MICHAEL J. SCHMIDT, PHD

Computational Scientist

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EDUCATION

PhD/MS	Computational and Applied Mathematics, Colorado School of Mines	2019/2018
BA, *summa cum laude*	Applied Mathematics, Metropolitan State University of Denver	2015
BS, *cum laude*	Interdisciplinary Business Management, Entrepreneurship Focus, Miami University	2008

RESEARCH INTERESTS

Partial Differential Equations; Numerical Methods;
High-performance Computing; Performance-portable Parallel Computing;
Models for Atmospheric Aerosols, Turbulence, and Climate;
Kernel-based Approximation Methods; Lagrangian (Particle-tracking) Methods

PROFESSIONAL EXPERIENCE

- **Senior Member of Technical Staff** September 2022 - Present
  Center for Computing Research, Sandia National Laboratories
  - Worked on the *EAGLES* team to complete a year-long sprint to port *E3SM*'s *MAM4* aerosol model from Fortran to C++ and *Kokkos*.
    - Reorganized/modularized a legacy code base containing numerous interdependencies.
    - Implemented validation tests for all high-level functions and unit tests for all sufficiently sophisticated functions.
    - Working jointly with Oscar Diaz-Ibarra, top contributors in: commits (#1), ported subroutines/aerosol processes (#1), lines of code (#3) *(adjusted for joint work)*.
  - Finished exploratory development of stochastic Lagrangian turbulent transport model for atmospheric aerosols.
    - Manuscript describing this work to be submitted September 2023.
    - Code to be shared with PNNL colleagues to collaborate on adapting the model to indoor bacteria- and virus-laden flows.
  - Ongoing research with external colleagues.
    - Continued collaboration with research group that include Colorado School of Mines (CSM), University of Notre Dame (UND), and Washington State University.
      - Advising CSM PhD student and extending work from PhD and UND postdoc.
    - ASCR SciML proposal submitted with NREL and SNL colleagues.
    - Finalizing proposal (submission September 26, 2023) with PNNL colleague to National Institutes of Health *Stephen I. Katz Early Stage Investigator Research Project Grant*.
  - Continued mentoring:
    - PhD advisor to Lucas Schauer (Colorado School of Mines).
    - Mentor to Meilin Zheng (University of New Mexico graduate, beginning graduate school at Johns Hopkins University in Fall 2023).

- **Postdoctoral Appointee** October 2020 - September 2022
  Center for Computing Research, Sandia National Laboratories
  - Developed an atmospheric chemistry driver for the *Haero* high-performance modal aerosol modeling package to be included in the Department of Energy's *E3SM* climate model (Q4 2020 - Q4 2022).
    * Coordinated with the Sandia *TChem* team to extend their chemistry solver to handle atmospheric problems of interest.
    * Implemented the chemistry driver using advanced C++ and the *Kokkos* performance portability library so that *E3SM* and *Haero* will take full advantage of next-generation exascale computing platforms when they go online.
    * Applied rigorous verification testing to the chemistry driver, comparing to known and trusted results in the community, including the presumptive chemistry mechanism for E3SM v4.
    * This development paused, and discussions pivoted to including this product as a standalone library in the E3SM atmosphere driver, itself.
  - Developed and implemented a stochastic Lagrangian model for the *Pluminate* project that captures the turbulent transport dynamics of ship-emitted aerosol plumes (Q4 2021 - Present).
    * The model employs random-walking particles, following an Ornstein-Uhlenbeck process.
    * Validated the model against corresponding LES simulations with favorable results.
  - Continued to conduct research and publish with colleagues from previous research positions.
  - Advised one PhD student and one undergraduate student.

- **Postdoctoral Research Associate** June 2019 - September 2020
  University of Notre Dame
  Advisor: Diogo Bolster (Civil & Environmental Engineering & Earth Sciences)
  - Applied Lagrangian (particle tracking) methods to novel problems, including arbitrarily complex chemical systems, fluid-solid interactions (dissolution/precipitation), and systems including diffusion coefficients with large jump discontinuities in space.
  - Demonstrated the advantages of particle methods, due to capturing subgrid perturbations to concentration, mixing, and transport properties.
  - Researched and published advances that improved and extended the capabilities of particle tracking methods, as applied to hydrogeological reactive transport.
  - Designed the *SMIMfit* library for parameterizing a stochastic mobile-immobile model (SMIM) based on groundwater reactive flow data.
    * This library was designed for present and future modeling work conducted by the research group of Diogo Bolster.

