

# Rohit Goswami

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*“An unproblematic state is a state without creative thought. Its other name is Death.”  
– David Deutsch*

## Personal Data

Name Rohit Goswami  
Date Of Birth 10.08.1995  
Birthplace Brookhaven, New York, United States of America

## Work Experience

### Lab COSMO

Postdoctoral position with Prof. Michele Ceriotti and Dr. Guillaume Fraux working on the metatensor ecosystem for interoperable atomistic machine learning, including GROMACS integration and DLPack support for zero-copy tensor interoperability.

### Department of Mechanical & Materials Engineering

TEER 1 NOC 41200 visa exemption researcher at Prof. Laurent Béland's group working on heating effects of large copper systems by scaling off-lattice / object kinetic monte carlo to over a million atoms.

### Science Institute

Principal investigator for the project on "Magnetic interactions of itinerant electrons modeled using Bayesian machine learning" supervised by Prof. Hannes Jónsson with Prof. Birgir Hrafnkelsson as a co-supervisor.

### Quansight Labs

Working on foundational FOSS scientific codebases and tools like numpy and f2py to provide holistic maintenance.

### Faculty of Physical Sciences

Worked with Prof. Hannes Jónsson on Bayesian analysis and machine learning for *ab-initio* quantum chemistry; partially employed on the EU funded "ReaxPro" project for potential energy surface saddle search acceleration.

### Department of Chemistry

I was affiliated to the Femtolab under the project "Femtosecond Laser Approaches to Quantum Information and Quantum Computation".

### Department of Chemical Engineering

I was associated with the Computational Nanoscience group. Over the course of two centrally funded projects, "Nucleation On Nanostructured Surfaces Computer Simulation Studies (SPO/DST/CHE/2017294)" and "Advanced Computation Research and Education (SPO/MHRD/CC/20130176)".

## Education

### Graduate studies

Thesis: "Efficient Exploration of Chemical Kinetics". Supervised by Prof. Hannes Jónsson with Prof. Birgir Hrafnkelsson as co-supervisor.

### B.Tech. Chemical Engineering

First Division (PROJECT: Gas Sweetening Plant Design)

### Intermediate (AISSCE)

87.2% Central Board of Secondary Education (CBSE)

### High School (AISSE)

9.8 Cumulative Grade Point Average (CGPA) in Central Board of Secondary Education (CBSE)

## Voluntary Positions

### Simulation and Data Lab Computational Chemistry

I administered the setup of a nix based software management module system.

### NumFOCUS

I was a co-admin for the entire raft of GSoC applications.

### Session CCo1

Virtual session chair for the DCOP session Computational Physics III: Modeling Molecules and Materials

### DVS 2024 Mentorship

I mentored a grad student on best practice visualizations for reproducible graphs with R

### IEEE P2881

Partially responsible for drafting the IEEE Standard for Neural Network Architecture Schema

### PySEAMS: Python Bindings for d-SEAMS

Under the Python Software Foundation, mentored and arranged for a Google Summer of Code intern to work on Python bindings to d-SEAMS.

### Artifact Description and Evaluation

Partially responsible for handling reproducibility for the 52<sup>nd</sup> International Conference on Parallel Processing

### Session GGo5

Virtual session chair for the DCOP session GGo5 on Electrons, Phonons, Electron-Phonon Scattering and Phononics I

### Scipy Proceedings Committee

Part of the proceedings committee tasked with handling, reviewing, updating the infrastructure to edit the proceedings of Scipy 2023

### IEEE P3173

Am actively involved in supporting the work on drafting the IEEE Standard for Endocrine Disrupting Chemical Hazard Labelling

### NumPy

I mentored a student for working on the F2PY frontend

### LFortran

I (co-)mentored students working on the Abstract Semantic Representation of LFortran

### Early Career Engineers Committee

### Early Career Member Group Committee

### Forum on Graduate Student Affairs

As part of the nomination committee, along with the past chair and other members, am responsible for validating and selecting nominees for the ballots of FGSA's elections

### Stúdentablaðsins

As a member of the editorial board; it is my pleasurable responsibility to provide guidance to the journalists and support my fellow editors in upholding the standards of the student paper of the University; published since 1943

### Summer of Nix

Will provide guidance to a group of five students who are to work towards packaging NLNet packages

### NBA Insights Through R

### LFortran: Computational Chemistry

Worked on implementing compile time intrinsic functions and also other front and middle end tasks towards a minimum viable product which compiles production computational chemistry codebases

### Young Professionals Committee

Am responsible for overseeing the preparation of all drafts of YPC publications as well as appointing subcommittee positions in coordination with the Chair.

