AND PRESENTATIONS

Invited Conference Talks

5. Jun 2023. Exploiting structures in multiobjective simulation optimization problems. *SIAM Conference on Optimization (OP 2023)*, Seattle, WA, USA.

- 4. Mar 2023. ParMOO: a Python library for parallel multiobjective simulation optimization. *SIAM Conference on Computational Science and Engineering (CSE 2023)*, Amsterdam, Netherlands.
- 3. Sep 2022. Geometric considerations when surrogate modeling. *SIAM Conference on Mathematics of Data Science (MDS 2022)*, San Diego, CA, USA.
- 2. Jul 2021. Surrogate modeling of simulations for multiobjective optimization applications. *SIAM Conference on Optimization* (*OP 2021*), virtual event.
- 1. Mar 2021. Computing sparse subsets of the Delaunay triangulation in high-dimensions for interpolation and graph problems. SIAM Conference on Computational Science and Engineering (CSE 2021), virtual event.

Seminars and Colloquia

- 4. July 2023. Toward interpretable machine learning via Delaunay interpolation challenges and next steps. *Argonne National Laboratory, LANS Seminar Series*, Lemont, IL, USA.
- 3. Feb 2020. Algorithms and software for Delaunay interpolation and multiobjective optimization. *Sandia National Laboratory, Wind Energy Technology Division Seminar*, virtual event.
- 2. Feb 2020. Algorithms and software for Delaunay interpolation and multiobjective optimization. *Argonne National Laboratory, Mathematics and Computer Science Division Seminar*, Lemont, IL, USA.
- 1. Jan 2020. Algorithms and software for Delaunay interpolation and multiobjective optimization. *Sandia National Laboratory, Center for Computing Research Seminar*, Albuquerque, NM, USA.

Tutorials and Guest Lectures

- 2. Oct 2022. An introduction to multiobjective simulation optimization with ParMOO. *The Science Academy, Science Circle Cohort, quest speaker*, virtual event. Recording: https://www.youtube.com/watch?v=gqha8urlehm.
- 1. May 2022. An introduction to multiobjective simulation optimization with ParMOO. *Univeristy of Chicago, Pritzker School of Molecular Engineering, guest lecture*, virtual event.

Contributed Talks

- 10. Jul 2022. ParMOO: a parallel framework for multiobjective simulation optimization problems. Seventh International Conference on Continuous Optimization (ICCOPT 2022), Bethlehem, PA, USA.
- 9. Dec 2020. Multiobjective optimization of the variability of the high-performance Linpack solver. 2020 Winter Simulation Conference (WSC 2020), virtual event.
- 8. May 2020. Managing computationally expensive blackbox multiobjective optimization problems with libEnsemble. *Spring Simulation Conference (SpringSim '20)*, virtual event.
- 7. Aug 2019. A surrogate for local optimization using Delaunay triangulations. *Sixth International Conference on Continuous Optimization (ICCOPT 2019)*, Berlin, Germany.
- 6. Apr 2018. Computing the umbrella neighbourhood of a vertex in the Delaunay triangulation and a single Voronoi cell in arbitrary dimension. *IEEE SoutheastCon 2020*, St. Petersburg, FL, USA.
- 5. Apr 2018. Nonparametric distribution models for predicting and managing computational performance variability. *IEEE SoutheastCon 2020*, St. Petersburg, FL, USA.
- 4. Mar 2018. A polynomial time algorithm for multivariate interpolation in arbitrary dimension via the Delaunay triangulation. *ACM Southeast Conference (ACMSE '18)*, Richmond, KY, USA.
- 3. Apr 2017. Global deterministic and stochastic optimization in a service oriented architecture. *Spring Simulation Conference (SpringSim '17)*, Virginia Beach, VA, USA.
- 2. Apr 2016. GPU saturation for multiple matrix-vector multiplications. *Virginia Wesleyan College, Undergraduate Research Symposium*, Virginia Beach, VA, USA.
- 1. Apr 2014. The new Mastermind. Virginia Wesleyan College, Undergraduate Research Symposium, Virginia Beach, VA, USA.

Posters and Lightning Talks

- 10. May 2023. A framework for fully autonomous design of experiments via active learning and multiobjective optimization: challenges and next steps (poster). 11th Intl. Conf. on Learning Representation (ICLR 2023), Workshop on Machine Learning for Materials (ML4Materials), Kigali, Rwanda.
- 9. Oct 2022. ParMOO: a Python library for parallel multiobjective simulation optimization (lightning talk). FASTMath All-Hands Meeting, Denver, CO, USA.
- 8. May 2022. ParMOO: parallel multiobjective optimization in python (poster). *The Argonne, Chicago, Michigan, Northwestern, Toyota, Wisconsin (ACMNTW) Workshop on Optimization and Machine Learning,* Evanston, IL, USA.
- 7. Nov 2020. Multiobjective optimization of simulations with PARMOO (lightning talk). *Argonne Postdoctoral Research and Career Symposium*, virtual event.
- 6. Feb 2020. VarSys: managing variability for high performance computers, cloud computing systems, and computer security (poster). *Virginia Tech, Graduate Student Recruitment Weekend, Lab Poster Session*, Blacksburg, VA, USA.
- 5. Aug 2019. An adaptive weighting scheme for multiobjective optimization (lightning talk). *Argonne National Laboratory, LANS SASSy Seminar Series*, Lemont, IL, USA.
- 4. Mar 2019. VarSys: managing variability for high performance computers, cloud computing systems, and computer security (poster). *Virginia Tech, Graduate Student Recruitment Weekend, Lab Poster Session*, Blacksburg, VA, USA.

