# 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, chemical design (see projects), and computational physics

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 (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

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

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 SCGSR Award: DOE Office of Science, Graduate Student Research (SCGSR) Program 2018. Pratt Fellowship: Virginia Tech, College of Engineering 2018. 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**

2022. **ParMOO**: Python library for parallel multiobjective simulation optimization. Release: 0.1.0 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** and S. M. Wild. ParMOO: a Python library for parallel multiobjective simulation optimization. *Submitted to Journal of Open Source Software*, May 2022. JOSS Open Review: https://github.com/openjournals/joss-reviews/issues/4468.
- **T. H. Chang**. Computing the Delaunay graph in high dimensions. *Submitted to Symposium on Computational Geometry (SoCG '23)*, Dec 2022. Double-blind peer-review, preprint available upon request.

### **Publications In Preparation**

- **T. H. Chang** and S. M. Wild. Working Title: Designing a framework for solving multiobjective simulation optimization problems.  $\sim$ 90% completion.
- **T. H. Chang**, J. Elias, S. M. Wild, and S. Chaudhuri. Working Title: Autonomous multiobjective optimization using real time data and multi-fidelity simulations.  $\sim$ 40% completion.
- M. Garg, **T. H. Chang**, and K. Raghavan. Working Title: Stochastic optimization of Fourier coefficients for space-filling designs.  $\sim$ 40% completion.
- **T. H. Chang** and A. K. Gillette. Working Title: On the quality of datasets for interpolation. ~30% completion.

#### **Peer-Reviewed Journal Articles**

- 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: VTMOP: 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**

- 2022. **T. H. Chang** and S. M. Wild. *ParMOO: Python library for parallel multiobjective simulation optimization*. Technical Report Version 0.1.0. Argonne National Laboratory, Lemont, Illinois, USA. url: https://parmoo.readthedocs.io/en/latest
- 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**

### **Pending Proposals**

FY 2023. Assessing the Quality of Scien4fic 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-Pl. Pl: 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-Pl. 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 student at UIUC), intern at Argonne via NSF MSGI program

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

Jun 2022 - Aug 2022. Hyrum Dickinson (undergrad at UIUC), intern at Argonne via DOE SULI program

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 Information 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, Markdown, reStructuredText, YAML, JSON Libraries: numpy, pandas, scipy, matplotlib, keras, pytorch, sklearn, PIL, OpenCV, MPI, OpenMP, CUDA,

BLAS, LAPACK

Tools/Frameworks: pytest, sphinx, PyPI/pip, conda-forge, slurm, git, CI/CD, GitHub Actions, GitFlow