

# Sam Foreman’s Résumé

Sam Foreman

2025-04-26

## Table of contents

|                                   |   |
|-----------------------------------|---|
| About . . . . .                   | 1 |
| Education . . . . .               | 1 |
| Professional Experience . . . . . | 1 |
| Publications . . . . .            | 2 |
| Awards and Honors . . . . .       | 6 |
| Talks . . . . .                   | 7 |
| Events . . . . .                  | 8 |
| References . . . . .              | 8 |

## About

Computational Scientist at Argonne National Laboratory.  
Scaling AI for science on supercomputers.  
[samforeman.me](#) [GitHub](#) • [Google Scholar](#) • [ORCID](#) • [Twitter](#)

## Education

- **Ph.D., Physics**  
*University of Iowa* | 2015–2019
  - [Learning Better Physics: A Machine Learning Approach to Lattice Gauge Theory](#)
- **B.S. in Engineering Physics**  
*University of Illinois at Urbana-Champaign* | 2010–2015
  - [Energy Storage in Quantum Resonators \(US Patent #US9741492B2\)](#)
- **B.S. in Applied Mathematics**  
*University of Illinois at Urbana-Champaign* | 2010–2015

## Professional Experience

- **Assistant Computational Scientist**

- *Argonne National Laboratory*, Leadership Computing Facility (ALCF) Lemont, IL | 2022–Present

- \* Research lead on scaling large language models (LLMs) and generative AI for science on supercomputers (Aurora, Frontier, LUMI, Leonardo, ...).
      - Co-lead the Models and Pretraining team of the [AuroraGPT](#) project
    - \* Optimize large-scale training of foundation models and language models for scientific applications.
    - \* Collaborate with interdisciplinary teams to enhance simulation efficiency and scalability
    - \* Focus on AI and HPC for scientific applications, including:
      - Training large language models on supercomputers
      - Genome scale language models (GenSLMs) for studying SARS-CoV-2 evolutionary dynamics
      - Direct Preference Optimization (DPO) for multimodal protein design workflows
      - Climate modeling and weather forecasting using foundation models
      - Developing improved sampling algorithms for lattice quantum chromodynamics (QCD)
    - \* <https://www.alcf.anl.gov/about/people/sam-foreman>

- **Postdoctoral Researcher**

- *Argonne National Laboratory*, Leadership Computing Facility (ALCF) Lemont, IL | 2019 – 2022

- \* Applied deep learning to lattice gauge theory and quantum field simulations.
    - \* Developed ML-enhanced Monte Carlo methods for QCD ([l2hmc-qcd](#)).
    - \* Engaged in AI-for-Science collaborations with national labs and university partners.

- **Graduate Researcher (DOE SCGSR Fellowship)**

- *Argonne National Laboratory*, Mathematics and Computer Sciences Division (MCS) Lemont, IL | 2018 – 2019

- \* Development of [l2hmc-qcd](#) in collaboration with ALCF for my PhD Thesis research

## Publications

Note

You can find a full list of my publications on my [Google Scholar](#)

1. **AERIS: Argonne Earth Systems Model for Reliable and Skillful Predictions** (Hatanpää et al. (2025))
  - *2025 ACM Gordon Bell Prize for Climate Modeling Finalist*
2. Aurora: Architecting Argonne’s First Exascale Supercomputer for Accelerated Scientific Discovery (Allen et al. (2025))
3. **HiPerRAG: High-Performance Retrieval Augmented Generation for Scientific Insights** (Gokdemir et al. (2025))
4. **Automated Tuning for HMC Mass Ratios** (Torsiello et al. (2025))
5. **MOFA: Discovering Materials for Carbon Capture with a GenAI and Simulation-Based Workflow** (Yan et al. (2025))
6. **MProt-DPO: Breaking the ExaFLOPS Barrier for Multimodal Protein Design with DPO** (Dharuman et al. (2024))
  - *2024 ACM Gordon Bell Finalist*
7. **Intro to HPC Bootcamp: Engaging New Communities Through Energy Justice Projects** (Leung et al. (2024))
8. **Thorough Characterization and Analysis of Large Transformer Model Training At-Scale** (Cheng et al. (2024))
9. **MLMC: Machine Learning Monte Carlo for Lattice Gauge Theory** (Sam Foreman, Jin, and Osborn (2023))
10. **Protein Generation via Genome-scale Language Models with Bio-physical Scoring** (Dharuman et al. (2023))
11. **DeepSpeed4Science Initiative: Enabling Large-Scale Scientific Discovery** (Song et al. (2023))
  - [DeepSpeed4Science.ai Blog Post](#)
  - [Looooooooong Sequence Lengths](#)
12. **Comprehensive Performance Study of LLMs on Novel AI Accelerators** (Emani et al. (2023))
13. **Exploratory Analysis of Climate Data with ClimRR, Intro to HPC Bootcamp @ NERSC** (Sam Foreman (2023))
14. **GenSLMs: Genome-scale language models reveal SARS-Cov-2 evolutionary dynamics** (Zvyagin et al. (2023))
  - Winner of the *ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research*

