Samuel Frederick

GitHub ⋄ Google Scholar ⋄ sf20@illinois.edu

EDUCATION

Ph.D. in Atmospheric Sciences *In progress*

University of Illinois at Urbana-Champaign

- *Dissertation topic*: ODE/DAE solvers and constrained optimization algorithms for performance portable acceleration of multiphase atmospheric chemistry
- *Advisor*: Nicole Riemer

M.S. in Atmospheric Sciences *May 2024*

University of Illinois at Urbana-Champaign

- *Thesis*: Idealized particle-resolved large-eddy simulations to evaluate the impact of emissions spatial heterogeneity on CCN activity
- *Advisor*: Nicole Riemer

B.S. in Physics, Minor in Applied Mathematics *May 2019*

Davidson College

- *Honors Thesis*: Modeling Stability of Magnetars and Accompanying Internal Magnetic Fields with Applications to Continuous Gravitational Wave Detection

RESEARCH EXPERIENCE

Graduate Research Assistant *August 2022 - Present*

Department of Climate, Meteorology, and Atmospheric Sciences, University of Illinois

- Contributed to TChem-atm, a performance-portable multiphase atmospheric chemistry model built on Kokkos. Developed Kokkos-enabled modules and conducted performance and scalability analysis on NCSA DeltaAI using Nvidia H100 GPUs, profiling with Nsight Compute and Nsight Systems.
- Extended WRF-PartMC to enable particle-resolved large-eddy simulations. Emissions scenarios ranging in spatial heterogeneity were run to investigate the coupling between emissions heterogeneity and CCN activity.

ORAU National Student Services Contract *October 2019 - July 2022*

U.S. EPA Office of Research and Development, RTP, NC

- Designed and published *sensortoolkit*, an open-source Python library for evaluating air sensor data against regulatory-grade measurements. Features a class-based architecture supporting multiple sensor models and pollutants, with modules for computing U.S. EPA performance metrics and automated report generation.
- Contributed to U.S. EPA performance targets, metrics, and protocols for $PM_{2.5}$ and O_3 sensor evaluations; designed technical reporting templates for summarizing sensor performance against established targets.
- Developed modular tools supporting EPA research, including large-volume data acquisition via air monitoring APIs and NowCast AQI estimation for correction equation validation for air sensors on the Fire and Smoke Map.

Undergraduate Honors Thesis Research *August 2018 - May 2019*

Department of Physics, Davidson College

- Designed a simulation of highly-magnetic pulsars with the magnetohydrodynamic model PLUTO, investigated field-induced deformations and gravitational wave production.
- Quantified continuous gravitational wave strain resulting from modeled stellar deformation.
- Manuscript published in the May 2021 issue of the Monthly Notices of the Royal Astronomical Society.

PUBLICATIONS

1. O.H. Díaz-Ibarra, **S.G. Frederick**, J.H. Curtis, Z. D'Aquino, P.A. Bosler, L. Patel, C. Safta, M. West, N. Riemer. "TChem-atm (v2.0.0): Scalable Performance-Portable Multiphase Atmospheric Chemistry". Geoscientific Model Development, Volume 19, Issue 3, 2026, Pages 1281–1299. DOI.

2. **S.G. Frederick**, M. Mohebalhojeh, J.H. Curtis, M. West, N. Riemer. "Idealized Particle-Resolved Large-Eddy Simulations to Evaluate the Impact of Emissions Spatial Heterogeneity on CCN Activity". EGUsphere, 2025 (*preprint*). DOI.

3. M. Mohebalhojeh, **S.G. Frederick**, N. Riemer, M. West. "A Metric for Quantifying Spatial Heterogeneity in Gridded Atmospheric Fields". ESS Open Archive, 2026 (*preprint*). DOI.

4. M. Kumar, **S.G. Frederick**, K.K. Barkjohn, A.L. Clements. "Sensortoolkit—A Python Library for Standardizing the Ingestion, Analysis, and Reporting of Air Sensor Data for Performance Evaluation". Sensors 2025, 25, 5645. DOI.

5. K.K. Barkjohn, A.L. Holder, **S.G. Frederick**, A.L. Clements. Correction and Accuracy of PurpleAir $PM_{2.5}$ Measurements for Extreme Wildfire Smoke. Sensors 2022, 22, 9669. DOI.

6. "Modeling Magnetohydrodynamic Equilibrium in Magnetars with Applications to Continuous Gravitational Wave Production". **S.G. Frederick**, K.L. Thompson, M.P. Kuchera. Monthly Notices of the Royal Astronomical Society, Volume 503, Issue 2, May 2021, Pages 2764–2775. DOI.

TECHNICAL REPORTS

1. "Performance Testing Protocols, Metrics, and Target Values for Fine Particulate Matter Air Sensors - Use in Ambient, Outdoor, Fixed Site, Non-Regulatory Supplemental and Informational Monitoring Applications". R. M. Duvall, A. L Clements, G. Hagler, A. Kamal, V. Kilaru, L. Goodman, **S.G. Frederick**, K.K. Barkjohn, I. VonWald, D. Greene, T. Dye. Feb 2021. EPA Science Inventory Link.

2. "Performance Testing Protocols, Metrics, and Target Values for Ozone Air Sensors - Use in Ambient, Outdoor, Fixed Site, Non-Regulatory Supplemental and Informational Monitoring Applications". R. M. Duvall, A. L Clements, G. Hagler, A. Kamal, V. Kilaru, L. Goodman, **S.G. Frederick**, K.K. Barkjohn, I. VonWald, D. Greene, T. Dye. Feb 2021. EPA Science Inventory Link.

