Rohit Goswami

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WORK EXPERIENCE

LAB COSMO, EPFL | Systems Specialist (Postdoctoral Researcher)
2025 – Present | Lausanne, Switzerland

- Developing the `metatensor` ecosystem for interoperable atomistic machine learning with Prof. Michele Ceriotti and Dr. Guillaume Fraux
- Integration of machine learning potentials with GROMACS; DLPack support for zero-copy tensor interoperability across C++, Python, Rust, and Fortran

QUEEN'S UNIVERSITY | Visiting Researcher
2025 | Kingston, Canada

- Scaling off-lattice / object kinetic Monte Carlo to over a million atoms for radiation damage modeling with Prof. Laurent Béland

UNIVERSITY OF ICELAND | Doctoral Researcher (Rannís Doctoral Grant PI)
2019 – 2024 | Reykjavík, Iceland

- Principal investigator: "Magnetic interactions of itinerant electrons modeled using Bayesian machine learning" (Rannís Research Fund)
- Developed Gaussian process accelerated saddle point search methods (climbing image NEB, dimer) with adaptive pruning
- Bayesian hierarchical models for quantitative benchmarking of saddle search algorithms

QUANSIGHT LABS | Software Engineer II
2021 – 2025 | Remote (Austin, TX)

- Maintained `f2py` (NumPy's Fortran-to-Python interface) and foundational FOSS scientific codebases
- Contributed to `scipy`, `meson-python`, and `LFortran` compiler development

IIT KANPUR | Senior Project Associate / Project Associate
2018 – 2020 | Kanpur, India

- Computational nanoscience group: ice nucleation analysis (CHILL+), GPU-accelerated MD tools; created `d-SEAMS`
- Femtolab: femtosecond laser approaches to quantum information and computation

EDUCATION

UNIVERSITY OF ICELAND | Ph.D. Physical Sciences
2019 – 2025 | Reykjavík, Iceland
Thesis: "Efficient Exploration of Chemical Kinetics". Supervised by Prof. Hannes Jónsson.

HBTU KANPUR | B.Tech. Chemical Engineering
2014 – 2018 | Kanpur, India
First Division.

SELECTED PUBLICATIONS

[9] **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.

[8] 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].

[7] **Goswami, Rohit**. **11th Aug. 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.

[6] **Goswami, Rohit** and Jónsson, Hannes. **27th Nov. 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.

[5] **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.

[4] **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.

[3] 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.

[2] 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.

[1] **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.

GRANTS AND AWARDS

COST ACTION CA23158 CO-PROPOSER | 575K EUR, 2025–2029
European Cooperation in Science and Technology network proposal.

RANNÍS DOCTORAL RESEARCH GRANT | 6650K ISK, 2020–2023
Icelandic Research Fund grant as PI for Bayesian ML applied to saddle point searches.

NUMFOCUS SMALL DEVELOPMENT GRANT | $5000 USD, 2020
For `d-SEAMS` molecular simulation analysis engine.

SPRINGER BEST STUDENT PAPER AWARD | Photonics 2016

SELECTED SERVICE

- **JOSS Editor** (2024–present) – Journal of Open Source Software, topic editor
- **NumFOCUS GSoC Admin** (2024–present) – Coordinating Google Summer of Code across NumFOCUS projects
- **IEEE P3173 Vice Chair** (2022–present) – Standard for Endocrine Disrupting Chemical Hazard Labelling
- **Nordic-RSE** – Board Member; founding Secretary of the Nordic Research Software Engineers association
- **IHPC Consultant** (2021–2024) – Simulation and Data Lab Computational Chemistry, National HPC center of Iceland
- **Reviewer**: Nature Comms, PRL, PRA, PRE, JOSS (80+), PLOS ONE, IOP journals, PeerJ

SELECTED PRESENTATIONS

- **ACS Fall 2025** – "Managing concurrency for high throughput adaptive kinetic Monte Carlo" (Washington, DC)
- **Psi-k 2025** – "Advocating for standardized APIs for common procedures" (Liverpool, UK)
- **Kernel aKMC 2025** – "Towards a million atoms and a thousand KMC steps a day" (Queen's, Canada)
- **APS Global Physics Summit 2025** – "Contending with concurrency across programming languages" (Anaheim, CA)
- **CECAM-LTS-MAP 2024** – "Accelerating Saddle Searches with Gaussian Process Regression" (Invited, Lausanne)
- **IPAM TMRC2 2023** – "Computational Chemistry and Possible Tensor Applications" (Invited, UCLA)
- **14th Icelandic HPC Workshop 2024** – "Scaling workflows from development to HPC"

OPEN SOURCE SOFTWARE

- **d-SEAMS** (co-creator) – Molecular dynamics trajectory analysis engine (JCIM 2020, NumFOCUS SDG funded)
- **f2py / NumPy** (maintainer) – Fortran-to-Python interface generator; core NumPy component
- **fastMatMR** – rOpenSci reviewed R bindings for fast Matrix Market I/O
- **wailord** – Python library for ORCA quantum chemistry workflows (SciPy 2022)
- **flowy** – High performance probabilistic lava emplacement prediction (CPC 2025)
- **eOn** (maintainer) – Long timescale dynamics code with Gaussian Process accelerated saddle searches
- **metatensor** (maintainer) – Atomistic machine learning toolkit (JCP 2026)

TECHNICAL SKILLS

HPC: LAMMPS, GROMACS, MPI, CUDA, Nix, Spack, EasyBuild, Slurm, containers (Docker/Singularity)
Languages: C++, Python, Fortran, Rust, R, Julia, Shell
Tools: CMake, Meson, Git, CI/CD (GitHub Actions, Azure), LaTeX, Emacs
ML/Data: PyTorch, scikit-learn, GPy, Stan, Bayesian optimization, Gaussian processes

PROFESSIONAL MEMBERSHIPS

IOP (MInstP) • RSC (MRSC) • BCS (MBCS) • ACM • APS • IEEE • AIChE