

# Rohit Goswami

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*“An unproblematic state is a state without creative thought. It’s 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

- 2021–PRESENT **Science Institute, University of Iceland, Rannís Research Fund Doctoral Grant Awardee**  
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.
- 2021–PRESENT **Quansight Labs, Software Engineer**  
Working on foundational FOSS scientific codebases and tools like numpy and f2py to provide holistic maintenance.
- 2019–2020 **Faculty of Physical Sciences, University of Iceland, Doctoral Researcher**  
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.
- 2019–2020 **Department of Chemistry, Indian Institute of Technology, Kanpur, Senior Project Associate**  
I was affiliated to the Femtolab under the project “Femtosecond Laser Approaches to Quantum Information and Quantum Computation”.
- 2018–2019 **Department of Chemical Engineering, Indian Institute Of Technology, Kanpur, Project Associate**  
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)”:
- I worked on the implementation of an enhanced version of the CHILL (CHILL+) algorithm for tracking ice types
  - Designed a linear discriminant analysis technique for near-surface ice structure determination which is undergoing rigorous testing
  - Implemented a graph based network connectivity model for ice structures
  - Spearheaded the development of High Performance GPU accelerated molecular dynamics simulation analysis tools
  - Worked on the determination of optimal GPU cluster configurations
  - Designed and administered academic outreach websites

## Education

- 2019–PRESENT **Graduate studies, University of Iceland, Reykjavík, Iceland**  
Current GPA: 9.25
- 2014–2018 **B.Tech. Chemical Engineering, Harcourt Butler Technical University, Kanpur, India**  
First Division (PROJECT: Gas Sweetening Plant Design)

- 2011–2013 **Intermediate (AISSCE)**, *Delhi Public School Kalyanpur*, Kanpur, India  
87.2% Central Board of Secondary Education (CBSE)
- 2009–2011 **High School (AISSE)**, *Delhi Public School Kalyanpur*, Kanpur, India  
9.8 Cumulative Grade Point Average (CGPA) in Central Board of Secondary Education (CBSE)

## Voluntary Positions

- 2024–PRESENT **NumFOCUS**, GSoC, Organization Admin  
I was a co-admin for the entire raft of GSoC applications.
- APRIL 2024 **Session CCo1**, *APS April Meeting 2024*, Session Chair  
Virtual session chair for the DCOP session Computational Physics III: Modeling Molecules and Materials
- FEB–MAY 24 **DVS 2024 Mentorship**, *Data Visualization Society*, Mentor  
I mentored a grad student on best practice visualizations for reproducible graphs with R
- 2024–PRESENT **IEEE P2881**, *IEEE Standards Committee*, Participant  
Partially responsible for drafting the IEEE Standard for Neural Network Architecture Schema
- JUNE–AUGUST 23 **PySEAMS: Python Bindings for d-SEAMS**, *Google Summer of Code*, Organization Admin  
Under the Python Software Foundation, mentored and arranged for a Google Summer of Code intern to work on Python bindings to d-SEAMS.
- 2023 **Artifact Description and Evaluation**, *ICPP 2023*, Review Board Member  
Partially responsible for handling reproducibility for the 52<sup>nd</sup> International Conference on Parallel Processing
- MARCH 2023 **Session GGo5**, *APS March Meeting 2023*, Session Chair  
Virtual session chair for the DCOP session GGo5 on Electrons, Phonons, Electron-Phonon Scattering and Phononics I
- 2022–2023 **Scipy Proceedings Committee**, *SciPy 2023*, Member  
Part of the proceedings committee tasked with handling, reviewing, updating the infrastructure to edit the proceedings of Scipy 2023
- 2022–PRESENT **IEEE P3173**, *IEEE Standards Committee*, Vice Chair  
Am actively involved in supporting the work on drafting the IEEE Standard for Endocrine Disrupting Chemical Hazard Labelling
- 2022–2023 **NumPy**, *Python Software Foundation*, GSoC Mentor  
I mentored a student for working on the F2PY frontend
- 2022–2023 **LFortran**, *NumFOCUS*, GSoC Mentor  
I (co-)mentored students working on the Abstract Semantic Representation of LFortran
- 2021–2022 **Early Career Engineers Committee**, *Professional Engineering Committee*, *Royal Academy of Engineering UK*, IOP Representative
- 2021–2025 **Early Career Member Group Committee**, *Institute of Physics*, Ordinary Member
- 2021–2023 **Forum on Graduate Student Affairs**, *American Physics Society*, Nominating Committee Member  
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
- 2021–2023 **Stúdentablaðsins**, *Stúdentaráð Háskóla Íslands*, Editorial Team Member  
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
- AUGUST–OCTOBER 21 **Summer of Nix**, *NixOS*, *NLNet*, and *Tweag*, Mentor  
Will provide guidance to a group of five students who are to work towards packaging NLNet packages
- 2021–2023 **NBA Insights Through R**, *Manning Publications*, Technical Editor
- JUNE–AUGUST 21 **LFortran: Computational Chemistry**, *Google Summer of Code*, Student Developer  
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
- 2021–2022 **Young Professionals Committee**, *American Institute of Chemical Engineers*, Publications Subcommittee Chair  
Am responsible for overseeing the preparation of all drafts of YPC publications as well as appointing subcommittee positions in coordination with the Chair.

