

Shreyas Sunil Gaikwad

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RESEARCH INTERESTS

Computational Science	PDE-constrained Inverse Problems	Uncertainty Quantification
Machine Learning	Climate Science	Data Assimilation
High-Performance Computing	Open Source Software Dev.	Automatic Differentiation

EDUCATION

Ph.D. in Computational Science, Engineering and Mathematics, 2019-2024

The University of Texas at Austin

Thesis: *Bayesian Inversion Over Long Time Scales for the Greenland Ice Sheet*

GPA: 4.0/4.0

M.S. in Computational Science, Engineering and Mathematics, 2019-2021

The University of Texas at Austin

GPA: 4.0/4.0

B.Tech in Mechanical Engineering with Honors, 2015-2019

Minor in Computer Science

Indian Institute of Technology Bombay

Thesis: *Computational Analysis of Subcooled Boiling*

GPA: 9.32/10.0, Department Rank: 4/150

RESEARCH EXPERIENCE

Graduate Research Assistant, CRIOS, UT Austin

2020-Present

Advisor - Dr. Patrick Heimbach

- Integrated the open source Automatic Differentiation (AD) tool Tapenade with the SICOPOLIS ice sheet model source code to generate the adjoint and tangent linear codes. The adjoint calculation of the gradient is exponentially faster than the finite differences calculation.
- Developing a computational framework for glaciological data assimilation and uncertainty quantification.
- Leveraging Deep Learning to reduce the computational cost of simulating sea ice in the general ocean circulation model, MITgcm.
- Examining the similarities between adjoint models and eXplainable-AI techniques (XAI) for deep learning emulators such as Layerwise Relevance Propagation (LRP) in the earth system context.

Visiting Scholar, Argonne National Laboratory

Summer 2022

Advisor - Dr. Sri Hari Krishna Narayanan, Dr. Patrick Heimbach, Dr. Michel Schanen

- First ever successful integration of the open source AD tool Tapenade with the MITgcm general circulation model source code, providing an alternative to a proprietary version that costs ~ \$14,000 per license per annum.

Undergraduate Research Assistant, IIT Bombay

2018-2019

Advisor - Dr. Janani Srree Muralidharan

- Simulated air-water multiphase flow around nuclear rods, analyzing trends in void fraction distribution for different turbulence models and solvers in OpenFOAM.

Undergraduate Research Assistant, IIT Bombay

Summer 2017

Advisor - Dr. Shivasubramanian Gopalakrishnan

- Simulated the impact of a subsonic, thin stream of air striking the surface of the water, to mirror the industrial process of purification of molten steel, leveraged axial symmetry to reduce computation time.

PUBLICATIONS AND TALKS

JOURNAL ARTICLES

Shreyas Gaikwad, Helen Pillar, Patrick Heimbach. “Pairing Neural Networks with Adjoint for Flexible Investigation and Robust Attribution of Ocean Variability”, *In Preparation for submission to Geophysical Research Letters*.

Shreyas Gaikwad, Sri Hari Krishna Narayanan, Laurent Hascoet, Jean-Michel Campin, Helen Pillar, An Nguyen, Jan Hückelheim, Paul Hovland, Patrick Heimbach. “MITgcm-AD v2: Open source tangent linear and adjoint modeling framework for the oceans and atmosphere enabled by the Automatic Differentiation tool Tapenade”, *Preprint on arXiv, Submitted to Joint Laboratory on Extreme Scale Computing Future Generation Computer Systems (JLESC-FGCS), 2024*.

Shreyas Gaikwad, Sri Hari Krishna Narayanan, Laurent Hascoet, Liz Curry-Logan, Ralf Greve, Patrick Heimbach. “SICOPOLIS-AD v2: linearized forward and adjoint modeling framework for ice sheet modeling enabled by automatic differentiation tool Tapenade”, *Journal of Open Source Software* 8, no. 83 (2023): 4679.

INVITED TALKS

Shreyas Gaikwad, Helen Pillar, Tim Smith, Nora Loose, Sri Hari Krishna Narayanan, Jean-Michel Campin, Laurent Hascoet, Patrick Heimbach (2023). “Computational Science To Enable Digital Twins Of The Ocean”, *6th SIAM Texas-Louisiana Sectional Meeting (SIAM TX-LA), 2023*.

