# 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 Mathematics** at **Sandia National Laboratory** in Livermore, CA. I developed Gaussian process based scientific ML models for machine precision solutions to nonlinear PDEs. I built fast, scalable multitask Gaussian processes for multi-fidelity modeling. Both projects produced publications and open-source software with HPC support.

2024.05 - 2024.08 **Scientific Machine Learning Researcher** at **FM (Factory Mutual Insurance Company).** I built scientific ML models, including Physics Informed Neural Networks (PINNs) and Deep Operator Networks (DeepONets), for solving Radiative Transport Equations (RTEs) used to speed up CFD fire dynamics simulations. Resulted in publication of "A neural surrogate solver for radiation transfer".

2023.05 - 2023.08 **Graduate Intern** at **Los Alamos National Laboratory.** I modeled the solution processes of PDEs with random coefficients using efficient and error aware Gaussian processes. Resulted in publication of "Computationally efficient and error aware surrogate construction for numerical solutions of subsurface flow through porous media".

2022.05 - 2022.08 **Givens Associate Intern** at **Argonne National Laboratory**. I researched methods to efficiently estimate failure probability using Monte Carlo with non-parametric importance sampling. Resulted in publication of "Credible intervals for probability of failure with Gaussian processes".

2021.05 - 2021.08 **ML Engineer Intern** at **SigOpt, an Intel Company**. I developed novel meta-learning techniques for model-aware hyperparameter tuning via Bayesian optimization. In a six-person ML engineering team, I contributed production code and learned key elements of the AWS stack. Resulted in publication of "SigOpt Mulch: an intelligent system for AutoML of gradient boosted trees".

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), lead developer. This package provides high quality quasi-random sequence generators, automatic variable transformations, adaptive stopping criteria algorithms, and diverse use cases. Over the past five years, this project has grown to dozens of collaborators and multiple publications [4, 13, 14, 15, 16, 2, 3].

`FastGPs` **Scalable Gaussian Process Regression in Python** (alegresor.github.io/fastgps). Gaussian process (GP) regression models typically require $\mathcal{O}(n^2)$ storage and $\mathcal{O}(n^3)$ computations. `FastGPs` implements GPs which requires only $\mathcal{O}(n)$ storage and $\mathcal{O}(n \log n)$ computations by pairing certain quasi-random sampling locations with matching kernels to yield structured Gram matrices. We support GPU scaling, batched inference, robust hyperparameter optimization, and multitask GPs.

`QMCGenerators` **Quasi-Random Sequence Generators in Julia** (alegresor.github.io/QMCGenerators.jl). This package includes routines to generate and randomize quasi-random sequences used in Quasi-Monte Carlo. Supported low discrepancy sequences include lattices with random shifts and digital nets (e.g. Sobol' points) with random digital shifts, linear matrix scrambling, nested uniform scrambling, and higher order construction through digital interlacing. These features are also supported in `QMCPy`.

`AI on HPC` **AI Driven Science on Supercomputers Course** at **Argonne National Laboratory**.

## Awards

2025 **Karl Menger Student Award for Exceptional Scholarship (Graduate)**, IIT.

2024 **College of Computing Excellence in Dissertation Research**, IIT.

2024 **Teaching Assistant Award**, IIT.

2023 **Outstanding Math Poster**, Los Alamos National Laboratory.

## Publications


[1] Eda Gjergo, Zhiyu Zhang, Pavel Kroupa, Aleksei G. Sorokin, Zhiqiang Yan, Ziyi Guo, Tereza Jerabkova, Akram Hasani Zoonozi, and Hosein Haghi. "Massive star formation at supersolar metallicities: constraints on the initial mass function". In: *ArXiv preprint* abs/2509.20440 (2025). URL: https://arxiv.org/abs/2509.20440.

[2] Fred J. Hickernell, Nathan Kirk, and Aleksei G. Sorokin. "Quasi-Monte Carlo methods: what, why, and how?" In: *ArXiv preprint* abs/2502.03644 (2025). URL: https://arxiv.org/abs/2502.03644.

[3] Aadit Jain, Fred J. Hickernell, Art B. Owen, and Aleksei G. Sorokin. "Empirical Bernstein and betting confidence intervals for randomized quasi-Monte Carlo". In: *ArXiv preprint* abs/2504.18677 (2025). URL: https://arxiv.org/abs/2504.18677.

[4] Aleksei G. Sorokin. "QMCPy: a Python software for randomized low-discrepancy sequences, quasi-Monte Carlo, and fast kernel methods". In: *ArXiv preprint* abs/2502.14256 (2025). URL: https://arxiv.org/abs/2502.14256.

[5] Aleksei G. Sorokin, Pieterjan Robbe, Gianluca Geraci, Michael S. Eldred, and Fred J. Hickernell. "Fast Bayesian multilevel quasi-Monte Carlo". In: *ArXiv preprint* abs/2510.24604 (2025). URL: https://arxiv.org/abs/2510.24604.

[6] 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.

[7] 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.

[8] 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. URL: https://www.sciencedirect.com/science/article/pii/S0309170824002239.

[9] 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.

[10] 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. URL: https://dx.doi.org/10.3847/1538-4365/aca7c7.

[11] Aleksei G. Sorokin and Vishwas Rao. "Credible intervals for probability of failure with Gaussian processes". In: *ArXiv preprint* abs/2311.07733 (2023). URL: https://arxiv.org/abs/2311.07733.

[12] 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. URL: https://www.sciencedirect.com/science/article/pii/S0950705123003544.

[13] 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.

[14] 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.

[15] 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.

[16] 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.