- 2020–2021 **Instructor Development Committee, *The Carpentries***, Special Projects Chair  
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
- SEP 20–MARCH 21 **Symengine, *Google Season of Docs***, Technical Writer  
Was tasked with a long project extending the existing documentation and setting up tests and websites for the Symengine project
- 2020–2022 **TeX Users Group Conference (TUG202X), *TeX Users Group***, Organizing Committee Member  
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
- 2020–2021 **Executive Student Council, *American Institute of Chemical Engineers***, Publications Webmaster  
Was tasked with managing the publications committee web resources
- 2019–2020 **IEEE P1940, *IEEE Standards Committee***, Working group member  
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
- 2019–PRESENT **R Novice Inflammation, *The Carpentries***, Maintainer  
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
- 2019–2020 **CarpentryCon 2020, *The Carpentries***, Program Committee co-chair & Website subcommittee member  
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
- 2019–PRESENT **Univ.ai, *Earth2Orbit Analytix Private Limited***, Teaching Fellow and Developer  
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
- 2018–2019 **Animal Welfare Group, *Indian Institute of Technology Kanpur***, Member and Web-developer  
Have worked with student bodies to rescue and care for local animals. Also designed and maintained a site with ReactJS to enhance knowledge dissemination

## Teaching Experience

- FALL 2024 **HBV505M Software Quality Management, *University of Iceland***, Supervisory Teacher  
6 credit undergraduate and graduate course for software engineering best practices.
- FALL 2023 **REI505M Machine Learning, *University of Iceland***, Assistant Teacher  
6 credit undergraduate and graduate introductory course on supervised and unsupervised learning.
- MAY 2022 **Statistical Inference for Biology, *The Jackson Laboratory***, Instructor  
R workshop focused on frequentist statistical inference used for experimental analysis and design.
- JUNE 2021 **Web Development for Physicists, *IOP Conference for Astronomy and Physics Students***, Invited Instructor  
Overview of web design, development and implementation focusing on technologies useful to the working physicist like SSGs and referencing frameworks
- APRIL–MAY 2021 **CS106A - Code in Place, *Stanford University***, Teaching Mentor and Section Leader (TA)  
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.
- APRIL 2021 **C++ part 2 - libraries and simulations, *IOP Student Community***, Invited Instructor  
Intensive C++ workshop which covered augmenting existing code with Python bindings and using a build automation tool (CMake) along with continuous integration.
- NOVEMBER 2020 **Data Carpentry (Social Sciences with R), *Carnegie Mellon University***, Lead Instructor  
R workshop focused on tidy data.
- SEPTEMBER–OCTOBER 2020 **Sciware: Git and GitHub, *Flatiron Institute***, Lead Instructor  
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.
- SEPTEMBER 2020 **Data Carpentry Workshop for Social Sciences, *Georgia Gwinnett College***, Lead Instructor  
6 hours on R practices, with a focus on how base-R gives way to tidy forms of data and the tidyverse.

- JULY-AUGUST 2020 **Water, Chemicals and more with Computers for Chemistry (WC3m)**, *Wave Learning Festival*, Co-Teacher  
15 hour long summer course for high school students and undergrads on the basics of computational chemistry.
- JUNE-JULY 2020 **Online Data Carpentry Workshop**, *SADiLaR, South Africa*, Lead Instructor  
Taught the basics of R, OpenRefine, and some data wrangling to graduate students in the social sciences over three days.
- JUNE-JULY 2020 **Data Carpentry Ecology Workshop**, *Biotech Partners*, Leading Instructor  
Taught the basics of Python and assisted with shell lessons for high school students over three days, with a follow up mentoring program.
- MAY 2020 **Helper**, *CodeRefinery Mega Workshop*
- APRIL-MAY 2020 **CS106A - Code in Place**, *Stanford University*, Section Leader (TA)  
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"

## Undergraduate Experience

### Internships

- 2017-2018 **Dr. Debojit Chakrabarty**, *Keva Fragrances Ltd, Mumbai*, R&D Industrial Intern  
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.
- SUMMER 2017 **Prof. Sibasish Ghosh**, *The Institute of Mathematical Sciences, Chennai*, Visiting Scholar  
Discussed computational techniques for the simulation and understanding of quantum tomography.
- SUMMER 2017 **Prof. Nisanth Nair**, *Indian Institute Of Technology Kanpur*, SURGE Scholar  
An exploratory project to understand and deal with bottlenecks in computational chemistry, the major objectives were to investigate hybridization of existing code via OpenMP and MPI.
- POSTER: Development of Computational Tools for Free Energy Calculations of Chemical Reactions
- SUMMER 2016 **Prof. Rajarshi Chakrabarti**, *Indian Institute Of Technology Bombay*, Research Intern  
Retoold 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

- 2017-2018 **ChemE Herald**, *Harcourt Butler Technical University, Kanpur*, Editor-in-Chief  
Inaugurated and managed an interdisciplinary technical newsletter.
- 2017-2018 **HBTU-MUN 2018**, Secretary General  
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.
- 2016-2017 **HBTU-MUN 2017**, Executive Board Chairperson  
Designed a Jekyll based static website and ensured adherence to standard MUN rules as Chairperson.
- 2014-2016 **The Curiosity Magazine**, *Harcourt Butler Technical University, Kanpur*, Editor-in-Chief  
Managed a diverse team of student content writers and also later typeset a spin-off multi-lingual newsletter in  $\text{\LaTeX}$ .