15. [Lattice QCD and Particle Physics](#) (Kronfeld et al. (2022))
16. [Applications of ML to Lattice QFT](#) (Boyda et al. (2022))
17. [LeapFrogLayers: Trainable Framework for Effective Sampling](#) (Sam Foreman et al. (2021))
18. [HMC with Normalizing Flows \[slides\]](#) (Sam Foreman et al. (2021))
19. [Deep Learning Hamiltonian Monte Carlo \[+ poster\]](#) (Sam Foreman, Jin, and C. (2021))
20. [Machine Learning and Neural Networks for Field Theory](#) (Sam Foreman, Jin, and Osborn (2020))
21. [Examples of renormalization group transformations for image sets](#) (Samuel Foreman et al. (2018))
22. [RG inspired Machine Learning for lattice field theory](#) (Sam Foreman et al. (2018))
23. [Large Energy Density in Three-Plate Nanocapacitors due to Coulomb Blockade](#) (Hubler et al. (2018))
24. [Superconductivity of In and Sn Samples](#) (Deamont and Foreman (2014))

## References

- Allen, Benjamin S., James Anchell, Victor Anisimov, Thomas Applencourt, Abhishek Bagusetty, Ramesh Balakrishnan, Riccardo Balin, et al. 2025. “Aurora: Architecting Argonne’s First Exascale Supercomputer for Accelerated Scientific Discovery.” <https://arxiv.org/abs/2509.08207>.
- Boyda, Denis, Salvatore Cali, Sam Foreman, Lena Funcke, Daniel C Hackett, Yin Lin, Gert Aarts, et al. 2022. “Applications of Machine Learning to Lattice Quantum Field Theory.” *arXiv Preprint arXiv:2202.05838*. <https://arxiv.org/abs/2202.05838>.
- Cheng, Scott, Jun-Liang Lin, Murali Emani, Siddhisanket Raskar, Sam Foreman, Zhen Xie, Venkatram Vishwanath, and Mahmut Taylan Kandemir. 2024. “Thorough Characterization and Analysis of Large Transformer Model Training at-Scale.” *Proc. ACM Meas. Anal. Comput. Syst.* 8 (1). <https://doi.org/10.1145/3639034>.
- Deamont, George, and Sam Foreman. 2014. “Superconductivity of in and Sn Samples.”
- Dharuman, Gautham, Kyle Hippe, Alexander Brace, Sam Foreman, Väinö Hatanpää, Varuni K. Sastry, Huihuo Zheng, et al. 2024. “MProt-DPO: Breaking the ExaFLOPS Barrier for Multimodal Protein Design Workflows with Direct Preference Optimization.” In *Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis*. SC ’24. Atlanta, GA, USA: IEEE Press. <https://doi.org/10.1109/SC41406.2024.00013>.
- Dharuman, Gautham, Logan Ward, Heng Ma, Priyanka V Setty, Ozan Gokdemir, Sam Foreman, Murali Emani, et al. 2023. “Protein Generation via Genome-Scale Language Models with Bio-Physical Scoring.” In *Proceedings of the SC’23 Workshops of the International Conference on High Performance Computing, Network, Storage, and Analysis*, 95–101.
- Emani, Murali, Sam Foreman, Varuni Sastry, Zhen Xie, Siddhisanket Raskar, William Arnold, Rajeev Thakur, Venkatram Vishwanath, and Michael E Papka. 2023. “A Comprehensive Performance Study of Large Language Models on Novel AI Accelerators.”