- **Adjunct Professor** August 2019 - December 2019
  Colorado School of Mines
  Course: Calculus I

- **Doctoral Research Assistant** July 2015 - May 2019
  Colorado School of Mines
  Advisors: Stephen Pankavich (Applied Mathematics) and David Benson (Hydrology)
  - *Dissertation Topic:* Lagrangian methods for modeling transport, mixing, and geochemical reactions.
    * Conducted research that improved the capabilities and understanding of Lagrangian (particle tracking) methods in the context of hydrogeological flows that include chemical reactions.
  - Participated in and gave multiple presentations in a weekly seminar focused on kernel-based approximation methods (4 Semesters).
  - Completed (or audited with graded work) a master's degree worth of statistics courses.
- **Summer Intern** 2017, 2018
  National Renewable Energy Laboratory (National Wind Technology Center)
  Mentor: Michael Sprague
  - Implemented a suite of unit tests for every subroutine in the *Beamdyn* module of the *OpenFAST* whole-turbine model.
  - Worked with mentor to add functionality and resolve code bugs within OpenFAST.
- **Greenwood Restoration** 2009-2011
  Founder and Owner, Self-employed
- **Breckenridge Ski Resort** 2008-2009
  Snowboarding Instructor

PEER-REVIEWED PUBLICATIONS

Citations: 154
h-index: 7

(*1*) **M. J. Schmidt**, Engdahl, N. B., Benson, D. A., and Bolster, D. (2023). Optimal Time Step Length for Lagrangian Interacting-Particle Simulations of Diffusive Mixing. *Transport in Porous Media 146*, 413–433, https://doi.org/10.1007/s11242-021-01734-8.

(*2*) **M. J. Schmidt**, McMichael, L., Wood, R., Blossey, P., and Patel, L. (2023). A Lagrangian random-walk model for the turbulent transport of aerosols in the atmospheric boundary layer. *In preparation for September submission*.

(*3*) Schauer, L., **M. J. Schmidt**, Engdahl, N. B., Pankavich, S. D., Benson, D. A., and Bolster, D. (2023). Parallelized domain decomposition for multi-dimensional Lagrangian random walk mass-transfer particle tracking schemes. *Geoscientific Model Development 16*, 833–849, https://gmd.copernicus.org/articles/16/833/2023/.

(*4*) Sole-Mari, G., **M. J. Schmidt**, Bolster, D., and Fernàndez-Garcia, D. (2021). Random-Walk Modeling of Reactive Transport in Porous Media With a Reduced-Order Chemical Basis of Conservative Components. *Water Resources Research 57*, e2020WR028679 2020WR028679, e2020WR028679, https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2020WR028679.

(*5*) Tran, N. T. V., Benson, D. A., **M. J. Schmidt**, and Pankavich, S. D. (2021). A Computational Information Criterion for Particle-Tracking with Sparse or Noisy Data. *Advances in Water Resources 151*, 103893, https://www.sciencedirect.com/science/article/pii/S0309170821000488.

(*6*) Benson, D. A., Pankavich, S., **M. J. Schmidt**, and Sole-Mari, G. (2020). Entropy: 1) The former trouble with particle-tracking simulation, and 2) A measure of computational information penalty. *Advances in Water Resources*, 103509, http://www.sciencedirect.com/science/article/pii/S0309170819303458.

(*7*) **M. J. Schmidt**, Engdahl, N. B., Pankavich, S. D., and Bolster, D. (2020). A mass-transfer particle-tracking method for simulating transport with discontinuous diffusion coefficients. *Advances in Water Resources 140*, 103577, http://www.sciencedirect.com/science/article/pii/S0309170819310425.

(*8*) **M. J. Schmidt**, Pankavich, S. D., Navarre-Sitchler, A., Engdahl, N. B., Bolster, D., and Benson, D. A. (2020). Reactive particle-tracking solutions to a benchmark problem on heavy metal cycling in lake sediments. *Journal of Contaminant Hydrology 234*, 103642, http://www.sciencedirect.com/science/article/pii/S0169772219304279.