## 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 |
|-------------|--|----------|---|

### Projects

EXPERIENCED	d-SEAMS, Android (Cyanogen, LineageOS, AOSP), Web-Design (static), ArchLinux	FAMILIAR	Linux Kernel (Android)
<b>Simulation Projects</b>			
EXPERIENCED	ESPResSo (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)
<b>Tools</b>			
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))
<b>Opensource Contributions</b>			
CREATED	PixN ROM & Kernel (AOSP based rom for the Xperia Z5) HaoZeke's LineageOS	MANTAINED	F2PY (NumPy) ASV (Airspeed Velocity) Xperia Z5 LineageOS (14.*)
<b>Opensource Projects Created</b>			
FASTMATMR	ROpensci 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

## Affiliations & Accolades

### Memberships

2014-PRESENT	<b>OSA (Optical Society of America)</b> , Student Member → Early Career Member (2018)
2015-PRESENT	<b>AIChE (American Institute Of Chemical Engineers)</b> , Student Member → Young Professional (2018)
2015-PRESENT	<b>APS (American Physical Society)</b> , Student Undergraduate Member → Early Career Member (2019)



2015–PRESENT **IEEE (Institute of Electrical and Electronics Engineers)**, Student Member → Early Career Member (2018)

2015–PRESENT **IOP (Institute of Physics)**, Student Member (2018) → Member (2019)

2006–PRESENT **World Taekwondo**, Red Belt

2009–PRESENT **XDA Developers**, Senior Member

2019–PRESENT **AAAI (Association for the Advancement of Artificial Intelligence)**, Professional Member

2019–PRESENT **ACM (Association for Computing Machinery)**, Professional Member  
Also part of the SIGHPC (Special Interest Group for High Performance Computing) & SIGHPC-Education

2019–PRESENT **ASAPBio (Accelerating Science and Publication in biology)**, Ambassador

2019–PRESENT **ICHEME (Institute of Chemical Engineers)**, Associate Member

2019–PRESENT **IICChE (Indian Institute of Chemical Engineers)**, Life Associate Member

2019–PRESENT **IEEE IAS (Industrial Applications Society)**, Member

2019–PRESENT **IEI (The Institution of Engineers [India])**, Associate Member

2019–PRESENT **InRaSS (Indian Radio Science Society)**, Student Member

2019–PRESENT **OSI (Open Source Initiative)**, Individual Member

2019–PRESENT **OSI (Optical Society of India)**, Life Fellow

2019–PRESENT **SPIE (Society of Photo-Optical Instrumentation Engineers)**, Early Career Professional

2019–PRESENT **The Carpentries**, Certified Instructor

2019–PRESENT **URSI (Union Radio-Scientifique Internationale)**, Corresponding Member

2020–PRESENT **Heterodox Academy**, Graduate Affiliate Member

2020–PRESENT **IGDORE (Institute for Globally Distributed Open Research and Education)**, Researcher-in-training

2020–PRESENT **COS (Center for Open Sciences)**, Ambassador

2020–PRESENT **ims (Institute of Mathematical Statistics)**, Student Member

2020–PRESENT **Bernoulli Society**, Student Member

2020–PRESENT **RSS (Royal Statistical Society)**, E-Student Member — > Fellow (2022)

2020–PRESENT **Computing at School**, Member

2021–PRESENT **TeX Users Group**, Member

2021–PRESENT **Nordic Research Software Engineers RY**, Board Member and founding Secretary (2021–2022)

2021–PRESENT **HPC Carpentry**, Member and Steering Council member (2022–2023)

2021–2025 **IOP SIG on Computational Physics**, Ordinary Member

2022–PRESENT **Biochemical Society**, UK, Graduate Member

2022–PRESENT **Federation of European Biochemical Societies (FEBS)**, Member

2022–PRESENT **BCS, the Chartered Institute of IT**, UK, Professional Member

2022–PRESENT **BCS Open Source Group**, Early Career Representative

2022–PRESENT **IOP Computational Physics Group**, Early Career Representative

2022–PRESENT **British Ecological Society**, Student Member

2022–PRESENT **RSC (Royal Society of Chemistry)**, Member (2022)

## Awards

SPRING 2021 **Tensor Methods and Emerging Applications to the Physical and Data Sciences**, *Institute for Pure and Applied Mathematics*, IPAM Fellow

DECEMBER 2016 **Photonics-2016**, *Indian Institute Of Technology Kanpur*, Springer Best Student Paper Award, Nonlinear-Optics Session

2014–2015 **IITG Zephyr Creative Writing**, *Indian Institute Of Technology Guwahati*, First Prize

2014–2015 **Antaragni IITK-MUN GA-DISEC**, *Indian Institute Of Technology Kanpur*, Best Speaker

## Reviews

2022–PRESENT **IOP - Journal of Physics B: Atomic, Molecular and Optical Physics**, *Reviewer*

