Aditya Sengar, PhD

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Interdisciplinary computational researcher with 8+ years of expertise in computational biology and chemistry. I am currently working at Imperial College London in the field of computational DNA nanotechnology where I perform large scale numerical simulations to study nucleic acid systems. Proven track record in problem-solving as demonstrated in my PhD research and the success of my data science consulting firm.

Research Software Skills

- *Python* (pandas, scikit, pytorch, keras, tensorflow): Used in 15+ projects (3 at postdoctoral level, 12 in freelancing projects).
- *Linux*: Used in running simulations and managing college cluster at postdoctoral and PhD level.
- *Mathematica*: Used in 10+ projects (3 at postdoctoral level, 3 at PhD level, 5+ at undergrad level).
- *C*: Used in 3 projects at PhD level.
- *C++:* Gave training sessions to Master students at PhD level, used in 1 project at undergraduate level.
- *Matlab*: 3 projects during freelancing; 10+ projects/assignments at undergraduate level.
- *Java*: Used in 4 projects at undergraduate and senior secondary school level.
- *Other softwares: SQL*, *Bash*

Employment

Postdoctoral Research Associate, Imperial College London, *Mar 2020 - Now*

- Developed methods including machine learning assisted kinetics calculation, enhanced sampling, free energy calculation techniques for a coarse-grained DNA model, oxDNA. Managed and ran **large scale numerical simulations** on university **cluster**; developed and executed Bash scripts for task automation; created data analysis pipelines to analyse large amounts (TBs) of simulation data which aided in the interpretation of experimental results.
- Spearheaded **collaborations with experimental researchers** from University of Cambridge, Imperial College, University of Surrey, AMOLF Amsterdam.
- Utilised oxDNA to perform to demonstrate the effects of the presence of a bulge on the kinetics and thermodynamics of diffusion of the Holliday junction. Combined **VMMC sampling** with WHAM algorithms to discover a unique phenomenon of bulge diffusion.
- Developed a forward flux sampling (FFS) algorithm (enhanced kinetics prediction methods) in **Python** to demonstrate the effect of sequence dependence on the binding characteristics of a single stranded DNA to an allosteric domain on a double stranded DNA strand.
- Developed a comprehensive database of computationally calculated hybridisation rates of DNA as a function of sequence and presence of secondary structures. Designed a multimodal AI architecture consisting of GRU networks and feed forward neutral nets that predict these rates with 91% accuracy.
- Leveraged NUPACK to design a DNA based kinetic proofreading system that can detect cancerous mutations. Contributed to theory development and chemical reaction network modelling.
- **Supervised 5 MSc/MRes students** including mentoring a junior machine learning engineering student.
- Presented at 2 international conferences. Data from collaborations used in 5 conferences.
- Wrote a series of blogs for the Imperial College website on the science of catalysis.

Postdoctoral Research Associate, Eindhoven University of Technology *Apr 2019-Mar 2020*

- Extended a previously developed coarse-grained kinetic Monte Carlo (kMC) method of alkylation reaction to a lab scale reactor system.

Education

PhD, Chemical Engineering and Chemistry, Eindhoven University of Technology *July 2015-Apr 2019*

- Youngest graduate to be awarded a cum laude distinction (awarded to 5% PhD candidates in Netherlands)
- Developed a coarse-grained **kinetic Monte Carlo** (kMC) algorithm in C to understand the deactivation kinetics of the alkylation reaction to produce aviation grade fuel. Combined concepts in nonlinear physics, **percolation theory**, reaction kinetics, transport phenomena to build a theory that solved a 30-year-old problem related to the reaction with potential to save Shell $10 million annually.
- Developed a coarse-grained fluid solver model in C called Stochastic Rotation Dynamics (SRD), to simulate fluid flow in the presence of chemical reactions and demonstrated for the first time the usage of multicomponent diffusion in PBS.
- Published 5 research papers in international journals; Presented research work at 6 international conferences across USA, Germany, Norway, Mexico. Supervised 2 Master students.
- Student administrator of the 60-researcher consortium MCEC (Netherlands Center for Multiscale Catalytic Energy Conversion). Tasks involved organizing MCEC biannual meetings, quarterly lab tours and workshops.

Bachelors in engineering physics (BTech), Indian Institute of Technology (IIT), Delhi *July 2011-May 2015*

- Top of the class grades in Statistical Physics (10/10), Probability theory (9/10), Computational Physics (10/10).
- *Research projects*: Built a statistical model for studying photon splitting in **Spontaneous Parametric Down Conversion** (thesis project), cellular automata model to simulate biophysical matter transport (internship in Netherlands), develop numerical techniques to solve nonlinear physics problems like Hopf bifurcation (internship in China).
- Coordinated career counselling session for underprivileged youth at ANK NGO, Delhi.
- Held posts of Student Program Convenor (2nd year), Student Mentor (3rd year) and organized multiple events for the Physics Society (2^{nd}-3^{rd} year).