- arXiv Preprint arXiv:2310.04607*. <https://arxiv.org/abs/2310.04607>.
- Foreman, Sam. 2023. “Energy Justice Analysis of Climate Data with ClimRR.” August 7, 2023. <https://saforem2.github.io/climate-analysis>.
- Foreman, Sam, Joel Giedt, Yannick Meurice, and Judah Unmuth-Yockey. 2018. “RG-inspired machine learning for lattice field theory.” In *European Physical Journal Web of Conferences*, 175:11025. European Physical Journal Web of Conferences. <https://doi.org/10.1051/epjconf/201817511025>.
- Foreman, Sam, Taku Izubuchi, Luchang Jin, Xiao-Yong Jin, James C Osborn, and Akio Tomiya. 2021. “HMC with Normalizing Flows.” *arXiv Preprint arXiv:2112.01586*. <https://arxiv.org/abs/2112.01586>.
- Foreman, Sam, Xiao-Yong Jin, and Osborn James C. 2021. “Deep Learning Hamiltonian Monte Carlo.” <https://arxiv.org/abs/2105.03418>.
- Foreman, Sam, Xiao-Yong Jin, and James C Osborn. 2020. “Machine Learning and Neural Networks for Field Theory.”
- Foreman, Sam, Xiao-Yong Jin, and James C. Osborn. 2023. “MLMC: Machine Learning Monte Carlo for Lattice Gauge Theory.” <https://arxiv.org/abs/2312.08936>.
- Foreman, Samuel, Joel Giedt, Yannick Meurice, and Judah Unmuth-Yockey. 2018. “Examples of Renormalization Group Transformations for Image Sets.” *Physical Review E* 98 (5): 052129.
- Gokdemir, Ozan, Carlo Siebenschuh, Alexander Brace, Azton Wells, Brian Hsu, Kyle Hippe, Priyanka V. Setty, et al. 2025. “HiPerRAG: High-Performance Retrieval Augmented Generation for Scientific Insights.” <https://arxiv.org/abs/2505.04846>.
- Hatanpää, Väinö, Eugene Ku, Jason Stock, Murali Emani, Sam Foreman, Chunyong Jung, Sandeep Madireddy, et al. 2025. “AERIS: Argonne Earth Systems Model for Reliable and Skillful Predictions.” <https://arxiv.org/abs/2509.13523>.
- Hubler, A, S Foreman, J Liu, and L Wortsman. 2018. “Large Energy Density in Three-Plate Nanocapacitors Due to Coulomb Blockade.” *Journal of Applied Physics* 123 (10).
- Kronfeld, Andreas S, Tanmoy Bhattacharya, Thomas Blum, Norman H Christ, Carleton DeTar, William Detmold, Robert Edwards, et al. 2022. “Lattice QCD and Particle Physics.” *arXiv Preprint arXiv:2207.07641*. <https://arxiv.org/abs/2207.07641>.
- Leung, Mary Ann, Katharine Cahill, Rebecca Hartman-Baker, Paige Kinsley, Lois Curfman McInnes, Suzanne Parete-Koon, Sreeranjani Ramprakash, et al. 2024. “Intro to HPC Bootcamp: Engaging New Communities Through Energy Justice Projects.” *Journal of Computational Science Education* 15 (1). <https://doi.org/10.22369/issn.2153-4136/15/1/10>.
- Song, Shuaiwen Leon, Bonnie Kruft, Minjia Zhang, Conglong Li, Shiyang Chen, Chengming Zhang, Masahiro Tanaka, et al. 2023. “DeepSpeed4Science Initiative: Enabling Large-Scale Scientific Discovery Through Sophisticated AI System Technologies.” *arXiv Preprint arXiv:2310.04610*. <https://arxiv.org/abs/2310.04610>.
- Torsiello, J., G. T. Fleming, S. Foreman, X.-Y. Jin, and J. C. Osborn. 2025. “Automated

Tuning for HMC Mass Ratios.” *PoS.* Argonne, ALCF; Argonne National Laboratory (ANL), Argonne, IL (United States); Temple U.; Fermi National Accelerator Laboratory (FNAL), Batavia, IL (United States). <https://doi.org/10.22323/1.466.0052>.

Yan, Xiaoli, Nathaniel Hudson, Hyun Park, Daniel Grzenda, J. Gregory Pauloski, Marcus Schwarting, Haochen Pan, et al. 2025. “MOFA: Discovering Materials for Carbon Capture with a GenAI- and Simulation-Based Workflow.” <https://arxiv.org/abs/2501.10651>.