2022–PRESENT **IOP - New Journal of Physics**, *Reviewer*

2021–PRESENT **IOP - Journal of Optics**, *Reviewer*

2021–PRESENT **IOP - Journal of Optics**, *Reviewer*

2021–PRESENT **IOP - Journal of Physics: Condensed Matter**, *Reviewer*

2021–PRESENT **APS Physical Review A**, *Reviewer*

2021–PRESENT **APS Physical Review E**, *Reviewer*

2021–PRESENT **APS Physical Review Applied**, *Reviewer*

2020–PRESENT **Nature Communications**, *Reviewer*

2020–PRESENT **APS Physical Review Letters**, *Reviewer*

2020–PRESENT **IOP - Machine Learning: Science and Technology**, *Reviewer*

2020–PRESENT **SPIE Journal of Micro/Nanolithography, MEMS, and MOEMS**, *Reviewer*

2020–PRESENT **Manning Publications**, *Technical Reviewer*

2020–PRESENT **JupyterCon 2020**, *Reviewer*

2020–PRESENT **Nature Communications**, *Reviewer*

2019–PRESENT **PeerJ - Life & Environment**, *Reviewer*

2019–PRESENT **PeerJ - Computer Science**, *Reviewer*

2019–PRESENT **PeerJ - Organic Chemistry**, *Reviewer*

2019–PRESENT **PLOS ONE**, *Reviewer*

2018–PRESENT **Journal Of Open Source Software**, *Reviewer*

**Editorial Positions**

2024–PRESENT **JOSS (Journal Of Open Source Software)**, *Editor*

## Grants Awarded

### Personal

2020–2023 **Icelandic Research Fund**, *Rannís*, 6650 thousand ISK, Doctoral Fellowship  
 TITLE: Magnetic interactions of itinerant electrons modeled using Bayesian machine learning.

### Project Leadership

2023 **Google Summer of Code**, *d-SEAMS*, 3,000 USD, Student Mentee  
 Funding generated to mentor a first time code contributor writing Python bindings for d-SEAMS.

2023 **NumFocus Small Development Grant**, *LFortran*, 10,000 USD, Software Engineer  
 Compiling SciPy's Fortran packages with LFortran.

2022 **Google Season of Docs**, *LFortran*, 10,000 USD, Technical writer  
 Funding generated to hire a technical writer full-time for two months.

2022 **NumFocus Small Development Grant**, *LFortran*, 4,600 USD, Software Engineer  
 Compiling SciPy with LFortran.

## Publications

### JOURNALS

Ondřej Čertík, John E. Pask, Isuru Fernando, Rohit Goswami, N. Sukumar, Lee. A. Collins, Gianmarco Manzini, and Jiří Vackář. “High-Order Finite Element Method for Atomic Structure Calculations.” In: *Computer Physics Communications* (Dec. 2023), p. 109051. DOI: 10.1016/j.cpc.2023.109051.

Laurence Kedward, Balint Aradi, Ondrej Certik, Milan Curcic, Sebastian Ehlert, Philipp Engel, Rohit Goswami, Michael Hirsch, Asdrubal Lozada-Blanco, Vincent Magnin, Arjen Markus, Emanuele Pagone, Ivan Pribec, Brad Richardson, Harris Snyder, John Urban, and Jeremie Vandenplas. “The State of Fortran.” In: *Computing in Science & Engineering* (2022). DOI: 10.1109/MCSE.2022.3159862. arXiv: 2203.15110.

Rohit Goswami, Amrita Goswami, and Jayant Kumar Singh. “d-SEAMS: Deferred Structural Elucidation Analysis for Molecular Simulations.” In: *Journal of Chemical Information and Modeling* (Mar. 2020). DOI: 10.1021/acs.jcim.0c00031. arXiv: 1909.09830.

Ligesh Theeyancheri, Subhasish Chaki, Nairhita Samanta, Rohit Goswami, Raghunath Chelakkot, and Rajarshi Chakrabarti. “Translational and Rotational Dynamics of a Self-Propelled Janus Probe in Crowded Environments.” In: *Soft Matter* (Aug. 5, 2020). DOI: 10.1039/D0SM00339E.

Rohit Goswami. “Don’t Pull Punches in Peer Review.” In: *Nature* 574 (Oct. 8, 2019), pp. 176–176. DOI: 10.1038/d41586-019-03024-2.

Prerna, Rohit Goswami, Atanu K. Metya, S. V. Shevkunov, and Jayant K. Singh. “Study of Ice Nucleation on Silver Iodide Surface with Defects.” In: *Molecular Physics* (Aug. 25, 2019), pp. 1–13. DOI: 10.1080/00268976.2019.1657599.

## CONFERENCE PROCEEDINGS

Rohit Goswami and Ruhila S. “High Throughput Reproducible Literate Phylogenetic Analysis (accepted).” In: *2022 Seventh International Conference on Parallel, Distributed and Grid Computing (PDGC)*. 2023.

Rohit Goswami, Ruhila S, Amrita Goswami, Sonaly Goswami, and Debabrata Goswami. “Reproducible High Performance Computing Without Redundancy with Nix (accepted).” In: *2022 Seventh International Conference on Parallel, Distributed and Grid Computing (PDGC)*. 2023.

Rohit Goswami. “Wailord: Parsers and Reproducibility for Quantum Chemistry.” In: *Proceedings of the 21st Python in Science Conference* (2022), pp. 193–197. DOI: 10.25080/majora-212e5952-021.

