Rahul Sharma

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DOB: Dec 25, 1992

Professional Experience

June 2023–Present **Center of Genomic Reserach, AstraZeneca PLC, Cambridge, UK**, *Post-doctoral researcher.*

Jan–May 2023 **École Polytechnique Fédérale de Lausanne (EPFL)**, *Post-doctoral researcher.*

Education

2018–2022 **EPFL**, *Doctor of Philosophy*, Applied Mathematics: supervised by Prof. John H. Maddocks.

2012–2017 **Indian Institute of Technology Roorkee (IITR)**, *Integrated Bachelor's and Master's degree, Chemistry (with specialization in Computational Chemistry)*.
– Department Gold medal
– Master's thesis undertaken at the University of Oxford: supervised by Prof. Jonathan Doye

Selected Publications

- Giniūnaitė, R., **Sharma, R.**, Maddocks, J. H., Kriaučionis S. and Petkevičiūtė-Gerlach, D. Nucleosome forming energy in CpG islands and the role of epigenetic base modifications. eLife, 2024.
- **Sharma, R.**, Patelli, A. S., Bruin, L. D., and Maddocks, J. H. cgNA+web: A web-based visual interface to the cgNA+ sequence-dependent statistical mechanics model of double-stranded nucleic acids J. Mol. Biol. 2023
- Dasgupta, A., **Sharma, R.**, Mishra, C., and Nagaraja, V. H. Machine learning for optical motion capture-driven musculoskeletal modeling from inertial motion capture data. Bioengineering, 2023.
- **Sharma, R.**, Dasgupta, A., Cheng, R., Mishra, C., and Nagaraja, V. H. Machine Learning for Musculoskeletal Modeling of Upper Extremity. IEEE Sens. J., 2022.
- Bauer, B., **Sharma, R.**, Chergui M., and Oppermann M. Exciton decay mechanism in DNA single strands: back-electron transfer and ultrafast base motions. Chem. Sci., 2022.
- Rosa et al. Sequence-dependent structural properties of B-DNA: what have we learned in 40 years? Biophys. Rev., 2021.
- **Sharma, R.**, Schreck, J. S., Romano, F., Louis, A. A., and Doye J. P. K. Characterizing the Motion of Jointed DNA Nanostructures Using a Coarse-Grained Model. ACS Nano, 2017.
- Goerigk, L. and **Sharma, R.**. The INV24 Test Set: How Well do Quantum-Chemical Methods Describe Inversion and Racemization Barriers? Can. J. Chem., 2016.
- Roy, T. K., **Sharma, R.** and Gerber, R. B. First-principles anharmonic quantum calculations for peptide spectroscopy: VSCF calculations and comparison with experiments. Phys. Chem. Chem. Phys., 2016.

Awards and achievements

- Department Gold medal, Integrated Bachelor's and Master's, IITR
- Awarded DAAD WISE scholarship (2015), MITCAS Globalink Research Internship (2016) (offer declined)
- Bursary award for summer school Energy & Sustainability at Leiden University (2015), for research interns at the University of Oxford (2016, 2017) and the University of Melbourne (2014)
- Awarded INSPIRE fellowship (2012-2017) by Department of Science & Technology, India
- Rank in top 0.005% (≈ 0.6 million applicants) in Joint Entrance Exam 2012 leading to IITR enrollment

Research Experience

- "**cgNA+: A sequence-dependent coarse-grain model of double-stranded nucleic acids**", PhD thesis , under supervision of Prof. John H. Maddocks, Institute of Mathematics, EPFL (2018-2022)
  Developed a coarse-grain model for sequence-dependent mechanics of double-stranded nucleic acids (dsNAs), including dsDNA, dsRNA, Hybrid DNA:RNA, and epigenetically modified dsDNA using supervised learning. cgNA+

model explicitly treats bases and phosphates as rigid bodies, and for a given sequence, it predicts the corresponding sequence-dependent equilibrium distribution. The first part of the thesis involved performing large-scale molecular dynamics (MD) simulations for dsNA, which were used for training (and testing) the cgNA+ model. Subsequently, cgNA+ parameters ($>$ 20,000) were trained by minimizing the Kullback-Leibler divergence between the observed Gaussian pdfs in MD simulations and cgNA+ predicted pdfs for the training library using an in-house MATLAB code. The second part of the thesis was dedicated to exploring sequence-dependence in various mechanical features of dsNAs, e.g., persistence length, groove widths, and equilibrium shape, and addressing exciting questions such as the influence of epigenetic modifications on groundstate and flanking sequence role in single-nucleotide polymorphism. We obtained strong sequence-specific patterns in the mechanical behavior of NAs by studying millions of sequences (only possible due to the highly efficient cgNA+ model) and scanning part of the human genome using bioinformatics tools and clustering. Furthermore, we developed insights into DNA deformation modes by investigating experimental (Protein-DNA X-ray) data using PCA and clustering and showed that findings were consistent with cgNA+ predictions. Finally, a deep learning tool was developed to locate the position of sugar atoms (treated implicitly in the cgNA+ model) in any coarse-grained configuration. Thus, cgNA+ tools allow generating an ensemble of *atomistic configurations* for a given sequence in negligible time which takes around 2-3 months of GPU computations using traditional MD simulations.

