

Tyler H. Chang

Argonne National Laboratory
Mathematics & Computer Science (MCS) Division
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Website: <https://thchang.github.io>
GitHub: <https://github.com/thchang>

Interests

Numerical optimization, machine learning, computational geometry, analysis of algorithms, and scientific software

Education

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

- *Thesis: Math. Softw. for Multiobjective Optimization Problems; Outstanding Dissertation Award nominee*

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

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

- Designed and implemented a Python framework for building and deploying multiobjective optimization solvers
- Deployed optimization solvers for particle accelerator design, material discovery (see projects), and DFT modeling

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

- Designed parallel algorithms and software for predictive modeling, blackbox optimization, and computational geometry
- Applied solvers to model and tune HPC systems (see projects) to control performance variability

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

May 2015 - Aug 2015. **Intern: US Army Research Labs**, Computational Science Division

- 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)

Notable Projects

Oct 2021 - Present. **Self-Driving Labs, automating material discovery via continuous-flow chemistry**

- Discovered ideal mixtures/settings to produce the battery electrolyte 2,2,2-TFMC in a continuous-flow reactor (CFR)
- Used a Bayesian/active learning framework to steer an automated feed, CFR, and NMR in a user-free feedback loop

Sep 2016 - May 2020. **The VarSys Project, NSF-funded study of performance variability in HPC systems**

- Member of the math and algorithms team on an interdisciplinary project to model and control performance variability
- Tuned the Linpack solver on the leadership-class HPC Bebop, resulting in a 3x reduction in performance variability

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

2023. **ParMOO**: Python library for parallel multiobjective simulation optimization. Release: 0.2.0
Devs: **T. H. Chang** (lead), S. M. Wild, and H. Dickinson Primary Prog. Lang: Python 3
git: <https://github.com/parmoo/parmoo>

2022. **VTMOP**: Solver for blackbox multiobjective optimization problems.
Devs: **T. H. Chang** (sole) Primary Prog. Lang: Fortran 2008
git: <https://github.com/vtopt/VTMOP>

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>

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

T. C. H. Lux, L. T. Watson, **T. H. Chang**, and W. I. Thacker. Algorithm XXXX: MQSI—Monotone quintic spline interpolation. *To appear in ACM Transactions on Mathematical Software*. doi: 10.1145/3570157

Publications Under Review

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. Submitted to the 11th International Conference on Learning Representations (ICLR '23), Workshop on Machine Learning for Materials (ML4Materials). Double-blind peer-review, preprint available upon request.

Peer-Reviewed Journal Articles

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

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

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

2022. **T. H. Chang**, L. T. Watson, J. Larson, N. Neveu, W. I. Thacker, S. Deshpande, and T. C. H. Lux. Algorithm 1028: VTMOPT: Solver for blackbox multiobjective optimization problems. *ACM Transactions on Mathematical Software* 48(3), Article 36, 34 pages. doi: 10.1145/3529258
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
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
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
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
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

Peer-Reviewed Conference Papers

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. virtual event. doi: 10.1109/WSC48552.2020.9383875
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. virtual event. doi: 10.22360/springsim.2020.hpc.001
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. virtual event. doi: 10.22360/springsim.2020.hpc.003
2020. T. C. H. Lux and **T. H. Chang**. Analytic test functions for generalizable evaluation of convex optimization techniques. In *Proc. IEEE SoutheastCon 2020 Vol. 2*, 8 pages. Raleigh, NC, USA. doi: 10.1109/Southeast-Con44009.2020.9368254
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 Vol. 2*, 6 pages. Raleigh, NC, USA. doi: 10.1109/SoutheastCon44009.2020.9368295
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
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
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
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
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

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
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

2023. **T. H. Chang**, S. M. Wild, and H. Dickinson. *ParMOO: Python library for parallel multiobjective simulation optimization*. Technical Report Version 0.2.0. Argonne National Laboratory, Lemont, Illinois, USA. url: https://parmoo.readthedocs.io/_/downloads/en/latest/pdf/
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>
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>
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