Rohit Goswami, Amrita Goswami, and Debabrata Goswami. “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, 2021, pp. 747–749. DOI: 10.1007/978-981-15-9259-1\_172.

Rohit Goswami, Amrita Goswami, and Debabrata Goswami. “Space Filling Curves: Heuristics For Semi Classical Lasing Computations.” In: *2019 URSI Asia-Pacific Radio Science Conference (AP-RASC)*. Mar. 2019, pp. 1–4. DOI: 10.23919/URSIAP-RASC.2019.8738612.

Rohit Goswami and Debabrata Goswami. “Quantum Distributed Computing with Shaped Laser Pulses.” In: *13th International Conference on Fiber Optics and Photonics* (2016). DOI: 10.1364/photonics.2016.w4c.3.

## PREPRINTS

Rohit Goswami, Ruhila S., Amrita Goswami, Sonaly Goswami, and Debabrata Goswami. *Unified Software Design Patterns for Simulated Annealing*. Feb. 6, 2023. arXiv: 2302.02811 [physics].

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## Conference Records

### Posters

- APRIL 2024 **Inferring Multicomponent Properties Through Thermal Lens**, *APS April Meeting 2024*, [R. Goswami](#), S. Goswami, and D. Goswami
- MARCH 2024 **Simulated Annealing for Global Search**, *APS March Meeting 2024*, [R. Goswami](#), R. S., A. Goswami, S. Goswami, and D. Goswami
- MARCH 2023 **Towards Modular Components for Phylogenetic Estimation**, *APS March Meeting 2023*, [R. Goswami](#), R. S.
- JULY 2022 **Wailord: Parsers and Reproducibility for Quantum Chemistry**, *SciPyCon 2022*, [R. Goswami](#)
- JULY 2022 **LPython: Interactive LLVM-based Python Compiler for Modern Architectures**, *SciPyCon 2022*, O. Čertík, B. Beckman, N. Gera, S. Lunagariya, G. Singh, [R. Goswami](#), T. Shaktivel, and D. Edwards
- MARCH 2020 **Ultrafast Insights for Predictive Fragrance Compounding**, *ACS Spring 2020 National Meeting*, [R. Goswami](#), A. K. Rawat, D. Chakrabarty, and D. Goswami
- DECEMBER 2019 **Qubit Network Barriers to Deep Learning**, *IEEE WRAP-2019*, [R. Goswami](#), A. Goswami, and D. Goswami
- MARCH 2019 **Space Filling Curves: Heuristics For Semi Classical Lasing Computations**, *URSI Asia-Pacific Radio Science Conference (AP-RASC 2019)*, [R. Goswami](#), A. Goswami, and D. Goswami



- DECEMBER 2018 **FDTD Numerical Computations for Ultrafast Non-linear Optics**, *Photonics-2018*, [R. Goswami](#), A. Goswami, and D. Goswami
- Oral Presentations**
- MAY 2024 **Throwaway Gaussian Processes for Saddle Searches**, *Machine Learning in Chemical and Materials Sciences 2024*, [R. Goswami](#)
- APRIL 2024 **PySEAMS: Pythonic Structural Elucidation Analysis for Molecular Simulations**, *APS April Meeting 2024*, [R. Goswami](#), R. S., and A. Goswami
- MARCH 2024 **Revisiting Scaling Assumptions of Ab-Initio Calculations**, *APS March Meeting 2024*, [R. Goswami](#)
- FEBRUARY 2024 **Scaling workflows from development to HPC**, *14<sup>th</sup> Icelandic HPC Community Workshop*, [R. Goswami](#)
- FEBRUARY 2024 **Development, Benchmarks and Workflows**, *CECAM-ESL: Advancing the Molecular Paradigm*, [R. Goswami](#)
- DECEMBER 2023 **Computational Chemistry and Possible Tensor Applications**, *IPAM TMRC2 (Tensor Methods Reunion Conference)*, [R. Goswami](#)
- APRIL 2023 **High-order finite element method for atomic structure calculations**, *APS April Meeting 2023*, [R. Goswami](#), O. Čertík, J. E. Pask, I. Fernando, L. A. Collins, G. Manzini, N. Sukumar, and J. Vackář
- MARCH 2023 **Enhancing slideware for computational physics education**, *APS March Meeting 2023*, [R. Goswami](#)
- MARCH 2023 **Intermediate Representations for Quantum Computing**, *APS March Meeting 2023*, [R. Goswami](#), S. Goswami and D. Goswami
- DECEMBER 2022 **Reproducible engines and interfaces on heterogeneous compute resources for structural analysis of deformed systems**, *APS Mid-Atlantic Section 2022 Meeting*, [R. Goswami](#), Accepted
- NOVEMBER 2022 **High Throughput Reproducible Literate Phylogenetic Analysis**, *IEEE PDGC-2022*, [R. Goswami](#), R. S.
- NOVEMBER 2022 **Reproducible High Performance Computing Without Redundancy with Nix**, *IEEE PDGC-2022*, [R. Goswami](#), R. S., A. Goswami, S. Goswami and D. Goswami
- NOVEMBER 2022 **Reproducible Literate Programming Workflows for Censored Data**, *IOP Machine Learning for Healthcare*, [R. Goswami](#), R. S.
- AUGUST 2022 **Reproducible Environments on Elja with Nix and Spack**, *6<sup>th</sup> Icelandic HPC Community Workshop*, [R. Goswami](#)
- JULY 2022 **Maintaining Fortran in Python in Perpetuity**, *SciPyCon 2022*, [R. Goswami](#), M. Mendonca, R. Gommers, and T. Shaktivel
- SEPTEMBER 2021 **f2py: Two Decades Later**, *FortranCon 2021*, [R. Goswami](#), R. Gommers, M. Mendonca, and P. Peterson
- SEPTEMBER 2021 **Implementing Fortran Standardese within LFortran**, *FortranCon 2021*, [R. Goswami](#) and O. Čertík
- AUGUST 2021 **Continuous Integration and TeX with Org-Mode**, *TUG21, 42nd Annual Conference of the TeX Users Group*, [R. Goswami](#)
- JULY 2021 **Modern documentation across languages**, *ACM SERI 2021*, [R. Goswami](#)
- OCTOBER 2020 **Nix from the dark ages (without Root)**, *NixCon 2020*, [R. Goswami](#), Lightning Talk
- OCTOBER 2020 **Reproducible Scalable Workflows with Nix, Papermill and Renku**, *PyCon India 2020*, [R. Goswami](#)
- AUGUST 2020 **Reproducible Environments with the Nix Packaging System**, *CarpentryCon 2020*, [R. Goswami](#) and A. Goswami
- JULY 2020 **LFortran: Interactive LLVM-based Fortran Compiler for Modern Architectures**, *FortranCon 2020*, O. Čertík, N. Maan, A. Pandey, M. Curcic, P. Brady, Z. Jibben, N. Carlson, [R. Goswami](#), A. Shahmoradi and A. Markus, Presented by Ondřej
- DECEMBER 2019 **Process Safety in terms of Latent Dirichlet Allocations**, *72nd Annual Session of of the Indian Institute of Chemical Engineers, CHEMCON-2019*, [R. Goswami](#), Accepted
- OCTOBER 2019 **Semi-Supervised Approaches to Ultrafast Optimal Control Theory**, *43rd Symposium of the Optical Society of India, International Conference on Optics & Electro-Optics*, [R. Goswami](#), A. Goswami and D. Goswami

