Aleksei Gregory Sorokin

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Research Scientific Machine Learning, Gaussian Processes, Quasi-Monte Carlo, Probabilistic Numerics

Programming Python (PyTorch, GPyTorch, Pandas, Matplotlib), Julia, C, MATLAB, R, SQL, Wolfram

Tools AWS (SageMaker, EC2), GitHub (general, actions, pages), LaTeX, Docker

Education

2026.01 - 2028.05 **Postdoc.** Department of Statistics, University of Chicago. Advisors *Yuehaw Khoo and Lek-Heng Lim*.

2021.08 - 2025.12 **PhD in Applied Math.** Illinois Institute of Technology (IIT). GPA $3.89/4$. Advisor *Fred J Hickernell*.

2017.08 - 2021.05 **Master of Data Science.** IIT. Summa Cum Laude. GPA $3.94/4$.

2017.08 - 2021.05 **B.S. in Applied Math, Minor in Computer Science.** IIT. Summa Cum Laude. GPA $3.94/4$.

Experiences

2025.01 - 2025.12 **DOE SCGSR Fellow in Applied Math** at **Sandia National Laboratory** in Livermore, CA. I produced scientific ML models for machine-precision solutions to nonlinear PDEs [2]. I developed scalable multi-fidelity Gaussian processes regression models and open-source software implementations [8, 9].

2024.05 - 2024.08 **Scientific Machine Learning Researcher** at **FM (Factory Mutual Insurance Company).** I deployed scientific ML models, including PINNs DeepONets, to accelerate CFD fire dynamics simulations [10].

2023.05 - 2023.08 **Graduate Intern** at **Los Alamos National Laboratory.** I modeled multi-fidelity solutions to PDE with random coefficients using efficient and error aware Gaussian processes regression models [11].

2022.05 - 2022.08 **Givens Associate Intern** at **Argonne National Laboratory**. I derived error bounds and a sequential sampling method for efficiently estimating failure probabilities with probabilistic models [14].

2021.05 - 2021.08 **ML Engineer Intern** at **SigOpt, an Intel Company**. In a six-person ML team, I contributed production code for meta-learning model-aware hyperparameter tuning via Bayesian optimization [15].

2022.09 - 2022.11 **Participant** in **Argonne National Laboratory's Course on AI Driven Science on Supercomputers**. Key topics included handling large scale data pipelines and parallel training for neural networks.

2018.05 - 2019.08 **Instructor** for the **STARS Computing Corps' Computer Discover Program.** I taught and developed curriculum for middle school and high school girls to learn programmatic thinking in Python.

2021.08 - 2025.01 **Teaching Assistant** at **IIT**. I led reviews for PhD qualifying exams in analysis and computational math.

Open-Source Software

`QMCPy` **Quasi-Monte Carlo Python Software** (qmcsoftware.github.io/QMCSoftware). I led dozens of collaborators across academia and industry to develop QMC sequence generators, automatic variable transformations, adaptive error estimators, and diverse use cases [1, 6, 7, 16, 17, 18, 19, 4, 5].

`FastGPs` **Scalable Gaussian Processes in Python** (alegresor.github.io/fastgps). This supports GPU scaling, batched inference, hyperparameter optimization, multi-fidelity GPs, and efficient Bayesian cubature. `FastGPs` is the first package to implement GPs which require only $\mathcal{O}(n)$ storage and $\mathcal{O}(n \log n)$ computations compared to the typical $\mathcal{O}(n^2)$ storage and $\mathcal{O}(n^3)$ computations requirements [9, 8].

`QMCGenerators.jl` **Randomized Quasi-Monte Carlo Sequences in Julia** (alegresor.github.io/QMCGenerators.jl).

`QMCToolsCL` **Randomized Quasi-Monte Carlo Sequences in C/OpenCL** (qmcsoftware.github.io/QMCToolsCL/).

`TorchOrthoPolys` **Orthogonal Polynomials in PyTorch** (alegresor.github.io/TorchOrthoPolys/) with GPU support.