Conference Talks

- Sep 2022. Geometric considerations when surrogate modeling. *SIAM Conference on Mathematics of Data Science (MDS 2022)*, San Diego, CA, USA.
- Jul 2022. ParMOO: a parallel framework for multiobjective simulation optimization problems. *Seventh International Conference on Continuous Optimization (ICCOPT 2022)*, Bethlehem, PA, USA.
- Jul 2021. Surrogate modeling of simulations for multiobjective optimization applications. *SIAM Conference on Optimization (OP 2021)*, virtual event.
- 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.
- Dec 2020. Multiobjective optimization of the variability of the high-performance Linpack solver. *2020 Winter Simulation Conference (WSC 2020)*, virtual event.
- Nov 2020. Multiobjective optimization of simulations with PARMOO. *Argonne Postdoctoral Research and Career Symposium*, virtual event.
- May 2020. Managing computationally expensive blackbox multiobjective optimization problems with libEnsemble. *Spring Simulation Conference (SpringSim '20)*, virtual event.
- Aug 2019. A surrogate for local optimization using Delaunay triangulations. *Sixth International Conference on Continuous Optimization (ICCOPT 2019)*, Berlin, Germany.
- 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.
- Apr 2018. Nonparametric distribution models for predicting and managing computational performance variability. *IEEE SoutheastCon 2020*, St. Petersburg, FL, USA.
- Mar 2018. A polynomial time algorithm for multivariate interpolation in arbitrary dimension via the Delaunay triangulation. *ACM Southeast Conference (ACMSE '18)*, Richmond, KY, USA.
- Apr 2017. Global deterministic and stochastic optimization in a service oriented architecture. *Spring Simulation Conference (SpringSim '17)*, Virginia Beach, VA, USA.

Apr 2016. GPU saturation for multiple matrix-vector multiplications. *Virginia Wesleyan College, Undergraduate Research Symposium*, Virginia Beach, VA, USA.

Apr 2014. The new Mastermind. *Virginia Wesleyan College, Undergraduate Research Symposium*, Virginia Beach, VA, USA.

Seminars and Colloquia

Feb 2020. Algorithms and software for Delaunay interpolation and multiobjective optimization. *Sandia National Laboratory, Wind Energy Technology Division Seminar*, virtual event.

Feb 2020. Algorithms and software for Delaunay interpolation and multiobjective optimization. *Argonne National Laboratory, Mathematics and Computer Science Division Seminar*, Lemont, IL, USA.

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

Oct 2022. An introduction to multiobjective simulation optimization with ParMOO. *The Science Academy, Science Circle Cohort, guest speaker*, virtual event. Recording: <https://www.youtube.com/watch?v=gQha8URLEHM>.

May 2022. An introduction to multiobjective simulation optimization with ParMOO. *University of Chicago, Pritzker School of Molecular Engineering, guest lecture*, virtual event.

Funding

Current

Mar 2023 - Sep 2023. A Scalable Multi-Physics Optimization Framework for Particle Accelerator Design.
ANL LDRD: 2023 LDRD Seed.
Type: ANL LDRD seed award. Budget: \$50K.
Role: co-PI. PI: G. Chen (ANL).

Rejected Proposals

FY 2023. Assessing the Quality of Scientific Data Sets for Machine Learning.
ANL LDRD: 2023 LDRD Seed.
Type: full proposal (3 pages + appendices). Budget: \$25K. Length: 7 months.
Role: PI.

FY 2022. Statistical and Mathematical Innovations for Next Generation Facilities.
DOE ASCR: 2022 Mathematical Multifaceted Integrated Capability Centers (MMICCS) (DE-FOA-0002704).
Type: full proposal (20 pages + appendices). Budget: \$12.7M. Length: 5 years.
Role: investigator. Dir: R. Joseph (GA Tech). ANL Lead: Z. Di.