- DECEMBER 2016 **Quantum Distributed Computing with Shaped Laser Pulses**, *13th International Conference on Fiber Optics and Photonics*, [R. Goswami](#) and D. Goswami  
[Sprint Mentorship](#)
- DECEMBER 4<sup>th</sup> 2022 **NumPy Sprint**, *PyData Global 2022*, G. Kathiresan, I. Pawson, [R. Goswami](#), and M. Pahari
- SEPTEMBER 16<sup>th</sup> 2022 **NumPy Sprint**, *Grace Hopper Open Source Day 2022*, [R. Goswami](#), R. Barnowski, B. Sipőcz, M. Mendonca and I. Pawson
- OCTOBER 30<sup>th</sup> 2021 **NumPy-SciPy Sprint**, *PyData Global 2021*, M. Mendonca, M. Picus, [R. Goswami](#), R. Gommers and M. Pahari
- SEPTEMBER 20<sup>th</sup> 2021 **NumPy Sprint**, *PyCon India 2021*, M. Mendonca, [R. Goswami](#) and M. Pahari

## Workshops and Schools

- FEBRUARY 2024 **Electronic Structure Software Development: Advancing the Modular Paradigm**, *CECAM-HQ, EPFL Lausanne*, Was an invited speaker to discuss scaling workflows from development machines to HPC centers and to provide a FOSS perspective into electronic structure codes.
- NOVEMBER 2023 **Quantum2 on Machine Learning Enhanced Sampling**, *CECAM-HQ, EPFL (Online)*, Explored the integration of machine learning potentials with enhanced sampling in molecular dynamics to address nuclear quantum effects, with discussions on advancing accuracy in chemical reactions study.
- SEPTEMBER 2023 **FAIR and TRUE Data Processing for Soft Matter Simulations**, *CECAM-DE-SMSM (Online)*, Focused on FAIR and TRUE data management in molecular simulations; highlighted standardization, metadata interoperability.
- JULY 2023 **Machine-learned potentials in molecular simulation: best practices and tutorials**, *CECAM-AT (Online)*, On the advancement and application of machine-learned potentials in molecular simulation, featuring discussions on best practices, tutorials, and collaborative efforts to integrate ML into various chemistry research areas.
- JUNE 2023 **Saddle point Search algorithms: towards the definition of a common BENCHMARK framework**, *CECAM-FR-GSO LAAS-CNRS (Online)*, Aimed at developing a unified benchmark for saddle point identification methods in potential energy surfaces for computational materials science.
- OCTOBER 2022 **Introduction to oneAPI, SYCL2020 and OpenMP offloading**, *High-Performance Computing Center Stuttgart (HLRS)*, A ten-hour long hands-on introduction to newer methodologies to heterogeneous computations in HPC work-spaces.
- OCTOBER 2022 **SciML GPU Programming Bootcamp**, *High-Performance Computing Center Stuttgart (HLRS) and NVIDIA*, A guided tour of Physics Inspired Neural Networks (PINNs) for solving differential equations.
- OCTOBER 2022 **Electronic Structure Software Development: Best Practices and Tools**, *CECAM-HQ, EPFL Lausanne*, Was an invited panelist (representing NumPy) for accelerating the Electronic Structure Library initiative projects with FOSS best practices.
- JUNE 2022 **Error control in first-principles modeling**, *CECAM-HQ, EPFL (Online)*, A statistical perspective on controlling numerical errors in ab-initio methods.
- MARCH 2022 **Recent Advances in Machine Learning Accelerated Molecular Dynamics**, *CECAM-DE-JUELICH*, An HPC workflow focused practical introduction to using exotic compute devices for ML in MD.
- JANUARY 2022 **MolSim2022**, *CECAM-NL*, A flagship two week virtual school attended to brush up on the fundamentals of computational chemistry (at the molecular level) and also to reconnect with the community.
- OCTOBER 2021 **PRACE Autumn School 2021**, *CSC-IT Center for Science, Finland*, This 5-day course held in Vuokatti, consists of lectures and hands-on training on modern, GPU-accelerated high-performance computing: GPU programming and GPU code optimization at scale, as well as understanding and applying machine learning methods emphasizing usage on LUMI.
- AUGUST-SEPTEMBER 2021 **Multiple scattering Green's function for electronic structure and spectroscopy calculations**, *Les Houches Physics School, France*, Two week school covering mathematical foundations and applications using Green's function and T-matrix approaches for condensed matter.

