Project Title: Machine Learning augmented Molecular Simulation Protocols

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Start date: October 2022

Brief description of project:

The aim of this project is to produce molecular simulation protocols that use unsupervised machine learning to reproduce atomistic molecular structures and thermodynamics at orders of magnitude greater efficiency than traditional molecular dynamics, and to apply these protocols to model specific protein-protein and drug-target interactions. Some specific objectives may include but are not limited to adopting or developing latent space simulation protocols to accurately model protein-protein complexes and the induced fit effect in drug molecule binding. This will be achieved by learning the slow collective variables of molecular systems of interest to accelerate the dynamics or sampling (of the conformational space) of such systems by propagating them within this slow latent space.

The supervisors have substantial experience in computational modelling, molecular simulations and application inspired algorithm development. Information on our research can be found here: http://www.cs.ox.ac.uk/mosaics/research_OCSMB_Roivant-Discovery.pdf

This project is supported by Roivant Discovery. The student recruited to this project will join the Department of Computer science at the University of Oxford as a DPhil student supervised by Dr. Peter Minary (University of Oxford) and co-supervised by Dr. Jesus Izaguirre (Roivant Sciences). As such, the successful applicant will be able to take full advantage of the training and networking opportunities available at the University of Oxford and Roivant Sciences. Further information can be found here, DPhil in Computer Science | University of Oxford

Attributes of suitable applicants:

- An undergraduate degree in physics/computer science/mathematics or a related discipline
- Experience or strong interest to pursue research in the following areas: machine learning especially deep generative modelling, molecular dynamics and structural modelling
- Excellent programming skills or experience in systematic software engineering is desirable
- Demonstrated ability to conduct and complete research projects (according to the experience of the candidate)
- Potential to work as a highly motivated, independent graduate student who will develop an outstanding research career

- Ability to work in a team
- Good verbal and written communication skills in English
- Experience or interest to work in multidisciplinary research settings
- Demonstrated ability to make clear, well-illustrated scientific presentations

Studentship details and How to apply:

This project is fully funded by the collaborating partner, Roivant Discovery, Inc. (https://discovery.roivant.com) who will cover the cost of all tuition fees. The studentship will provide an annual stipend (at the UKRI rate) of at least £16,062 per annum for 3.5 years (42 months).

The project will also cover the cost of course fees at the level set for either Home students or Overseas students (as applicable).

Applicants must satisfy the usual requirements for studying for the DPhil in Computer Science at Oxford.

Interested candidates are encouraged to contact Peter Minary (peter.minary@cs.ox.ac.uk) or Jesus Izaguirre (jesus.izaguirre@roivant.com) to discuss their suitability for the project.

Applicants should apply for the DPhil in Computer Science online by midday UK time on Wednesday 3 August 2022, quoting studentship reference **22-CS-OR** in their application.

For all application related enquiries, please consult our Graduate Studies Administrator.