Zvyagin, Maxim, Alexander Brace, Kyle Hippe, Yuntian Deng, Bin Zhang, Cindy Orozco Bohorquez, Austin Clyde, et al. 2023. “GenSLMs: Genome-Scale Language Models Reveal SARS-CoV-2 Evolutionary Dynamics.” *The International Journal of High Performance Computing Applications* 37 (6): 683–705.

## Awards and Honors

- Nominated to serve on the US **Coordinating Panel for Software and Computing** by the Division of Particles and Fields of the American Physical Society (APS).
- **Finalist, ACM Gordon Bell Prize in Climate Modeling, 2025**
  - Recognized for our work on **AERIS** (Hatanpää et al. (2025)): The first billion-parameter pixel-level diffusion model for global weather and subseasonal-to-seasonal forecasting. Trained efficiently at scales from 1.3–80B parameters with our sequence-window parallelism (SWiPe) strategy, we achieve a sustained mixed-precision performance of 10.21 ExaFLOPS and peak performance of 11.21 ExaFLOPS, scaling to 10,080 nodes (120,960 GPUs) on the Aurora supercomputer.
- **Finalist, ACM Gordon Bell Prize, 2024**
  - Acknowledged for the MProt-DPO (Dharuman et al. (2024)) project, which achieved over 4 ExaFLOP sustained performance in multimodal protein design workflows using Direct Preference Optimization.
    - \* [Argonne team breaks new ground in AI-driven protein design – Argonne @ SC](#)
- **ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research, 2022**
  - Recognized for contributions to the GenSLMs (Zvyagin et al. (2023)) project, which developed genome-scale language models to study SARS-CoV-2 evolutionary dynamics.
    - \* [ACM Gordon Bell Special Prize for HPC-Based COVID-19 Research Awarded to Team for Modelling How Pandemic-Causing Viruses, Especially SARS-CoV-2, are Identified and Classified](#)

- **DOE Office of Science Graduate Student Research Fellow, 2018**
  - Awarded by the Department of Energy for outstanding research contributions during graduate studies.

## Talks

Note

You can see all of my talks online at <https://samforeman.me/talks/>

- 2025-:
  - 10: [Training Foundation Models on Supercomputers](#) @ University of Illinois at Urbana-Champaign
  - 10: [Training Foundation Models on Supercomputers](#) @ Georgia Institute of Technology
  - 10: [AERIS: Argonne’s Earth Systems Model](#) @ 2025 ALCF Hands-On HPC Workshop
  - 09: [Scientific AI at Scale: AI for Science](#) @ Open SkAI 2025
  - 09: [Scientific AI at Scale: Distributed Training](#) @ Open SkAI 2025
  - 07: [Large Scale Training on Diverse Accelerators](#) @ Scalable Deep Learning, SIAM AN2025
  - 05: [LLMs on Aurora: AuroraGPT](#) @ 2025 ALCF INCITE GPU Hackathon
  - 05: [LLMs on Aurora: ezip](#) @ 2025 ALCF INCITE GPU Hackathon
  - 02: [AuroraGPT: Foundation Models for Science](#) @ Foundation Models for the Electric Grid
- 2024-:
  - 11: [Parallel Training Methods](#) @ AI-for-Science on Supercomputers
  - 10: [AuroraGPT](#) @ 2024 ALCF Hands-On HPC Workshop
  - 10: [Machine Learning and Foundation Models at Scale](#) @ 2024 ALCF Hands-On HPC Workshop
  - 09: [AuroraGPT](#) @ HPC User Forum, 2024
  - 08: [Training LLMs at Scale](#) @ ATPESC, 2024
  - 07: [LLMs on Polaris](#) @ Center for Scientific Foundation Models, Summer School 24’
  - 03: [Parallel Training Techniques](#) @ AI-4-Science Training Series
  - 02: [LLMs from Scratch](#) @ LLM Tutorial Workshop
- 2023-:
  - 11: [Creating Small\(-ish\) LLMs](#) @ LLM Tutorial Workshop (1)
  - 10: [Exascale Science on Aurora](#) @ Intel oneAPI Workshop @ UIC