FY 2022. Visual Analytics for Complex Network Workflows to Accelerate Science into Decision Making.
DOE ASCR: Data Visualization for Scientific Discovery, Decision-Making, and Comm. (DE-FOA-0002726).
Type: full proposal (16 pages + appendices). Budget: \$2.7M. Length: 3 years.
Role: key personnel. PI: G. Chin (PNNL). ANL Lead: T. Munson.

FY 2022. Accelerating Multi-Objective Neural Architecture Search.
ANL CELS: 2022 LDRD Advanced Computing Expedition.
Type: short proposal (1 paragraph + admin info.). Budget: \$33.6K. Length: 8 weeks.
Role: co-PI. With: S. Khairy (ANL).

FY 2020. FAIR Delaunay Benchmarking of Scientific AI Workflows.
DOE ASCR: FAIR Frameworks for Data and AI Models (LAB 20-2306).
Type: full proposal (13 pages + appendices). Budget: \$2.1M. Length: 3 years.
Role: key personnel. PI: A. Gillette (LLNL). ANL Lead: Z. Di.

Professional Services and Activities

Journal Referee

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

Conference Reviewer

- Int. Conf. for High Performance Computing, Networking, Storage, and Analysis 2021 (SC 21)
- 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**

- Providing input on topics and recruiting seminar speakers

Dec 2022. **Hiring Committee: MCS Division**

- Interviewing potential candidates for postdoctoral openings

Nov 2022. **Technical Reviewer: Sustainable Research Pathways**

- Providing technical reviews of faculty and student submissions to SRP program

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

- Providing red team reviews of staff pre-proposals, for internal downselection for DOE ASCR FOAs

Virginia Tech

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

- Organized professional and social events for graduate students and communicated student concerns to faculty

Mar 2019. **Primary Student Organizer: Computer Science Graduate Preview Weekend**

- Organized recruitment events for prospective graduate students and coordinated meetings with faculty

Advising

- Jun 2022 - Aug 2022. Manisha Garg (Urbana-Champaign), NSF MSGI at Argonne
- Project: Model agnostic sampling techniques for generating design-of-experiments
 - Project resulted in software package (pre-release) and conference article (in preparation)

- Jun 2022 - Aug 2022. Hyrum Dickinson (Urbana-Champaign), DOE SULI at Argonne
- Project: Visualization tools for the ParMOO library
 - Project resulted in a new feature in ParMOO v0.2.0 and credit in our user documentation

Mentoring

- Aug 2022. Srinivas Eswar (postdoc at Argonne), via Argonne Navigator Program
- Mar 2021. Bosco Ndemeye (PhD student at Univ. of Oregon), via SIAM CSE Mentoring Program

Teaching

- Jan 2022 - Present. **Adjunct Professor: College of DuPage**, Dept. of Computer and Info. Science
- CIS 2531: Introduction to Python Programming
- Jan 2020 - May 2020. **Instructor of Record: Virginia Tech**, Dept. of Computer Science
- CS 3114: Data Structures and Algorithms (in Java)
- Jan 2013 - Dec 2015. **Subject Tutor: Virginia Wesleyan University**, Learning Center
- Tutored undergraduate courses in calculus, computer science, and statistics

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

Misc. Travel Awards

- Feb 2021. *SIAM Early Career Travel Award*, \$160 to cover SIAM CSE 2021 registration
- Apr 2020. *Virginia Tech Computer Science Graduate Travel Award*, \$400 to attend SpringSim 2020
- Aug 2019. *Virginia Tech Graduate Student Association Travel Fund*, \$225 to attend ICCOPT 2019
- Jun 2019. *Virginia Tech Computer Science Graduate Travel Award*, \$600 to attend ICCOPT 2019
- Apr 2019. *ICCOPT Travel Grant Program*, €450 to attend ICCOPT 2019
- Apr 2018. *Virginia Tech Graduate Student Association Travel Fund*, \$225 to attend IEEE SoutheastCon 2018
- Mar 2018. *Virginia Tech Computer Science Graduate Travel Award*, \$400 to attend IEEE SoutheastCon 2018
- Aug 2016. *Virginia Tech Cunningham Travel Fund*, \$1000 unrestricted travel fund for Cunningham fellow

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