### Instructor Development Committee

Was tasked with facilitating the formation of task forces/committees as appropriate to accomplish desired project outcomes; in particular with a focus on improving recognition for community contributions

### Symengine

Was tasked with a long project extending the existing documentation and setting up tests and websites for the Symengine project

### T<sub>E</sub>X Users Group Conference (TUG202X)

Have administered the TUG Zulip and coordinated social activities (including Topia) from the first online TUG, the 41st in 2020 and continuing to support the committee in subsequent interactions

## Executive Student Council

Was tasked with managing the publications committee web resources

### IEEE P1940

Was actively engaged in working with stake holders in industry and academia to create a collection of standard profiles that define integration of authentication services with ISO 8583 used for financial transactions

### R Novice Inflammation

As a maintainer for the Software Carpentries lesson on R, I work with the community to make sure that lessons stay up-to-date, accurate, functional and cohesive

### CarpentryCon 2020

Working for an international conference with diverse leads from across the world, as part of the program committee I reached out to keynote speakers and managed the overall schedule. Wrote content with the website subcommittee and also contributed due to my web development expertise

### Univ.ai

Tested course-content and developed interactive labs to work with an online cohort of students. Am presently teaching labs and mentoring small batches. I also work with the front and backend teams to facilitate workflows including shopify stores and NodeJS authentication systems

### Animal Welfare Group

Have worked with student bodies to rescue and care for local animals. Also designed and maintained a site with ReactJS to enhance knowledge dissemination

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## Teaching Experience

### HBV505M Software Quality Management

6 credit undergraduate and graduate course for software engineering best practices.

### REI505M Machine Learning

6 credit undergraduate and graduate introductory course on supervised and unsupervised learning.

### Statistical Inference for Biology

R workshop focused on frequentist statistical inference used for experimental analysis and design.

### Web Development for Physicists

Overview of web design, development and implementation focusing on technologies useful to the working physicist like SSGs and referencing frameworks

### CS106A - Code in Place

As a returning section leader for the `code-in-place` initiative, I was given the additional honor of being a mentor to the first time section leaders for this unique course. Also delivered a Nix workshop for the SLs.

### C++ part 2 - libraries and simulations

Intensive C++ workshop which covered augmenting existing code with Python bindings and using a build automation tool (CMake) along with continuous integration.

### Data Carpentry (Social Sciences with R)

R workshop focused on tidy data.

### Sciware: Git and GitHub

10 hour long workshop which taught the fundamentals of version control and collaboration using `git`, with some introductory coverage of more advanced topics like rebases.

### Data Carpentry Workshop for Social Sciences

6 hours on R practices, with a focus on how base-R gives way to tidy forms of data and the `tidyverse`.

### Water, Chemicals and more with Computers for Chemistry (WC3m)

15 hour long summer course for high school students and undergrads on the basics of computational chemistry.

### Online Data Carpentry Workshop

Taught the basics of R, OpenRefine, and some data wrangling to graduate students in the social sciences over three days.

### Data Carpentry Ecology Workshop

Taught the basics of Python and assisted with shell lessons for high school students over three days, with a follow up mentoring program.

### Helper

### CS106A - Code in Place

As part of the special COVID-19 `code-in-place` initiative, I worked as a section leader (teaching assistant). The course covered the fundamentals of computer programming using Python and was built off the first half of CS106A. Also moderated and participated

in an AMA session on "Machine Learning for the Physical Sciences" and taught a workshop for the other section leaders entitled "Functional Python Packaging with Nix"

### Opensource Contributions

CREATED	PixN ROM & Kernel (AOSP based rom for the Xperia Z5) HaoZeke's LineageOS	MANTAINED	F2PY (NumPy) ASV (Airspeed Velocity) Xperia Z5 LineageOS (14.*)
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### Opensource Projects Created

FASTMATMR	ROpenci reviewed R bindings for the fastest C++ library for reading and writing .mtx files		
D-SEAMS	An open-source, community supported engine for the analysis of molecular dynamics trajectories (co-creator)		
WAILORD	FOSS python library to interact with the ORCA suite of quantum chemistry programs, focused on the generation of property specific machine learning data-sets		
ZENYODA	Pandoc based, tup driven stand-alone multi format (revealJS, beamer etc.) presentation system with static site generation.	DOCUYODA	A document generation system based on pandoc and latexmk driven by gulp with yaml configuration and easy templating.
STARDOCK	Docker compose based containerized self-updating setup for media hosting, with traefik for reverse proxying. Includes music, ebook and video acquisition and management.	PYQTNUMSIM	A Qt interface for verbose numerical methods assignments.
GRIMOIRE	Metalsmith and webpack based open source educational experiment with a strong focus on readability, equations and references.	RGOSWAMI.ME	A hugo-blog template meant to be used with Emacs orgmode