- 10: [LLM Lunch Talk @ ALCF Hands On HPC Workshop](#)
- 08: [Scaling LLMs for Science @ Data-Intensive Computing + AI/ML at Scale](#)
- 07: [MLMC: Machine Learning Monte Carlo @ Lattice 2023](#)
- 07: [Generative Modeling and Efficient Sampling @ PASC23](#)
- 04: [Efficient Sampling for LGT @ Deep Fridays @ U. Bologna](#)
- 2022-:
  - 11: [Large Scale Training @ AI4Science on Supercomputers \(ALCF\)](#)
  - 10: [Hyperparameter Management @ ALCF SDL Workshop](#)
  - 08: [Statistical Learning @ ATPESC 2022](#)
  - 05: [Scientific Data Science: An Emerging Symbiosis @ ANL \(05/2022\)](#)
  - 03: [Machine Learning in HEP @ UNC Greensboro](#)
- 2021-:
  - 12: [Accelerated Sampling Methods for LGT, @ DWQ @ 25 \[BNL\]](#)
  - 09: [Training Topological Samplers for LGT @ ML4HEP, ECT\\* Trento](#)
  - 05: [Deep Learning HMC for Improved Gauge Generation @ ML in LQCD Workshop \[2021\]](#)
- 2020:
  - 02: [Machine Learning for Lattice QCD @ U. Iowa \[2020\]](#)

## Events

- Organizer for:
  - [SC25 Workshop: High Performance Python for Science at Scale \(HPPSS\)](#), November 2025
  - [SC25 Tutorial: Accelerating and Scaling Python for HPC](#)
  - [SC24 Workshop: High Performance Python for Science at Scale \(HPPSS\)](#), November 2024
  - [SC23 Workshop: High Performance Python for Science at Scale \(HPPSS\)](#), November 2023
  - [Machine Learning and Quantum Computing for Earth Sciences](#) at 17th U. S. National Congress on Computational Mechanics, July 2023



## References

### References

- Allen, Benjamin S., James Anchell, Victor Anisimov, Thomas Applencourt, Abhishek Bagusetty, Ramesh Balakrishnan, Riccardo Balin, et al. 2025. “Aurora: Architecting Argonne’s First Exascale Supercomputer for Accelerated Scientific Discovery.” <https://arxiv.org/abs/2509.08207>.
- Boyda, Denis, Salvatore Cali, Sam Foreman, Lena Funcke, Daniel C Hackett, Yin Lin, Gert Aarts, et al. 2022. “Applications of Machine Learning to Lattice Quantum Field Theory.” *arXiv Preprint arXiv:2202.05838*. <https://arxiv.org/abs/2202.05838>.
- Cheng, Scott, Jun-Liang Lin, Murali Emani, Siddhisanket Raskar, Sam Foreman, Zhen Xie, Venkatram Vishwanath, and Mahmut Taylan Kandemir. 2024. “Thorough Characterization and Analysis of Large Transformer Model Training at-Scale.” *Proc. ACM Meas. Anal. Comput. Syst.* 8 (1). <https://doi.org/10.1145/3639034>.
- Deamont, George, and Sam Foreman. 2014. “Superconductivity of in and Sn Samples.”
- Dharuman, Gautham, Kyle Hippe, Alexander Brace, Sam Foreman, Väinö Hatanpää, Varuni K. Sastry, Huihuo Zheng, et al. 2024. “MProt-DPO: Breaking the ExaFLOPS Barrier for Multimodal Protein Design Workflows with Direct Preference Optimization.” In *Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis*. SC ’24. Atlanta, GA, USA: IEEE Press. <https://doi.org/10.1109/SC41406.2024.00013>.
- Dharuman, Gautham, Logan Ward, Heng Ma, Priyanka V Setty, Ozan Gokdemir, Sam Foreman, Murali Emani, et al. 2023. “Protein Generation via Genome-Scale Language Models with Bio-Physical Scoring.” In *Proceedings of the SC’23 Workshops of the International Conference on High Performance Computing, Network, Storage, and Analysis*, 95–101.
- Emani, Murali, Sam Foreman, Varuni Sastry, Zhen Xie, Siddhisanket Raskar, William Arnold, Rajeev Thakur, Venkatram Vishwanath, and Michael E Papka. 2023. “A Comprehensive Performance Study of Large Language Models on Novel AI Accelerators.” *arXiv Preprint arXiv:2310.04607*. <https://arxiv.org/abs/2310.04607>.
- Foreman, Sam. 2023. “Energy Justice Analysis of Climate Data with ClimRR.” August 7, 2023. <https://saforem2.github.io/climate-analysis>.
- Foreman, Sam, Joel Giedt, Yannick Meurice, and Judah Unmuth-Yockey. 2018. “RG-inspired machine learning for lattice field theory.” In *European Physical Journal Web of Conferences*, 175:11025. European Physical Journal Web of Conferences. <https://doi.org/10.1051/epjconf/201817511025>.
- Foreman, Sam, Taku Izubuchi, Luchang Jin, Xiao-Yong Jin, James C Osborn, and Akio Tomiya. 2021. “HMC with Normalizing Flows.” *arXiv Preprint arXiv:2112.01586*. <https://arxiv.org/abs/2112.01586>.
- Foreman, Sam, Xiao-Yong Jin, and Osborn James C. 2021. “Deep Learning Hamiltonian Monte Carlo.” <https://arxiv.org/abs/2105.03418>.