ORAL PRESENTATIONS

Shreyas Gaikwad, Sri Hari Krishna Narayanan, Laurent Hascoet, Michel Schanen, Patrick Heimbach (2022). “MITgcm-AD: Open Source Inverse Modeling Framework for the Oceans using the AD tool Tapenade”, *ECCO Annual Meeting, 2023, 25th EuroAD Workshop, 2023, WCRP Workshop MIT, 2023, Summer Argonne Students Symposium (SASSy), 2022*.

Shreyas Gaikwad, Sri Hari Krishna Narayanan, Laurent Hascoet, Liz Curry-Logan, Ralf Greve, Patrick Heimbach (2022). “SICOPOLIS-AD V2: Inverse Modeling Framework for Ice Sheet Modeling enabled by Automatic Differentiation”, *AGU Annual Meeting, 2022, Scientific Committee on Antarctic Research 10th Open Science Conference (SCAR-OSC), 2022, Machine Learning for Polar Regions Workshop, 2022, 24th EuroAD Workshop, 2021*.

POSTERS

Shreyas Gaikwad, Sri Hari Krishna Narayanan, Laurent Hascoet, Liz Curry-Logan, Ralf Greve, Patrick Heimbach (2022). “SICOPOLIS-AD v2 and MITgcm-AD: linearized forward and adjoint modeling framework for ice sheet and ocean modeling enabled by automatic differentiation tool Tapenade”, *14th Joint Laboratory for Extreme Scale Computing (JLESC) Workshop*.

HONORS AND AWARDS

- **ACDC+GRISO Summer School**, prestigious climate dynamics summer school in Greenland. 2023
- **Peter O'Donnell Fellow**, Awarded Fellowship worth \$24,000 by the Oden Institute. 2019-2020
- **Ph.D. Preliminary Exam**, Cleared exams in applied maths, scientific computing, and maths modeling. 2020
- **KVPY Fellowship**, by Govt. of India for demonstrating an aptitude for research, (Rank: 27/50,000). 2015

OTHER RESEARCH PROJECTS

Machine Learning Applications in Geophysics

Spring 2021

- Developed CNNs in **Keras** for earthquake detection using data from stations, with **96% validation accuracy**.
- Developed U-Nets in **Keras** for seismic faults detection through image segmentation, with **97% test accuracy**.
- Leveraged Autoencoders in **Keras** to aid clustering through dimensional reduction into the latent space.
- Built pipeline to pick mudrocks from real wireline logs using ML algorithms, with **87% test accuracy**.

Physics-Informed Machine Learning

Spring 2021

- Trained a Deep Neural Network in **PyTorch** to emulate a partial differential equation (PDE) based glacier model by leveraging **higher-order derivatives of the PyTorch computational graph**.
- Enriched the framework using an expanded computational graph to infer unknown PDE parameters.

Laplacian 2D Finite Difference (FD) Solver Application

Fall 2020

- Features: OOP (C++), Solver (gauss, jacobi, PETSc), tests (bats, Travis CI, docker), 98% code coverage (lcov), 0% memory errors (valgrind), build (autotools), HPC env (SLURM), parser & logger (GRVY).

SOFTWARE CONTRIBUTIONS

All of these tools are constantly under development.

- **SICOPOLIS-AD v2**, a new inverse modeling framework for the ice sheet model SICOPOLIS that is enabled by source transformation using the open-source Automatic Differentiation (AD) tool Tapenade.
- **MITgcm-AD**, a new inverse modeling framework for the general circulation model MITgcm that is enabled by source transformation using the open-source Automatic Differentiation (AD) tool Tapenade.
- **ARGOVIS**, developed OOP-based Python tools for interactive plotting and binning of Argo data. The Jupyter Notebook will help the community to better analyze and visualize the Argo data.
- **Enzyme**, Identified fundamental bugs in Enzyme through glacier simulations in Julia, reported as MWEs [here](#) and [here](#) by Dr. Michel Schanen (my co-advisor at Argonne).