PRESENTATIONS (***presenter**)

1. "Accelerating Multiphase Atmospheric Chemistry with Performance Portable Solvers in TChem-atm". **S.G. Frederick***, O.H. Díaz-Ibarra, J.H. Curtis, Z. D'Aquino, M. West, N. Riemer. 12th Symposium on High Performance Computing for Weather, Water, and Climate, 106th AMS Annual Meeting. (Houston, TX, Jan 2026). Conference Link.

2. "Idealized particle-resolved large-eddy simulations to evaluate the impact of emissions spatial heterogeneity on CCN activity". **S.G. Frederick***, M. Mohebalhojeh, J. Curtis, M. West, N. Riemer. International Aerosol Modeling Algorithms Conference. Dec 2023.

3. "Communication of $PM_{2.5}$ Air Sensor Performance Evaluations in the Field Using EPA's Recommended Performance Metrics and Target Values". **S.G. Frederick***, R.M. Duvall, K.K. Barkjohn, C. Johnson, A.L. Clements. Association for Aerosol Research Conference. (Virtual, Oct 2021). EPA Science Inventory Link.

4. "Application of EPA's Recommended $PM_{2.5}$ Air Sensor Performance Metrics and Targets to Sensor Field Evaluations at Research Triangle Park". **S.G. Frederick***, K.K. Barkjohn, R.M. Duvall, C. Johnson, A.L. Clements. U.S. EPA Moment of Science, Air and Energy Connections Seminar. (Virtual, Apr 2021). EPA Science Inventory Link.

5. "Performance Evaluations of Air Sensors at EPA's AIRS Site". **S.G. Frederick***, K.K. Barkjohn, C. Johnson, R. Yaga, A.L. Clements. U.S. EPA $PM_{2.5}$ Implementation Workgroup. (Virtual, Aug 2020).

6. "Performance Evaluations of PM$_{2.5}$ Sensors in Research Triangle Park". **S.G. Frederick***, K.K. Barkjohn, C. Johnson, R. Yaga, A.L. Clements. U.S. EPA Air Sensor Webinar. (RTP, NC, Jan 2020).

7. "Modeling Structural and Magnetic Field Stability in Magnetars with Applications to Continuous Gravitational Wave Production". **S.G. Frederick***. Thesis Defense, Davidson College Department of Physics. (Davidson, Apr 2019).

POSTER PRESENTATIONS (***presenter**)

1. "Quantifying structural uncertainty in the aerosol modeling hierarchy: particle-resolved modeling on LES scales". J. Curtis, **S. Frederick**, Z. D'Aquino, M. Mohebalhojeh, N. Riemer, M. West. Atmospheric Radiation Measurement Atmospheric System Research Principal Investigator meeting, Bethesda, MD, Aug 2023.

2. "Interrogating the impact of spatial heterogeneity in aerosols on structural uncertainty using large-eddy simulations". **S. Frederick***, M. Mohebalhojeh, J. Curtis, M. West, and N. Riemer. American Chemical Society Spring Meeting, Indianapolis, IN, Mar 2023.

3. "sensortoolkit: A Python Library for Standardizing the Ingestion, Analysis, and Reporting of Air Sensor Data for Performance Evaluations". **S.G. Frederick***, K. Barkjohn, R. Duvall, A. Clements. Air Sensor International Conference, Pasadena, California, May 11 - 13, 2022. EPA Science Inventory Link.

4. "Performance Evaluations of Six PM$_{2.5}$ Sensors in Research Triangle Park, NC". **S.G. Frederick***, K.K. Barkjohn, C. Johnson, I. VonWald, A.L. Clements. American Association for Aerosol Research. (Virtual, Oct 2020). EPA Science Inventory Link.

5. "Impacts of Data Completeness on Hourly Averaged PurpleAir PM$_{2.5}$ Concentrations During Smoke Events". **S.G. Frederick***, K.K. Barkjohn, A.L. Holder, A.L. Clements. American Association for Aerosol Research. (Virtual, Oct 2020). EPA Science Inventory Link.

SKILLS

Programming:	Python, C++, Fortran, Bash
HPC & Parallel Computing:	CUDA, Kokkos, MPI (job-level execution), Slurm job scheduling, GPU profiling (Nsight Compute, Nsight Systems)
HPC Systems:	NCSA DeltaAI, TACC Stampede3, UIUC Keeling
Data Analysis & Visualization:	VisIt, Matplotlib, NumPy, Xarray, NetCDF, pandas

LEADERSHIP AND OUTREACH

Treasurer *Fall 2023 - Spring 2025*
University of Illinois, Atmospheric Sciences Graduate Student Organization
- Managed graduate student organization finances, including dues collection, reimbursements, and banking ledger maintenance, and assisted in planning social events

Graduate Student Ambassador *Fall 2022 - Fall 2024*
University of Illinois, Department of Climate, Meteorology, and Atmospheric Sciences
- Served as a contact point for prospective graduate students and collaborated with fellow ambassadors to plan and host prospective student webinar events

Vice President for Professional Affairs *Spring 2017 - Spring 2019*
Davidson College, Society of Physics Students (SPS)
- Organized GRE preparatory seminars, coordinated public outreach events, and contributed to chapter recognition as an Outstanding SPS Chapter (2017–2018). Inducted into Sigma Pi Sigma.

Boy Scouts of America **Valdese, NC**
Eagle Scout *Spring 2014*