- AUGUST 2021 **Seventh LAMMPS Workshop and Symposium**, *Online*, Three day tutorial and overview of recent results led by the LAMMPS developers.
- JULY 2021 **AiiDA Virtual Tutorial**, *EPFL, Lausanne, Switzerland*, A five day online in-depth tutorial by core and plugin developers covering programming practices including a hackathon on workflows and plugins.
- JUNE 2021 **Comscope Summer School**, *Virtual, Comscope, US*, Covers dynamical mean field theory and electronic structure codes using FlapwMBPT, LDA+, LQSGW+DMFT, RISB+LDA by tutorials and training from professionals at BNL and Rutgers.
- JUNE 2021 **Virtual Summer School on Theoretical Methods for Energy Conversion**, *International Center for Advanced Studies of Energy Conversion (ICASEC) and the RTG2455 BENCH*, The Summer School provided a comprehensive picture of state-of-the-art theoretical methods in the field, combining tutorial and research lectures into a 3-day event. The topics covered spanned electronic structure methods, dynamics and machine learning approaches.
- JUNE 2021 **MPI and OpenMP in Scientific Software Development**, *PRACE @ SURF, NL*, An in-depth application oriented three day event with concrete examples in C++ involving guest lectures from distinguished speakers and covering parallel I/O, debugging performance bottlenecks, multi-grid and mesh methods, along with more of the OpenMPI standard; culminated with examples of using OpenMP for GPUs; from the PRACE training center at SURF.
- JUNE 2021 **Basic Parallel Programming with MPI and OpenMP**, *SURF, NL*, A refresher on OpenMPI and OpenMP for both Fortran and C++ usage, involving the HLRI materials.
- MAY 2021 **Efficient Tensor Representations for Learning and Computational Complexity**, *Institute for Pure and Applied Mathematics, US*, The fourth of the core IPAM long program workshops; focusing on algorithmic complexity and usage.
- MAY 2021 **Mathematical Foundations and Algorithms for Tensor Computations**, *Institute for Pure and Applied Mathematics, US*, The third of the core IPAM long program workshops; focusing on numerical analysis and linear algebra for tensor networks and their computation.
- APRIL 2021 **Tensor Network States and Applications**, *Institute for Pure and Applied Mathematics, US*, The second of the core IPAM long program workshops; focusing on tensor network states; their topology and applications.
- MARCH-APRIL 2021 **Tensor Methods and their Applications in the Physical and Data Sciences**, *Institute for Pure and Applied Mathematics, US*, The first of the workshops which form the core of the IPAM long program; focusing on representations of basic tensor networks in various disciplines and their computation
- MARCH 2021 **SWiMM: School on Simulation Workflows in Materials Modelling**, *CECAM School*, Two week long program focused on the familiarization with tools for high-throughput HPC workflows including AiiDA and PyIron along with tools ontological exploration.
- MARCH 2021 **Workflows for Atomistic Simulations**, *Ruhr-Universität Bochum*, A three day intensive workshop consisting of hands-on sessions working with PyIron followed by lectures and discussions on potential and forcefield development.
- MARCH 2021 **Tensor Method Tutorials**, *Institute for Pure and Applied Mathematics, US*, Part of my long program participation in the Tensor Methods and Emerging Applications to the Physical and Data Sciences. A two week long exposure to the basics of the program, and recent advances for context.
- JANUARY 2021 **IPWin2021: Inverse problems in partial differential equations and geometry**, *Technical University of Denmark*, Virtual winter school providing an introduction to modern and hot topics in inverse problems based on three series of embedded lectures given by internationally recognized researchers.
- JANUARY 2021 **BerkeleyGW Workshop and Berkeley Excited States Conference**, *Virtual*, An event focused on the BerkeleyGW software, split between a three day practical tutorial and a two day conference.
- OCTOBER 2020 **Computational materials discovery of unconventional magnets**, *EPFL, Lausanne, Switzerland*, The proposed workshop aims to bring together researchers both from theory and experiments working on different aspects of the field to present the latest advancements and to discuss the efforts required to expedite the discovery of new unconventional magnetic materials.