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## Affiliations & Accolades

### Memberships

OSA (Optical Society of America)

AIChE (American Institute Of Chemical Engineers)

APS (American Physical Society)

IEEE (Institute of Electrical and Electronics Engineers)

IOP (Institute of Physics)

World Taekwondo

XDA Developers

AAAI (Association for the Advancement of Artificial Intelligence)

ACM (Association for Computing Machinery)

Also part of the SIGHPC (Special Interest Group for High Performance Computing) & SIGHPC-Education

ASAPBio (Accelerating Science and Publication in biology)

IChemE (Institute of Chemical Engineers)

IIChe (Indian Institute of Chemical Engineers)

IEEE IAS (Industrial Applications Society)

IEI (The Institution of Engineers [India])

InRaSS (Indian Radio Science Society)

OSI (Open Source Initiative)

OSI (Optical Society of India)

SPIE (Society of Photo-Optical Instrumentation Engineers)

The Carpentries

URSI (Union Radio-Scientifique Internationale)

Heterodox Academy

IGDORE (Institute for Globally Distributed Open Research and Education)  
COS (Center for Open Sciences)  
ims (Institute of Mathematical Statistics)  
Bernoulli Society  
RSS (Royal Statistical Society)  
Computing at School  
T<sub>E</sub>X Users Group  
Nordic Research Software Engineers RY  
HPC Carpentry  
IOP SIG on Computational Physics  
Biochemical Society, UK  
Federation of European Biochemical Societies (FEBS)  
BCS, the Chartered Institute of IT, UK  
BCS Open Source Group  
IOP Computational Physics Group  
British Ecological Society  
RSC (Royal Society of Chemistry)  
Awards  
Tensor Methods and Emerging Applications to the Physical and Data Sciences  
Photonics-2016

Nonlinear-Optics Session

IITG Zephyr Creative Writing  
Antaragni IITK-MUN GA-DISEC  
Reviews  
IOP - Journal of Physics B: Atomic, Molecular and Optical Physics  
IOP - New Journal of Physics  
IOP - Journal of Optics  
IOP - Journal of Physics: Condensed Matter  
APS Physical Review A  
APS Physical Review E  
APS Physical Review Applied  
Nature Communications  
APS Physical Review Letters  
IOP - Machine Learning: Science and Technology  
SPIE Journal of Micro/Nanolithography, MEMS, and MOEMS  
Manning Publications  
JupyterCon 2020  
PeerJ - Life & Environment  
PeerJ - Computer Science  
PeerJ - Organic Chemistry

## Grants Awarded

### Personal

#### Icelandic Research Fund

Amount: 6650 thousand ISK TITLE: Magnetic interactions of itinerant electrons modeled using Bayesian machine learning.

#### Project Leadership

#### COST Action

Amount: 575,000 EUR Funding generated for the COST action CA24106, also part of the Management Committee (Iceland).

#### Google Summer of Code

Amount: 6,000 USD Funding generated to mentor a first time code contributor writing Python bindings for d-SEAMS.

#### NumFocus Small Development Grant

Amount: 10,000 USD Compiling SciPy's Fortran packages with LFortran.

#### Google Season of Docs

Amount: 10,000 USD Funding generated to hire a technical writer full-time for two months.

#### NumFocus Small Development Grant

Amount: 4,600 USD Compiling SciPy with LFortran.