- Foreman, Sam, Xiao-Yong Jin, and James C Osborn. 2020. “Machine Learning and Neural Networks for Field Theory.”
- Foreman, Sam, Xiao-Yong Jin, and James C. Osborn. 2023. “MLMC: Machine Learning Monte Carlo for Lattice Gauge Theory.” <https://arxiv.org/abs/2312.08936>.
- Foreman, Samuel, Joel Giedt, Yannick Meurice, and Judah Unmuth-Yockey. 2018. “Examples of Renormalization Group Transformations for Image Sets.” *Physical Review E* 98 (5): 052129.
- Gokdemir, Ozan, Carlo Siebenschuh, Alexander Brace, Azton Wells, Brian Hsu, Kyle Hippe, Priyanka V. Setty, et al. 2025. “HiPerRAG: High-Performance Retrieval Augmented Generation for Scientific Insights.” <https://arxiv.org/abs/2505.04846>.
- Hatanpää, Väinö, Eugene Ku, Jason Stock, Murali Emani, Sam Foreman, Chunyong Jung, Sandeep Madireddy, et al. 2025. “AERIS: Argonne Earth Systems Model for Reliable and Skillful Predictions.” <https://arxiv.org/abs/2509.13523>.
- Hubler, A, S Foreman, J Liu, and L Wortsman. 2018. “Large Energy Density in Three-Plate Nanocapacitors Due to Coulomb Blockade.” *Journal of Applied Physics* 123 (10).
- Kronfeld, Andreas S, Tanmoy Bhattacharya, Thomas Blum, Norman H Christ, Carleton DeTar, William Detmold, Robert Edwards, et al. 2022. “Lattice QCD and Particle Physics.” *arXiv Preprint arXiv:2207.07641*. <https://arxiv.org/abs/2207.07641>.
- Leung, Mary Ann, Katharine Cahill, Rebecca Hartman-Baker, Paige Kinsley, Lois Curfman McInnes, Suzanne Parete-Koon, Sreeranjani Ramprakash, et al. 2024. “Intro to HPC Bootcamp: Engaging New Communities Through Energy Justice Projects.” *Journal of Computational Science Education* 15 (1). <https://doi.org/10.22369/issn.2153-4136/15/1/10>.
- Song, Shuaiwen Leon, Bonnie Kruft, Minjia Zhang, Conglong Li, Shiyang Chen, Chengming Zhang, Masahiro Tanaka, et al. 2023. “DeepSpeed4Science Initiative: Enabling Large-Scale Scientific Discovery Through Sophisticated AI System Technologies.” *arXiv Preprint arXiv:2310.04610*. <https://arxiv.org/abs/2310.04610>.
- Torsiello, J., G. T. Fleming, S. Foreman, X.-Y. Jin, and J. C. Osborn. 2025. “Automated Tuning for HMC Mass Ratios.” *PoS. Argonne, ALCF; Argonne National Laboratory (ANL), Argonne, IL (United States); Temple U.; Fermi National Accelerator Laboratory (FNAL), Batavia, IL (United States)*. <https://doi.org/10.22323/1.466.0052>.
- Yan, Xiaoli, Nathaniel Hudson, Hyun Park, Daniel Grzenda, J. Gregory Pauloski, Marcus Schwarting, Haochen Pan, et al. 2025. “MOFA: Discovering Materials for Carbon Capture with a GenAI- and Simulation-Based Workflow.” <https://arxiv.org/abs/2501.10651>.
- Zvyagin, Maxim, Alexander Brace, Kyle Hippe, Yuntian Deng, Bin Zhang, Cindy Orozco Bohorquez, Austin Clyde, et al. 2023. “GenSLMs: Genome-Scale Language Models Reveal SARS-CoV-2 Evolutionary Dynamics.” *The International Journal of High Performance Computing Applications* 37 (6): 683–705.