SELECT GRADUATE COURSEWORK

Data Science and HPC - Machine Learning applications in Geophysics, Foundational Techniques in Machine Learning, Engineering Data Mining, Tools and Techniques in Computational Science, Numerical Methods for Differential Equations, Numerical Linear Algebra, High-Performance Scientific Computing, Operating Systems.

Inverse Problems and UQ - Uncertainty Quantification in Computational Models, Computational & Variational Methods for Inverse Problems (observer).

Mathematics - Functional Analysis, Partial Differential Equations, Analytical Methods.

Fluid Dynamics - Physical Oceanography, Mathematical Modeling in Science and Engineering, Computational Fluid Dynamics, Galerkin Methods.

COMPUTATIONAL SKILLS

Languages - Python (scikit-learn, Keras, PyTorch, FENICS, xarrays, numpy, autograd, Pandas), Julia (MPI, Enzyme), C++ (GRVY, MASA, HDF5, PETSc), Fortran-77/90.

Softwares - MATLAB, Scilab, ANSYS, OpenFOAM, L^AT_EX, Tapenade, MITgcm, SICOPOLIS.

HPC and other tools - OpenMP, MPI, CUDA, SLURM, Github, Docker, Shell scripting, Travis-CI, Autotools, Valgrind, HTML, CSS, Jekyll, lcov, gcov.

SUMMER SCHOOLS

Advanced Climate Dynamics Courses (ACDC) + Greenland Ice Sheet Ocean (GRISO) Summer School, Disko Island, Greenland, 2023.

Trustworthy Artificial Intelligence for Environmental Science (TAI4ES) Summer School, 2021 & 2022.

PROFESSIONAL MEMBERSHIPS

Society of Industrial and Applied Mathematics (SIAM)

International Association of Cryospheric Sciences (IACS)

American Geophysical Union (AGU)
Indian Society of Arctic Researchers (ISAR)
Arctic Research Consortium of the United States (ARCUS)
Association of Polar Early Career Scientists (APECS)
Seismological Society of America (SSA)

MENTORSHIP, LEADERSHIP, TEACHING AND COMMUNITY EXPERIENCE

MENTORSHIP EXPERIENCE

- Mentor: Oden Institute for Computational Engineering and Sciences** 2022-2023
- Mentored first-year Oden Institute graduate students and served as a contact point for becoming acclimated to the program.
- Mentor: UT Austin SIAM Applied Math Mentorship Program** 2021-2022
- Mentored undergraduate students with a broad focus on careers in applied mathematics.
- Mentor: Department Academic Mentorship Program (DAMP), IIT Bombay** 2018-2019
- Mentored students for a smooth transition to the department curriculum, motivating their academic and personal endeavors.
 - Part of the team tasked with suggesting modifications to the curriculum if necessary after consultation with the Head of Department, Faculty Advisors, and Professors.
 - Counseled an academically weak student on a one-on-one basis, helping him to clear his academic backlogs as part of the Academic Rehabilitation Program.

LEADERSHIP EXPERIENCE

- President and Vice President, Austin Chapter of SIAM** 2021-2023
- Hosted NREL, Sandia National Laboratories, AMD, ANSYS, Two Sigma, Julia Computing, StriveWorks, Cerfe Labs (ARM), and Sandia National Laboratories as part of our Industry Seminar Series.
 - Helped organize Applied Maths Mentorship Program, which comprised 74 mentors and 97 mentees in total.
 - Nominated as a finalist for Best Graduate Organization at UT for two years in a row.

TEACHING EXPERIENCE

- Graduate Teaching Assistant, UT Austin** Fall 2022
Course - Intro. to Mathematical Modeling in Science and Engineering I
- Responsible for grading assignments, conducting recitation and office hours, as well as full lectures in the absence of the instructor.

COMMUNITY PARTICIPATION

- Guest Lecture, Course on Physical Oceanography** 2021
- My guest lecture “Scaling Analysis” focused on 1) an overview of how scaling analysis is performed and 2) on how it can help greatly simplify the governing equations of ocean flow.
- Volunteer: UT Girl Day** 2024
- Going to help organize and demonstrate to elementary and middle school kids and their parents how to conduct simple yet powerful experiments to understand the role of sea ice and glacial melts in the changing Arctic climate and explore observational and modeling tools fundamental to many CRIOS research projects.