## Publications

### JOURNALS

- [12] **Goswami, Rohit. Mar. 2026.** "Two-Dimensional RMSD Projections for Reaction Path Visualization and Validation". In: *MethodsX*, p. 103851. DOI: 10.1016/j.mex.2026.103851.
- [11] **Goswami, Rohit** and Jónsson, Hannes. **Nov. 27, 2025.** "Adaptive Pruning for Increased Robustness and Reduced Computational Overhead in Gaussian Process Accelerated Saddle Point Searches". In: *ChemPhysChem (Cover feature)*. DOI: 10.1002/cphc.202500730. arXiv: 2510.06030.
- [10] Sallermann, Moritz, Goswami, Amrita, Peña-Torres, Alejandro, and **Goswami, Rohit. Oct. 2025.** "Flowy: High Performance Probabilistic Lava Emplacement Prediction". In: *Computer Physics Communications* 315, p. 109745. DOI: 10.1016/j.cpc.2025.109745. arXiv: 2405.20144.
- [9] **Goswami, Rohit. Aug. 11, 2025.** "Bayesian Hierarchical Models for Quantitative Estimates for Performance Metrics Applied to Saddle Search Algorithms". In: *AIP Advances* 15.8, p. 85210. DOI: 10.1063/5.0283639. arXiv: 2505.13621.
- [8] **Goswami, Rohit**, Masterov, Maxim, Kamath, Satish, Pena-Torres, Alejandro, and Jónsson, Hannes. **July 2025.** "Efficient Implementation of Gaussian Process Regression Accelerated Saddle Point Searches with Application to Molecular Reactions". In: *Journal of Chemical Theory and Computation*. DOI: 10.1021/acs.jctc.5c00866. arXiv: 2505.12519.
- [7] **Goswami, Rohit**, Rawat, Ashwini Kumar, Goswami, Sonaly, and Goswami, Debabrata. **June 2025.** "Compositional Analysis of Fragrance Accords Using Femtosecond Thermal Lens Spectroscopy". In: *Chemistry – an Asian Journal* 20.17. DOI: 10.1002/asia.202500521. arXiv: 2503.20431.
- [6] Čertík, Ondřej, Pask, John E., Fernando, Isuru, **Goswami, Rohit**, Sukumar, N., Collins, Lee. A., Manzini, Gianmarco, and Vackář, Jiří. **Dec. 2023.** "High-Order Finite Element Method for Atomic Structure Calculations". In: *Computer Physics Communications*, p. 109051. DOI: 10.1016/j.cpc.2023.109051. arXiv: 2307.05856.
- [5] Kedward, Laurence, Aradi, Balint, Certik, Ondrej, Curcic, Milan, Ehlert, Sebastian, Engel, Philipp, **Goswami, Rohit**, Hirsch, Michael, Lozada-Blanco, Asdrubal, Magnin, Vincent, Markus, Arjen, Pagone, Emanuele, Pribec, Ivan, Richardson, Brad, Snyder, Harris, Urban, John, and Vandenplas, Jeremie. **Apr. 2022.** "The State of Fortran". In: *Computing in Science & Engineering*. DOI: 10.1109/MCSE.2022.3159862. arXiv: 2203.15110.
- [4] Theeyancheri, Ligesh, Chaki, Subhasish, Samanta, Nairhita, **Goswami, Rohit**, Chelakkot, Raghunath, and Chakrabarti, Rajarshi. **Aug. 5, 2020.** "Translational and Rotational Dynamics of a Self-Propelled Janus Probe in Crowded Environments". In: *Soft Matter*. DOI: 10.1039/D0SM00339E. arXiv: 2008.02089.
- [3] **Goswami, Rohit**, Goswami, Amrita, and Singh, Jayant Kumar. **Mar. 2020.** "d-SEAMS: Deferred Structural Elucidation Analysis for Molecular Simulations". In: *Journal of Chemical Information and Modeling*. DOI: 10.1021/acs.jcim.0c00031. arXiv: 1909.09830.
- [2] **Goswami, Rohit. Oct. 8, 2019.** "Don't Pull Punches in Peer Review". In: *Nature* 574, pp. 176–176. DOI: 10.1038/d41586-019-03024-2.
- [1] Prerna, **Goswami, Rohit**, Metya, Atanu K., Shevkunov, S. V., and Singh, Jayant K. **Aug. 25, 2019.** "Study of Ice Nucleation on Silver Iodide Surface with Defects". In: *Molecular Physics*, pp. 1–13. DOI: 10.1080/00268976.2019.1657599.

- [7] **Goswami, Rohit** and S, Ruhila. **Mar. 2023**. “High Throughput Reproducible Literate Phylogenetic Analysis”. In: *2022 Seventh International Conference on Parallel, Distributed and Grid Computing (PDGC)*.
- [6] **Goswami, Rohit**, S, Ruhila, Goswami, Amrita, Goswami, Sonaly, and Goswami, Debabrata. **Mar. 2023**. “Reproducible High Performance Computing Without Redundancy with Nix”. In: *2022 Seventh International Conference on Parallel, Distributed and Grid Computing (PDGC)*.
- [5] **Goswami, Rohit**. **July 2022**. “Wailord: Parsers and Reproducibility for Quantum Chemistry”. In: *Proceedings of the 21st Python in Science Conference*, pp. 193–197. DOI: 10.25080/majora-212e5952-021.
- [4] **Goswami, Rohit**, Goswami, Amrita, and Goswami, Debabrata. **2021**. “Semi-Supervised Approaches to Ultrafast Pulse Shaping”. In: *ICOL-2019*. Ed. by Kehar Singh, A. K. Gupta, Sudhir Khare, Nimish Dixit, and Kamal Pant. Springer Proceedings in Physics. Singapore: Springer, pp. 747–749. DOI: 10.1007/978-981-15-9259-1\_172.
- [3] **Goswami, Rohit**, Goswami, Amrita, and Goswami, Debabrata. **Dec. 2019**. “Qubit Network Barriers to Deep Learning”. In: *2019 Workshop on Recent Advances in Photonics (WRAP)*. 2019 Workshop on Recent Advances in Photonics (WRAP), pp. 1–3. DOI: 10.1109/WRAP47485.2019.9013687.
- [2] **Goswami, Rohit**, Goswami, Amrita, and Goswami, Debabrata. **Mar. 2019**. “Space Filling Curves: Heuristics For Semi Classical Lasing Computations”. In: *2019 URSI Asia-Pacific Radio Science Conference (AP-RASC)*, pp. 1–4. DOI: 10.23919/URSIAP-RASC.2019.8738612.
- [1] **Goswami, Rohit** and Goswami, Debabrata. **2016**. “Quantum Distributed Computing with Shaped Laser Pulses”. In: *13th International Conference on Fiber Optics and Photonics*. DOI: 10.1364/photonics.2016.w4c.3.