Awards

2025.01 - 2025.12 **DOE SCGSR Fellow in Applied Math**, Sandia National Laboratory, Livermore California.

2025.01 **Karl Menger Student Award for Exceptional Scholarship (Graduate)**, IIT.

2024.01 **College of Computing Excellence in Dissertation Research**, IIT.

2024 **Teaching Assistant Award**, IIT.

2023.08 **Outstanding Math Poster**, Los Alamos National Laboratory.

2017.08 - 2025.05 **Deans List Member**, IIT, every semester.

References

PhD Advisor **Fred J. Hickernell** (hickernell@iit.edu) Vice Provost for Research and Professor of Applied Math, IIT.

Mentor **Nicolas W. Hengartner** (nickh@lanl.gov) Senior Scientist, Los Alamos National Lab.

Mentor **Michael J. McCourt** (mikemccourt1234@gmail.com) CTO and Co-Founder at Distributional.

Mentor **Pieterjan M. Robbe** (pmrobbe@sandia.gov) Senior Member of Technical Staff, Sandia National Lab.

Publications

[1] Aleksei G. Sorokin, Fred J. Hickernell, Sou-Cheng T. Choi, Jagadeeswaran Rathinavel, Pieterjan Robbe, and Aadit Jain. "QMCPy: a Python framework for (quasi-)Monte Carlo algorithms". In: *Journal of Open Source Software* 11.117 (2026), p. 9705. DOI: 10.21105/joss.09705. URL: https://doi.org/10.21105/joss.09705.

[2] Aras Bacho, Aleksei G. Sorokin, Xianjin Yang, Théo Bourdais, Edoardo Calvello, Matthieu Darcy, Alexander Hsu, Bamdad Hosseini, and Houman Owhadi. "Operator learning at machine precision". In: (2025). DOI: 10.48550/arXiv.2511.19980.

[3] Eda Gjergo, Zhi-Yu Zhang, Pavel Kroupa, Aleksei Sorokin, Zhiqiang Yan, Ziyi Guo, Tereza Jerabkova, Akram Hasani Zonoozi, and Hosein Haghi. "Massive Star Formation at Supersolar Metallicities: Constraints on the Initial Mass Function". In: *Research in Astronomy and Astrophysics* 26.2 (Dec. 2025), p. 025003. DOI: 10.1088/1674-4527/ae1f79.

[4] Fred J. Hickernell, Nathan Kirk, and Aleksei G. Sorokin. "Quasi-Monte Carlo methods: what, why, and how?" In: (2025). DOI: 10.48550/arXiv.2502.03644.

[5] Aadit Jain, Fred J. Hickernell, Art B. Owen, and Aleksei G. Sorokin. "Empirical Bernstein and betting confidence intervals for randomized quasi-Monte Carlo". In: (2025). DOI: 10.48550/arXiv.2504.18677.

[6] Aleksei G. Sorokin. "Algorithms and scientific software for quasi-Monte Carlo, fast Gaussian process regression, and scientific machine learning". PhD thesis. Illinois Institute of Technology, 2025. DOI: 10.48550/arXiv.2511.21915.

[7] Aleksei G. Sorokin. "QMCPy: a Python software for randomized low-discrepancy sequences, quasi-Monte Carlo, and fast kernel methods". In: (2025). DOI: 10.48550/arXiv.2502.14256.

[8] Aleksei G. Sorokin, Pieterjan Robbe, Gianluca Geraci, Michael S. Eldred, and Fred J. Hickernell. "Fast Bayesian multilevel quasi-Monte Carlo". In: (2025). DOI: 10.48550/arXiv.2510.24604.

[9] Aleksei G. Sorokin, Pieterjan Robbe, and Fred J. Hickernell. "Fast Gaussian process regression for high dimensional functions with derivative information". In: *Proceedings of the First International Conference on Probabilistic Numerics*. Ed. by Motonobu Kanagawa, Jon Cockayne, Alexandra Gessner, and Philipp Hennig. Vol. 271. Proceedings of Machine Learning Research. PMLR, 2025, pp. 35–49. URL: https://proceedings.mlr.press/v271/sorokin25a.html.