- OCTOBER 2020 **ESPResSo and Python: Versatile Tools for Soft Matter Research**, *CECAM School*, The school focused on the introduction of particle-based coarse-grained Molecular Dynamics simulation techniques for Hard and Soft Matter systems with the freely available software package ESPResSo. Included lectures and hands-on sessions.
- SEPTEMBER 2020 **Excited Charge Dynamics in Semiconductors**, *ICTP, Trieste*, An online workshop to discuss recent progress in the investigation of dynamics of excited charges in semiconductors.
- SEPTEMBER 2020 **(Machine) learning how to coarse-grain**, *CECAM and TRR146 Virtual Event*, The purpose of this workshop will be to discuss the current state of the art, some of the challenges that the community is facing in furthering the penetration of ML models in CG simulations, and future perspectives.
- SEPTEMBER 2020 **Gaussian Process and Uncertainty Quantification Summer School**, *University of Sheffield, UK*, The Gaussian Process Summer Schools are a series of schools and workshops aimed at researchers who want to understand and use Gaussian process models, both in theory and practice.
- JULY 2020 **AiiDA Virtual Tutorial**, *EPFL, Lausanne, Switzerland*, A four day online in-depth tutorial by core and plugin developers covering the nuances of reproducible workflows for AiiDA with example Quantum ESPRESSO calculations on Quantum Mobile virtual machines.
- JUNE 2020 **Mathematical Methods of Modern Statistics 2**, *CIRM Virtual Event*, A five day online event from the Centre International de Rencontres Mathématiques on recent statistical advances relating to the analysis of high dimensional data from frequentist and Bayesian perspectives.
- MAY 2020 **ALCF Computational Performance Workshop**, *Online*, A three day workshop on the hardware and software improvements organized by Argonne Leadership Computing Facility.
- OCTOBER 2019 **TriangleSCI 2019**, *Invited to the Triangle Scholarly Communication Institute*, 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, **declined to attend**
- MAY-JUNE 2019 **Artificial Intelligence**, *E & ICT Academy, IIT Kanpur*, A four week course on AI foundations culminating in a time-series prediction project.
- JUNE 2019 **AI Foundations Certificate Course**, *univ.ai*, A summer school taught in-person by faculty from Harvard and UCLA, culminating in a computer vision and neural network based identification project.
- JULY 2019 **Rare Events Summer School**, *Indian Institute of Science, Bangalore*, A short course consisting of lectures and hands-on sessions by experts in the field, organized by Prof. Baron Peters.

### Short Courses

- SEPTEMBER 23<sup>rd</sup> 2019 **Surface Area and Porous Material Characterization**, *Dept. of ChemE, IIT Kanpur*, An intensive day long course on the basics of experimental classification and DFT methods for pore distribution by Dr. Martin Thomas from Anton-Paar.
- SEPTEMBER 21<sup>st</sup> 2019 **OpenACC GPU Bootcamp**, *Chemistry Department, IIT Kanpur*, Day long programming session and discussion covering the acceleration of Institute in-house code facilitated by a Senior Nvidia Solution Architect (Mr. Bharatkumar) and Prof. Debabrata Goswami.

## Certifications

### Coursera

- MARCH 2020 **Deep Learning Specialization**, *deeplearning.ai*, 99.5%  
The specialization can be verified by ID Q3DLMZJ42TR. 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

- JAN-APR 2019 **Graph Theory**, *IISER Pune*, 55%  
License: NPTEL19MA13S21460067

- AUG-SEP 2018 **Computational Chemistry and Classical Molecular Dynamics, IIT Bombay, Elite, 77%**  
License: NPTEL18CS13S21440127
- AUG-SEP 2018 **Introduction to Parallel Programming in OpenMP, IIT Madras, 40%**  
License: NPTEL18CS55S11440122
- JAN-APR 2018 **Quantum Computing, IIT Kanpur, Elite, 65%**  
License: NPTEL18CY07S4480024

## Graduate Coursework

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

- SUMMER 2020 **Seminar on Machine Learning, University of Iceland, Computer Science Dept., Pass**  
Research seminar.  
PRESENTATION: Graph Neural Networks
- SUMMER 2020 **Statistics, science and COVID-19, University of Iceland, Health Sciences Institute, 10**  
Course covering “Statistical Rethinking” by Richard McElreath as well as the COVID-19 model of the University.
- SPRING 2020 **Probabilistic Data Analysis, University of Turku, Finland, Turku Data Science group**  
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
- SPRING 2020 **Applied data analysis, University of Iceland, Mathematics and Applied Statistics Dept., 10**  
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
- SPRING 2020 **Applied data analysis - Project, University of Iceland, Mathematics and Applied Statistics Dept., Pass**  
Extra credit course  
PROJECT: Molecular Dynamics Trajectory Analysis
- SPRING 2020 **Machine Learning, University of Iceland, Computer Science Dept., Pass**  
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)
- SPRING 2020 **Software Quality Management, University of Iceland, Pass**  
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)
- SPRING 2020 **Introduction to Pattern Recognition, University of Iceland, Electrical Engineering Dept., 8**  
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