Freelancing

Sengar Consulting BV *Mar 2020-Now*

- 4.7/5 rated freelancer on Kolabtree.com providing data science and research consultancy services. Successful completion of 30+ projects for startups and researchers in USA, UK, India, S. Korea.
- Led the development of a computational platform for protein-small molecule binding prediction, implementing a unique hashing algorithm and Grand Canonical Monte Carlo simulations, and securing project funding. The platform efficiently ranks chemical fragments based on protein affinity.
- Designed an AI-based platform for a startup for personalized treatment recommendations and implemented a pipeline for genomics and epigenomics data analysis.
- Evaluated and compared the performance of random forest, SVM, and deep neural network models with dimensionality reduction using PCA to predict API vulnerability scores for a computer network security client, achieving up to 67% accuracy. Employed tensorflow, keras, sklearn for model development.
- Led the development of a conversational AI chatbot using a Seq2Seq model in PyTorch, normalizing text data for training, and optimizing the model for inference. Successfully trained the chatbot to generate responses.

Professional Development/Certifications

- *ML courses*: Neural Networks and Deep Learning by Andrew Ng; Generative AI by Google
- *Other courses*: Consultancy, Making the most of your Postdoc; The Postdoc Entrepreneur; How to Peer Review Research Papers; Preparing Successful Fellowship Applications.
- Undertook a 3-workshop course on "Make Time Count" by a professional productivity and well-being coach.
- Supervised 4 MBA students in India for their grad course and wrote a white paper on the implementation of blockchain technology in a government social scheme.

Publications*

[1] **A. Sengar**, T. E. Ouldridge. On the free energy landscape of the Handhold Mediated Strand Displacement reaction using oxDNA. *Submission in Nucleic Acids Research in September 2023*

[2] **A. Sengar**, E. Hatton, T. E. Ouldridge. A deep learning-based model for predicting oxDNA generated hybridization kinetics. *Under Preparation*

[3] F. Smith, **A. Sengar**, G.B. Stan, T. E. Ouldridge, W. Bae. Overcoming the speed limit of fourway DNA branch migration with bulges in toeholds. *Submitted to JACS in June 2023*
Contributions: Discovered a unique phenomenon of bulge diffusion (that cannot be observed in experiments) by performing Umbrella Sampling simulations and combining them using WHAM in oxDNA.

[4] A. Stannard, **A. Sengar**, L. Michele, T. E. Ouldridge. Allosteric topological modulation of toehold-mediated strand displacement. *Submission to ACS Nano in August 2023.*
Contributions: Developed forward flux sampling algorithm and performed simulations in oxDNA to explain the effects of the presence of a bubble in binding kinetics of a toehold strand.

[5] R. Mukherjee, **A. Sengar**, T. E. Ouldridge. Kinetic Proofreading to Enhance Single Nucleotide Discrimination in a Non-enzymatic DNA Strand Displacement Network. *Submitted to Nature Nano in July 2023*
Contributions: Developed a chemical reaction network model for the kinetic proofreading mechanism, obtain reaction rate constants for the intermediary reactions and developed a simplified theory around the mechanism.

[6] **A. Sengar**, T. E. Ouldridge, O. Henrich, L. Rovigatti, P. Sulc. A primer on the oxDNA model of DNA: When to use it, how to simulate it and how to interpret the results. Front. Mol. Biosci. 2021, 8, 693710. 464 views and 103 downloads on Zenodo

[7] **A. Sengar**, J.A.M. Kuipers, R.A. van Santen. Deactivation Kinetics of the Catalytic Alkylation Reaction. ACS Catalysis, 2020, 10, XXX, 6988–7006

[8] **A. Sengar**, R.A. van Santen, E. Steur, J.A.M. Kuipers, J.T. Padding. Deactivation Kinetics of Solid Acid Catalyst with Laterally Interacting Protons. ACS Catalysis 2018, 8(10), 9016-9033

[9] R.A. Van Santen, **A. Sengar**, E. Steur. The challenge of catalyst prediction. Faraday Discussions 2018, 208, 35-52
Contributions: Developed a chemical reaction network model for the 2 proton model and performed simulations to explain the phenomena of catalyst deactivation under different reactor conditions.

[10] **A. Sengar**, J.A.M. Kuipers, R.A. van Santen, J.T. Padding. Particle-based modeling of heterogeneous chemical kinetics including mass transfer. Physical Review E 2017, 96 (2), 022115

[11] **A. Sengar**, J.A.M. Kuipers, R.A. van Santen, J.T. Padding. Towards a particle-based approach for multiscale modeling of heterogeneous catalytic reactors. Chem. Eng. Sci. 2018, 198, 184-197 (Selected as cover picture of vol. 198 Chem. Eng. Sci)

[12] E.N.M. Cirillo, O. Krehel, A. Muntean, R.A. van Santen, **A. Sengar**. Residence time estimates for asymmetric simple exclusion dynamics on strips. Physica A: Statistical Mechanics and its Applications 2016, 442, 436-457
Contributions: Developed a cellular automata model in C along with the first author and ran all simulations for the paper. Aided in the theory development process.

*Contributions mentioned where A. Sengar is not the first author