

Tyler H. Chang

Argonne National Laboratory
Mathematics & Computer Science (MCS) Division
9700 S. Cass Ave, Bldg. 240, Lemont, IL 60439

E-mail: tchang@anl.gov
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/SoutheastCon44009.2020.9368254
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. *Univeristy of Chicago, Pritzker School of Molecular Engineering, guest lecture*, virtual event.

Funding

Pending Proposals

FY 2023. Assessing the Quality of Scientific Data Sets for Machine Learning.

Role: PI.

Argonne National Laboratory: *2023 LDRD Innovate-Seed*.

Type: full proposal (3 pages + appendices). Budget: \$25K. Length: 7 months.

FY 2023. A Scalable Multi-Physics Optimization Framework for Particle Accelerator Design.

Role: co-PI. PI: G. Chen.

Argonne National Laboratory: *2023 LDRD Innovate-Seed*.

Type: full proposal (3 pages + appendices). Budget: \$50K. Length: 7 months.

Past Proposals (rejected)

FY 2022. Statistical and Mathematical Innovations for Next Generation Facilities.

Role: investigator. Director: R. Joseph. ANL Lead: Z. Di.

DOE ASCR: *2022 Mathematical Multifaceted Integrated Capability Centers (MMICCS)* (DE-FOA-0002704).

Type: full proposal (20 pages + appendices). Budget: \$12.7M. Length: 5 years.

FY 2022. Visual Analytics for Complex Network Workflows to Accelerate Science into Decision Making.

Role: key personnel. PI: G. Chin. ANL Lead: T. Munson.

DOE ASCR: *Data Visualization for Scientific Discovery, Decision-Making, and Communication* (DE-FOA-0002726).

Type: full proposal (16 pages + appendices). Budget: \$2.7M. Length: 3 years.

FY 2022. Accelerating Multi-Objective Neural Architecture Search.

Role: co-PI. With: S. Khairy.

ANL CELS: *2022 LDRD Advanced Computing Expedition*.

Type: short proposal (1 paragraph + admin info.). Budget: \$33.6K. Length: 8 weeks.

FY 2020. FAIR Delaunay Benchmarking of Scientific AI Workflows.

Role: key personnel. PI: A. Gillette. ANL Lead: Z. Di.

DOE ASCR: *FAIR Frameworks for Data and AI Models* (LAB 20-2306).

Type: full proposal (13 pages + appendices). Budget: \$2.1M. Length: 3 years.

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 (PhD at UIUC), NSF MSGI at Argonne
• Project: Model agnostic sampling techniques for generating design-of-experiments

Jun 2022 - Aug 2022. Hyrum Dickinson (UG at UIUC), DOE SULI at Argonne
• Project: Visualization tools for the ParMOO library

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

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