PREPRINTS

- [3] **Goswami, Rohit**. **Dec. 2025**. *Two-Dimensional RMSD Projections for Reaction Path Visualization and Validation*. DOI: 10.48550/arXiv.2512.07329. arXiv: 2512.07329 [physics].
- [2] Bigi, Filippo, Abbott, Joseph W., Loche, Philip, Mazitov, Arslan, Tisi, Davide, Langer, Marcel F., Goscinski, Alexander, Pegolo, Paolo, Chong, Sanggyu, **Goswami, Rohit**, Chorna, Sofiia, Kellner, Matthias, Ceriotti, Michele, and Fraux, Guillaume. **Aug. 2025**. *Metatensor and Metatomic: Foundational Libraries for Interoperable Atomistic Machine Learning*. DOI: 10.48550/arXiv.2508.15704. arXiv: 2508.15704 [physics].
- [1] **Goswami, Rohit**, S. Ruhila, Goswami, Amrita, Goswami, Sonaly, and Goswami, Debabrata. **Feb. 6, 2023**. *Unified Software Design Patterns for Simulated Annealing*. arXiv: 2302.02811 [physics].

## Conference Records

### Posters

#### Inferring Multicomponent Properties Through Thermal Lens

Presented at APS April Meeting 2024. Authors: [R. Goswami](#), S. Goswami, and D. Goswami

#### Simulated Annealing for Global Search

Presented at APS March Meeting 2024. Authors: [R. Goswami](#), R. S., A. Goswami, S. Goswami, and D. Goswami

#### Towards Modular Components for Phylogenetic Estimation

Presented at APS March Meeting 2023. Authors: [R. Goswami](#), R. S.

#### Wailord: Parsers and Reproducibility for Quantum Chemistry

Presented at SciPyCon 2022. Author: [R. Goswami](#)

#### LPython: Interactive LLVM-based Python Compiler for Modern Architectures

Presented at SciPyCon 2022. Authors: O. Čertík, B. Beckman, N. Gera, S. Lunagariya, G. Singh, [R. Goswami](#), T. Shaktivel, and D. Edwards

#### Ultrafast Insights for Predictive Fragrance Compounding

Presented at ACS Spring 2020 National Meeting. Authors: [R. Goswami](#), A. K. Rawat, D. Chakrabarty, and D. Goswami

#### Qubit Network Barriers to Deep Learning

Presented at IEEE WRAP-2019. Authors: [R. Goswami](#), A. Goswami, and D. Goswami

#### Space Filling Curves: Heuristics For Semi Classical Lasing Computations

Presented at URSI Asia-Pacific Radio Science Conference (AP-RASC 2019). Authors: [R. Goswami](#), A. Goswami, and D. Goswami

#### FDTD Numerical Computations for Ultrafast Non-linear Optics

Presented at Photonics-2018. Authors: [R. Goswami](#), A. Goswami, and D. Goswami

### Oral Presentations

#### Managing concurrency for high throughput adaptive kinetic monte carlo

Presented at ACS Fall 2025. Author: [R. Goswami](#)

#### Advocating for standardized APIs for common procedures

Presented at Psi-K 2025. Authors: Miha Gunde, and [R. Goswami](#)  
Towards a million atoms and a thousand KMC steps a day

Presented at Kernel aKMC Conference 2025. Author: [R. Goswami](#)  
Low Data Saddle Search Acceleration with Bayesian Performance Analysis

Presented at Machine Learning in Chemical and Materials Sciences 2025. Author: [R. Goswami](#)  
Contending with concurrency across programming languages