- "**Machine learning applications in biomechanical modeling**" in collaboration with Dr. Challenger Mishra, University of Cambridge & Dr. Vikranth H. Nagaraja, University of Oxford (2021-present)
  Explored neural network (NN) applications in predicting biomechanical variables from experimental motion capture data. In particular, we developed machine learning (ML) models (implemented by me) to map Inertial & Optical Motion Capture data (IMC & OMC) to outputs from musculoskeletal (MSK) model, which is computationally expensive and laborious to use, making feasible real-time predictions for potential clinical and sports applications. In a series of projects, we (i) demonstrated a proof-of-concept for NN applications in human upper-extremity MSK modeling, (ii) developed a unique approach to predict *gold-standard* (but lab-based) OMC-quality MSK outputs from highly portable (but less reliable) IMC data making possible real-time highly accurate predictions in outdoor settings, and (iii) analyzed various NN architectures and protocols to set up ML best-practices for such applications.
- "**Characterizing the motion of jointed DNA nanostructures using a coarse-grained model**" & "**Topological challenges in DNA origami assembly**" with Prof. Jonathan Doye and Prof. Ard A. Louis, University of Oxford, Internship (2016) and Master's thesis (2017)
  (a) Performed large-scale MD simulations to simulate flexible DNA nanostructures using the oxDNA model. We obtained insights into their structural and mechanical behavior and their functioning, thus, aided the design process of complex DNA nanostructures (b) Performed Monte Carlo (MC) simulations and advanced MC techniques (Umbrella sampling) to explore the thermodynamics of DNA self-assembly, focusing on the topological defects which obstruct the assembly completely or sometimes lead to ill-formed nanostructures. This study provided thermodynamic cost of various topological defects and set up guidelines for origami design to minimize such defects.

Technical Skills

Prog. Lang.	Python & Bash (proficient), MATLAB (intermediate), C++ & JavaScript (elementary)
Frameworks	Keras, PyTorch
Others	Bio-informatics, TensorFlow, Data science, Git, High-performance computing, LaTeX, Machine learning, Molecular dynamics, Monte Carlo, Statistical modeling, Statistics

Soft Skills

- Leadership, teamwork, organization, and management
  - Supervised two semester research projects at EPFL (2020, 2022)
  - Core Committee member (2019-2021), YUVA, EPFL
  - Coordinator (2014) and Convener (2016), Dept. of Chemistry, Tech-Fest, IITR of a 12-member team
  - Secretary, Sankalp 2015, Annual fest of National Service Scheme, IITR of a 28-member team
- Excellent communication and presentation skills
- Enthusiastic and quick learner
- Independent and initiator with excellent problem-solving and time-management skills
- Academic and professional writing skills (with experience in writing manuscripts and grants)

Selected poster and presentation

2022 Presentation at “Machine Learning Meets Statistical Mechanics: Success and Future Challenges in Biosimulations” at CECAM-IT-SIMUL, Sorrento

2019 Presentation at “oxDNA users and developers workshop” at the University of Oxford

2019 Poster at “Annual MolSim summer school” in Amsterdam

2018 Poster at “Frontiers of coarse-graining in molecular dynamics”, CECAM workshop in Berlin

2016 Presentation at "Nanotechnology for medicine and health care", Tech-Fest, IITR (1^{st} Prize)

Teaching and supervising at EPFL

2022 Co-supervising semester project on “Coarse-grain modeling of nucleic acids”

2020 Supervised semester project on “Unsupervised ML for analyzing protein-DNA Xray data”

2020, 2022 Teaching assistant for “Mathematical modeling of DNA”, MATH-481 (autumn semesters)

2018-2021 Teaching assistant for “Linear Algebra”, MATH-111 (spring semesters)

2019 Principal teaching assistant for “Analysis II”, MATH-106 (autumn semester)

Beyond academic activities

- Outreach activities
  - Former member of Child Rights and You (2015-2017) and National Service Scheme, IITR (2013-2016) — received “Executive Member Certificate” for being a highly dedicated volunteer for three years
  - Volunteered in Squishy Soft Science event, 2016, University of Oxford
- Sports: Cricket, Hiking, and Swimming
- Hobbies: Cooking and traveling

References

Prof. John H. Maddocks
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