(*9*) Benson, D. A., **M. J. Schmidt**, Bolster, D., Harmon, C., and Engdahl, N. B. (2019). Aging and mixing as pseudo-chemical-reactions between, and on, particles: Perspectives on particle interaction and multi-modal ages in hillslopes and streams. *Advances in Water Resources*, 103386, http://www.sciencedirect.com/science/article/pii/S0309170819303951.

(*10*) Engdahl, N. B., **M. J. Schmidt**, and Benson, D. A. (2019). Accelerating and Parallelizing Lagrangian Simulations of Mixing-Limited Reactive Transport. *Water Resources Research 55*, http://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2018WR024361.

(*11*) **M. J. Schmidt** Lagrangian methods for modeling transport, mixing, and geochemical reactions, PhD dissertation, Colorado School of Mines, 2019, https://hdl.handle.net/11124/173042.

(*12*) **M. J. Schmidt**, Pankavich, S. D., Navarre-Sitchler, A., and Benson, D. A. (2019). A Lagrangian Method for Reactive Transport with Solid/Aqueous Chemical Phase Interaction. *Journal of Computational Physics: X*, 100021, http://www.sciencedirect.com/science/article/pii/S259005521930037X.

(*13*) Sole-Mari, G., **M. J. Schmidt**, Pankavich, S. D., and Benson, D. A. (2019). Numerical Equivalence Between SPH and Probabilistic Mass Transfer Methods for Lagrangian Simulation of Dispersion. *Advances in Water Resources*, http://www.sciencedirect.com/science/article/pii/S0309170818310820.

(*14*) **M. J. Schmidt**, Pankavich, S. D., and Benson, D. A. (2018). On the accuracy of simulating mixing by random-walk particle-based mass-transfer algorithms. *Advances in Water Resources 117*, 115–119, http://www.sciencedirect.com/science/article/pii/S0309170818301830.

(*15*) **M. J. Schmidt**, Pankavich, S., and Benson, D. A. (2017). A kernel-based Lagrangian method for imperfectly-mixed chemical reactions. *Journal of Computational Physics 336*, 288–307, http://www.sciencedirect.com/science/article/pii/S0021999117301055.

PROFESSIONAL PRESENTATIONS

- **2023:** Platform for Advanced Scientific Computing, Davos, Switzerland;
  Center for Computing Research Postdoc and Early Career Seminar, Sandia National Laboratories (March);
  Society for Industrial and Applied Mathematics Conference on Computational Science and Engineering, Amsterdam, The Netherlands (February).
- **2022:** American Geophysical Union Fall Meeting, Chicago, IL (December);
  The International Conference for High Performance Computing, Networking, Storage, and Analysis, Dallas, TX (November);
  Generalized Aerosol/Chemistry Interface Workshop and Hackathon (April).
- **2021:** Sandia National Laboratories Postdoctoral Development Seminar Series, Albuquerque, NM (May).
- **2020:** Los Alamos National Laboratory, Los Alamos, NM (February), ***Invited***;
  Lorentz Center Workshop on Mixing in Porous Media, Leiden, Netherlands (February);
  Sandia National Laboratories, Albuquerque, NM (January), ***Invited***.
- **2019:** American Geophysical Union Fall Meeting, San Francisco, CA (December);
  Society for Industrial and Applied Mathematics Northern States Section Meeting, Laramie, WY (September), ***Invited***;
  Graduate Research and Development Symposia Conference, Colorado School of Mines, Golden, CO (April).
- **2018:** American Geophysical Union Fall Meeting, Washington, D.C. (December);
  Graduate Student Colloquium, Colorado School of Mines, Golden, CO (November);
  Computational Methods in Water Resources, Saint-Malo, France (June);
  Faculty Colloquium–Graduate Student Symposium, Colorado School of Mines, Golden, CO (April).
- **2017:** American Geophysical Union Fall Meeting, New Orleans, LA (December);
  Graduate Research and Development Symposia Conference, Colorado School of Mines, Golden, CO (April);
  Graduate Student Colloquium, Colorado School of Mines, Golden, CO (March);
  Front Range Applied Mathematics Student Conference, University of Colorado Denver, CO (March);
  Faculty Colloquium, Metropolitan State University of Denver, CO (February), ***Invited***.
- **2016:** American Geophysical Union Fall Meeting, San Francisco, CA (December);
  Faculty Colloquium–Graduate Student Symposium, Colorado School of Mines, Golden, CO (December);
  Society for Industrial and Applied Mathematics Central States Section Meeting, Little Rock, AR (October);
  Short Course on Applied Reactive Transport Modeling, Technical University of Denmark, Lyngby, Denmark (June);
  Colorado Nonlinear Day, University of Colorado Colorado Springs, CO (April);
  Graduate Student Colloquium, Colorado School of Mines, Golden, CO (March);
  Front Range Applied Mathematics Student Conference, University of Colorado Denver, CO (March).