Presented at APS Global Physics Summit 2025. Author: [R. Goswami](#)  
Modeling material-dependent thermal beam profiles in fiber optics

Presented at ACS Fall 2024. Authors: [R. Goswami](#), R. S., S. Goswami, and D. Goswami  
Accelerating Saddle Searches with Gaussian Process Regression

Presented at CECAM-LTS-MAP: Long time multi-scale simulations of activated events. Author: [R. Goswami](#)  
Throwaway Gaussian Processes for Saddle Searches

Presented at Machine Learning in Chemical and Materials Sciences 2024. Author: [R. Goswami](#)  
PySEAMS: Pythonic Structural Elucidation Analysis for Molecular Simulations

Presented at APS April Meeting 2024. Authors: [R. Goswami](#), R. S., and A. Goswami  
Revisiting Scaling Assumptions of Ab-Initio Calculations

Presented at APS March Meeting 2024. Author: [R. Goswami](#)  
Scaling workflows from development to HPC

Presented at 14<sup>th</sup> Icelandic HPC Community Workshop. Author: [R. Goswami](#)  
Development, Benchmarks and Workflows

Presented at CECAM-ESL: Advancing the Molecular Paradigm. Author: [R. Goswami](#)  
Computational Chemistry and Possible Tensor Applications

Presented at IPAM TMRC2 (Tensor Methods Reunion Conference). Author: [R. Goswami](#)  
High-order finite element method for atomic structure calculations

Presented at APS April Meeting 2023. Authors: [R. Goswami](#), O. Čertík, J. E. Pask, I. Fernando, L. A. Collins, G. Manzini, N. Sukumar, and J. Vackář  
Enhancing slideware for computational physics education

Presented at APS March Meeting 2023. Author: [R. Goswami](#)  
Intermediate Representations for Quantum Computing

Presented at APS March Meeting 2023. Authors: [R. Goswami](#), S. Goswami and D. Goswami  
Reproducible engines and interfaces on heterogeneous compute resources for structural analysis of deformed systems

Presented at APS Mid-Atlantic Section 2022 Meeting. Author: [R. Goswami](#) (Accepted)  
High Throughput Reproducible Literate Phylogenetic Analysis

Presented at IEEE PDGC-2022. Authors: [R. Goswami](#), R. S.  
Reproducible High Performance Computing Without Redundancy with Nix

Presented at IEEE PDGC-2022. Authors: [R. Goswami](#), R. S., A. Goswami, S. Goswami and D. Goswami  
Reproducible Literate Programming Workflows for Censored Data

Presented at IOP Machine Learning for Healthcare. Authors: [R. Goswami](#), R. S.  
Reproducible Environments on Elja with Nix and Spack

Presented at 6<sup>th</sup> Icelandic HPC Community Workshop. Author: [R. Goswami](#)  
Maintaining Fortran in Python in Perpetuity

Presented at SciPyCon 2022. Authors: [R. Goswami](#), M. Mendonca, R. Gommers, and T. Shaktivel  
f2py: Two Decades Later

Presented at FortranCon 2021. Authors: [R. Goswami](#), R. Gommers, M. Mendonca, and P. Peterson  
Implementing Fortran Standardese within LFortran

Presented at FortranCon 2021. Authors: [R. Goswami](#) and O. Čertík  
Continuous Integration and T<sub>E</sub>X with Org-Mode

Presented at TUG21, 42nd Annual Conference of the T<sub>E</sub>X Users Group. Author: [R. Goswami](#)  
Modern documentation across languages

Presented at ACM SERI 2021. Author: [R. Goswami](#)

Nix from the dark ages (without Root)

Presented at NixCon 2020. Author: [R. Goswami](#) (Lightning Talk)

Reproducible Scalable Workflows with Nix, Papermill and Renku

Presented at PyCon India 2020. Author: [R. Goswami](#)

Reproducible Environments with the Nix Packaging System

Presented at CarpentryCon 2020. Authors: [R. Goswami](#) and A. Goswami

LFortran: Interactive LLVM-based Fortran Compiler for Modern Architectures

Presented at FortranCon 2020. Authors: O. Čertík, N. Maan, A. Pandey, M. Curcic, P. Brady, Z. Jibben, N. Carlson, [R. Goswami](#), A. Shahmoradi and A. Markus (Presented by Ondřej)

Process Safety in terms of Latent Dirichlet Allocations

Presented at 72nd Annual Session of of the Indian Institute of Chemical Engineers, CHEMCON-2019. Author: [R. Goswami](#) (Accepted)