[10] Aleksei G. Sorokin, Xiaoyi Lu, and Yi Wang. "A neural surrogate solver for radiation transfer". In: *NeurIPS 2024 Workshop on Data-Driven and Differentiable Simulations, Surrogates, and Solvers*. 2024. URL: https://openreview.net/forum?id=SHidR8UMKo.

[11] Aleksei G. Sorokin, Aleksandra Pachalieva, Daniel O'Malley, James M. Hyman, Fred J. Hickernell, and Nicolas W. Hengartner. "Computationally efficient and error aware surrogate construction for numerical solutions of subsurface flow through porous media". In: *Advances in Water Resources* 193 (2024), p. 104836. ISSN: 0309-1708. DOI: 10.1016/j.advwatres.2024.104836.

[12] Eda Gjergo, Aleksei G. Sorokin, Anthony Ruth, Emanuele Spitoni, Francesca Matteucci, Xilong Fan, Jinning Liang, Marco Limongi, Yuta Yamazaki, Motohiko Kusakabe, et al. "GalCEM: galactic chemical evolution model". In: *Astrophysics Source Code Library* (2023), ascl–2301. URL: https://ascl.net/2301.022.

[13] Eda Gjergo, Aleksei G. Sorokin, Anthony Ruth, Emanuele Spitoni, Francesca Matteucci, Xilong Fan, Jinning Liang, Marco Limongi, Yuta Yamazaki, Motohiko Kusakabe, and Toshitaka Kajino. *GalCEM. I. An Open-source Detailed Isotopic Chemical Evolution Code*. 2023. DOI: 10.3847/1538-4365/aca7c7.

[14] Aleksei G. Sorokin and Vishwas Rao. "Credible intervals for probability of failure with Gaussian processes". In: (2023). DOI: 10.48550/arXiv.2311.07733.

[15] Aleksei G. Sorokin, Xinran Zhu, Eric Hans Lee, and Bolong Cheng. "SigOpt Mulch: an intelligent system for AutoML of gradient boosted trees". In: *Knowledge-Based Systems* (2023), p. 110604. ISSN: 0950-7051. DOI: 10.1016/j.knosys.2023.110604.

[16] Sou-Cheng T. Choi, Yuhan Ding, Fred J. Hickernell, Jagadeeswaran Rathinavel, and Aleksei G. Sorokin. "Challenges in developing great quasi-Monte Carlo software". In: *Monte Carlo and Quasi-Monte Carlo Methods 2022*. Ed. by Aicke Hinrichs, Peter Kritzer, and Friedrich Pillichshammer. Springer. 2022, pp. 209–222. DOI: 10.1007/978-3-031-59762-6_9.

[17] Sou-Cheng T. Choi, Fred J. Hickernell, Jagadeeswaran Rathinavel, Michael J. McCourt, and Aleksei G. Sorokin. "Quasi-Monte Carlo software". In: *Monte Carlo and Quasi-Monte Carlo Methods 2020*. Ed. by Alexander Keller. Cham: Springer International Publishing, 2022, pp. 23–47. ISBN: 978-3-030-98319-2. DOI: 10.1007/978-3-030-98319-2_2.

[18] Aleksei G. Sorokin and Jagadeeswaran Rathinavel. "On bounding and approximating functions of multiple expectations using quasi-Monte Carlo". In: *Monte Carlo and Quasi-Monte Carlo Methods 2022*. Ed. by Aicke Hinrichs, Peter Kritzer, and Friedrich Pillichshammer. Springer. 2022, pp. 583–599. DOI: 10.1007/978-3-031-59762-6_29.

[19] Aleksei G. Sorokin, Fred J. Hickernell, Sou-Cheng T. Choi, Michael J. McCourt, and Jagadeeswaran Rathinavel. "(Quasi-)Monte Carlo Importance Sampling with QMCPy". In: *IIT Undergraduate Research Journal* (2021), pp. 49–54. URL: http://urj.library.iit.edu/index.php/urj/article/view/48.