TECHNICAL SKILLS

- Programming Languages:
  - C++
  - Python
    - NumPy, scikit-learn, pandas, seaborn, Jupyter Notebook
  - Fortran
  - High-performance Computing
    - MPI, OpenMP, batch schedulers
  - Kokkos
    - C++ library for parallel CPU/GPU performance portability
  - Matlab
  - CMake
  - Shell Scripting
    - Bash, Zsh
  - LaTeX
  - Julia (nascent interest)
- Git
- YAML, JSON
- Markdown, Doxygen, MkDocs
- Docker
- Machine Learning
  - Enthought, Machine Learning Mastery Workshop

PROFESSIONAL MEMBERSHIPS

- Society of Industrial and Applied Mathematics
- US Research Software Engineer Association
- American Geophysical Union
- US Association for Computational Mechanics
- Institute of Electrical and Electronics Engineers

ADVISING & MENTORING

- *PhD Advisor/Mentor:*
  - Lucas Schauer, Colorado School of Mines (2019 - Present).
- *Undergraduate STEM Mentor*:
  - Meilin Zheng, University of New Mexico, Johns Hopkins University (2021 - Present).

PROFESSIONAL SERVICE & OUTREACH

- **Organizing Activities:**
  1. Co-organizer, Minisymposium on *Machine Learning and Model-Based Dimension Reduction for Exploration and Interpretation of Dynamical and Industrial Systems*, US National Congress on Computational Mechanics 2023, Albuqueque, NM;
  2. Co-organizer, Minisymposium on *Modern Approaches to Modeling Atmospheric Aerosols and Clouds*, Platform for Advanced Scientific Computing 2023, Davos, Switzerland.
- **Referee/Reviewer:**
  - Water Resources Research
  - Advances in Water Resources
  - Journal of Contaminant Hydrology
  - Scientific Reports
  - Computer Physics Communications
  - Computers & Geosciences
  - LDRD Technical Reviewer (Sandia)
- **Presentation Judge:**
  - Graduate Research and Discovery Symposium, Colorado School of Mines (2020, 2021);
  - Undergraduate Poster Session, Joint Mathematics Meetings, Denver, CO (2020);

MAJOR COLLABORATORS

- Dr. Andrew Glaws
  - National Renewable Energy Laboratory, Computational Science Center
- Dr. Zachary Grey
  - National Institute of Standards and Technology, Applied and Computational Mathematics Division
- Dr. Laura Fierce
  - Pacific Northwest National Laboratory, Aerosols and Aerosol-cloud Interactions
- Dr. Lekha Patel
  - Sandia National Laboratories, Statistical Sciences
- Dr. Jeff Johnson
  - Cohere Consulting, LLC
- Dr. Peter Bosler
  - Sandia National Laboratories, Center for Computing Research
- Prof. Stephen Pankavich
  - Colorado School of Mines, Applied Mathematics and Statistics
- Prof. David Benson
  - Colorado School of Mines, Geology and Geological Engineering
- Prof. Diogo Bolster
  - University of Notre Dame, Civil & Environmental Engineering and Earth Sciences
- Prof. Nicholas Engdahl
  - Washington State University, Civil and Environmental Engineering
- Dr. Guillem Sole-Mari
  - Lawrence Berkeley National Laboratory, Earth & Environmental Sciences
- Prof. Lazaro Perez
  - Desert Research Institute, Hydrologic Sciences