Semi-Supervised Approaches to Ultrafast Optimal Control Theory

Presented at 43rd Symposium of the Optical Society of India, International Conference on Optics & Electro-Optics. Authors: [R. Goswami](#), A. Goswami and D. Goswami

Quantum Distributed Computing with Shaped Laser Pulses

Presented at 13th International Conference on Fiber Optics and Photonics. Authors: [R. Goswami](#) and D. Goswami

Sprint Mentorship

NumPy Sprint

Presented at PyData Global 2022. Authors: G. Kathiresan, I. Pawson, [R. Goswami](#), and M. Pahari

NumPy Sprint

Presented at Grace Hopper Open Source Day 2022. Authors: [R. Goswami](#), R. Barnowski, B. Sipócz, M. Mendonca and I. Pawson

NumPy-SciPy Sprint

Presented at PyData Global 2021. Authors: M. Mendonca, M. Picus, [R. Goswami](#), R. Gommers and M. Pahari

NumPy Sprint

Presented at PyCon India 2021. Authors: M. Mendonca, [R. Goswami](#) and M. Pahari

## Workshops and Schools

Long time multi-scale simulations of activated events: from theory to practice

Electronic Structure Software Development: Advancing the Modular Paradigm

Quantum2 on Machine Learning Enhanced Sampling

FAIR and TRUE Data Processing for Soft Matter Simulations

Machine-learned potentials in molecular simulation: best practices and tutorials

Saddle point Search algorithms: towards the definition of a common BENCHMARK framework

Introduction to oneAPI, SYCL2020 and OpenMP offloading

SciML GPU Programming Bootcamp

Electronic Structure Software Development: Best Practices and Tools

Error control in first-principles modeling

Recent Advances in Machine Learning Accelerated Molecular Dynamics

MolSim2022

PRACE Autumn School 2021

Multiple scattering Green's function for electronic structure and spectroscopy calculations

Seventh LAMMPS Workshop and Symposium

AiiDA Virtual Tutorial

Comscope Summer School

Virtual Summer School on Theoretical Methods for Energy Conversion

MPI and OpenMP in Scientific Software Development  
Basic Parallel Programming with MPI and OpenMP  
Efficient Tensor Representations for Learning and Computational Complexity  
Mathematical Foundations and Algorithms for Tensor Computations  
Tensor Network States and Applications  
Tensor Methods and their Applications in the Physical and Data Sciences  
SWiMM: School on Simulation Workflows in Materials Modelling  
Workflows for Atomistic Simulations  
Tensor Method Tutorials  
IPWin2021: Inverse problems in partial differential equations and geometry  
BerkeleyGW Workshop and Berkeley Excited States Conference  
Computational materials discovery of unconventional magnets  
ESPReso and Python: Versatile Tools for Soft Matter Research  
Excited Charge Dynamics in Semiconductors  
(Machine) learning how to coarse-grain  
Gaussian Process and Uncertainty Quantification Summer School  
AiiDA Virtual Tutorial  
Mathematical Methods of Modern Statistics 2  
ALCF Computational Performance Workshop  
TriangleSCI 2019

A week long fully-funded incubator to discuss actionable goals towards Bringing Equity and Diversity to Peer Review. This was undertaken as part of the larger discussion on Equity in Scholarly Communications

#### Artificial Intelligence

A four week course on AI foundations culminating in a time-series prediction project.

#### AI Foundations Certificate Course

A summer school taught in-person by faculty from Harvard and UCLA, culminating in a computer vision and neural network based identification project.

#### Rare Events Summer School

#### Short Courses

#### Surface Area and Porous Material Characterization

#### OpenACC GPU Bootcamp

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## Certifications

### Coursera

#### Deep Learning Specialization

The specialization can be verified by ID Q3DLMMZJ42TR. This signifies the completion of the following five courses:

- Neural Networks and Deep Learning - **100.0%**
- Improving Deep Neural Networks: Hyperparameter tuning, Regularization and Optimization - **99.2%**
- Structuring Machine Learning Projects - **98.3%**
- Convolutional Neural Networks - **100.0%**
- Sequence Models - **100.0%**

### NPTEL Courses

#### Graph Theory

License: NPTEL19MA13S21460067

#### Computational Chemistry and Classical Molecular Dynamics

License: NPTEL18CS13S21440127

## Introduction to Parallel Programming in OpenMP

License: NPTEL18CS55S11440122

## Quantum Computing

License: NPTEL18CY07S4480024

## Graduate Coursework

“Due to COVID-19, grading varies from Pass/Fail to a 10 point scale.” (Note)

### Seminar on Machine Learning

Research seminar. PRESENTATION: Graph Neural Networks

### Statistics, science and COVID-19

Course covering “Statistical Rethinking” by Richard McElreath as well as the COVID-19 model of the University.