- 3. Sep 2018. A polynomial time algorithm for multivariate interpolation in arbitrary dimension via the Delaunay triangulation (lightning talk). *Virginia Tech, CS GSC: Lightning Talks*, Blacksburg, VA, USA.
- 2. Mar 2018. VarSys: managing variability for high performance computers, cloud computing systems, and computer security (poster). *Virginia Tech, Graduate Student Recruitment Weekend, Lab Poster Session*, Blacksburg, VA, USA.
- 1. Aug 2014. Real-time target identification in Matlab with OpenCV (poster). *US Army Research Laboratories, Summer Student Poster Symposium*, Aberdeen, MD, USA.



GRANTS

Current

1. Mar 2023 - Sep 2023. **Co-PI** (PI: G. Chen (ANL)), \$50K (my share: \$25K). *A Scalable Multi-Physics Optimization Framework for Particle Accelerator Design*, institutional award (3 pages + appendices). ANL LDRD: 2023 LDRD Seed (LDRD 2023-0246).

Completed

1. Jun 2019 - Dec 2019. **Primary awardee** (Advisors: J. Larson (ANL) and L. Watson (VT)), \$3K/mo stipend. *An Adaptive Weighting Scheme for Multiobjective Optimization*, DOE award for PhD students (3 pages + appendices). DOE SCGSR/ASCR: SCGSR Program 2018 Solicitation 2 (DE-SC0014664).



ADVISING

Jun 2022 - Aug 2022. Manisha Garg (Urbana-Champaign), NSF MSGI at Argonne

• Project: Model agnostic sampling techniques for generating design-of-experiments

Jun 2022 - Aug 2022. Hyrum Dickinson (Urbana-Champaign), DOE SULI at Argonne

• Project: Visualization tools for the ParMOO library



TEACHING EXPERIENCE

Jan 2022 - Present. Adjunct Professor: College of DuPage, Dept. of Computer and Info. Science

- Summer 2023. CIS 2531: Introduction to Python Programming (in-person)
- Spring 2022. CIS 2531: Introduction to Python Programming (online)

Jan 2020 - May 2020. Instructor of Record: Virginia Tech, Dept. of Computer Science

• Spring 2020. CS 3114: Data Structures and Algorithms (half in-person, half online)

Jan 2013 - Dec 2015. Subject Tutor: Virginia Wesleyan University, Learning Center

Spring 2013 - Fall 2014. All undergraduate courses in calculus, computer science, and statistics



Professional Services and Activities

Journal Referee

- INFORMS Journal on Computing (2023–Present)
- ACM Transactions on Mathematical Software (2021–Present)
- Quantum Information Processing (2021–Present)
- The Visual Computer Journal (2021)
- MDPI: Mathematical and Computer Applications (2021)
- Journal of Machine Learning Research (2019)

Conference Reviewer

- Int. Congress on Industrial and Applied Mathematics (ICIAM) 2023
- Int. Conf. for HPC, Networking, Storage, and Analysis (Supercomputing) 2021
- IEEE SoutheastCon 2020
- IEEE SoutheastCon 2019
- IEEE SoutheastCon 2018

Minisymposium Organizer

- SIAM Conference on Optimization (2021)
- SIAM Conference on Computational Science and Engineering (2021)

Professional Membership

- ACM (2015-Present)
- SIAM (2016–Present)
- MOS (2022–Present)



INSTITUTIONAL SERVICES

Argonne

Nov 2022 - Present. Organizing Committee: FASTMath Institute Seminar Series

Dec 2022 - Jan 2023. Hiring Committee: MCS Division

Oct 2022 - Dec 2022. Technical Reviewer: Sustainable Research Pathways

Mar 2022 - Apr 2022. Red Team Reviewer: ASCR Pre-proposals

Virginia Tech

Aug 2017 - May 2020. Founding Member: Computer Science Graduate Counsel

Dec 2018 - Mar 2019. Lead Student Organizer: Computer Science Graduate Preview Weekend



POST-DISSERTATION COURSES AND CERTIFICATIONS

Jul 2022. Distributionally Robust Optimization, ICCOPT Summer School

Jul 2022. Mathematical Optimization in Julia with JuMP, ICCOPT Summer School

Aug 2020. Probability, Geometry, and Computation in High Dimensions Boot Camp, Simons Institute Workshop

Jul 2020. Advanced Python, LinkedIn Learning



TECHNICAL SKILLS

Languages: Python, Fortran, C/C++, Java, Matlab

OS: MacOS, Unix/Linux

Markup: HTML/CSS, GNU Make, TeX/LaTeX/bibTeX

Libraries: numpy, pandas, scipy, matplotlib, keras, sklearn, MPI, OpenMP, CUDA, BLAS, LAPACK

Tools/Frameworks: pytest, sphinx, slurm, CI/CD, GitHub Actions, GitFlow