### Probabilistic Data Analysis

Research seminar based on “Bayesian Data Analysis” by Andrew Gelman, John Carlin, Hal Stern, David Dunson, Aki Vehtari, and Donald Rubin PRESENTATION: Markov Chain Simulations

### Applied data analysis

Course covering “Introduction to Statistical Learning An Introduction to Statistical Learning with Applications in R” by Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani PROJECT: Icelandic Housing Analysis

### Applied data analysis - Project

Extra credit course PROJECT: Molecular Dynamics Trajectory Analysis

### Machine Learning

An overview of some of the main concepts, techniques and algorithms in machine learning. Supervised learning, unsupervised learning and reinforcement learning. Data preprocessing and data visualization. Model evaluation and model selection. Linear regression, nearest neighbors, support vector machines and decision trees. Deep learning. Cluster analysis, the k-means and EM algorithms. TD-learning, Q-learning. PROJECT: Toxic Comment Classification (Grade 9/10)

### Software Quality Management

Metrics and models: Tools for managing software quality and its improvement. Quality Assurance: standards. Software Quality assurance activities. Quality assurance infrastructure and progress control. Software quality in Agile development. PRESENTATION: Scrum (Grade 10/10)

### Introduction to Pattern Recognition

Course covering “Elements of Statistical Learning: Data Mining, Inference, and Prediction” by Trevor Hastie, Robert Tibshirani, and Jerome Friedman along with “Pattern Recognition and Machine Learning” by Christopher Bishop. PROJECT: Predicting Molecular Properties

## Undergraduate Experience

### Internships

#### Dr. Debojit Chakrabarty

Modeling complex multi-component perfumes in a predictive method via experimental and theoretical considerations. In collaboration with Prof. Rajdip Bandyopadhyaya of the ChemE Dept. at IIT Bombay.

#### Prof. Sibasish Ghosh

Discussed computational techniques for the simulation and understanding of quantum tomography.

SUMMER 2017 **Prof. Nisanth Nair, IIT Bombay**

An exploratory project to investigate hybridization

POSTER: Development of

SUMMER 2016 **Prof. Rajarshi Chakrabarti, Indian Institute Of Technology Bombay**, Research Intern

Retooled a server with ArchLinux and also simulated patchy colloids (Janus Particles).

PROJECT REPORT: Computational Survey of Coarse Grained Soft Matter Molecular Dynamics Simulations

### Volunteer Work

#### ChemE Herald

Inaugurated and managed an interdisciplinary technical newsletter.

HBTU-MUN 2018

Designed a ReactJS based static website, with Trello backed user registration, also performed outreach pre-events to raise awareness and participation, in addition to overseeing the working of the executive board.

### HBTU-MUN 2017

Designed a Jekyll based static website and ensured adherence to standard MUN rules as Chairperson.

### The Curiosity Magazine

Managed a diverse team of student content writers and also later typeset a spin-off multi-lingual newsletter in X<sub>Y</sub>L<sup>A</sup>T<sub>E</sub>X.

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## Technical Skills

### Programming Languages

EXPERIENCED	C++, Python, R, FORTRAN, Shell (zsh, bash), OpenMP, OpenMPI, Tcl, CSS, JS, HTML, Sass, C	FAMILIAR	Ruby, Julia, Java, Haskell, Matlab, Golang, ReactJS, Node, CUDA
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### Projects

EXPERIENCED	d-SEAMS, Android (Cyanogen, LineageOS, AOSP), Web-Design (static), ArchLinux	FAMILIAR	Linux Kernel (Android)
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### Simulation Projects

EXPERIENCED	ESPreSo (Extensible Simulation Package for Research on Soft matter), LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), OVITO, AiiDA (Automated Interactive Infrastructure and Database for Computational Science)	FAMILIAR	OpenFOAM, GROMACS (GRONingen Machine for Chemical Simulations), VMD (Visual Molecular Dynamics)
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### Tools

EXPERIENCED	X <sub>Y</sub> L <sup>A</sup> T <sub>E</sub> X, pandoc, Git (version control), tmux, ssh, Vim, Sublime Text Editor 3, gnuplot, gadfly, bspwm (tiling window manager), babun, MATLAB (matrix laboratory), Continuous Integration Services (Wercker, Travis CI, Semaphore CI), docker	FAMILIAR	AWS (Amazon Web Services), moltemplate, jekyll, middleman, grunt, gulp, Frameworks (Bourbon, Skeleton, neat) Markup Languages (Textile, HAML, Jade(pug))
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