CompBioMed

A Centre of Excellence in Computational Biomedicine

e-Seminar Series

e-Seminar #25
Addressing the challenge of drug discovery with Machine Learning and Exascale computing

28 July 2022 2pm CEST / 1pm BST (1h duration)

Register for free here: https://register.gotowebinar.com/register/2982719282349703182

This seminar will introduce an innovative workflow that couples machine learning (ML) and physics-based (PB) methods to accelerate the traditional process of computer aided drug discovery. PB methods compensate for the sparsity of data for ML training, whereas ML methods yield progressively better predictions of ligand structures with active learning. Not only can the accuracy of predictions be improved through machine learning but, through the application of deep learning molecular generation methods, the relevant chemical space can be sampled, and the most relevant compounds identified. This workflow is known as IMPECCABLE which involves performing compute-intensive MD simulations in tandem with much less expensive ML runs, all performed concurrently and in large numbers. The ensemble computing pattern deployed can be exploited for full utilisation of a supercomputer, which employs a high throughput "embarrassingly" parallel workload on a wide range of node counts. Therefore, as we move into an era of exascale computing, this workflow will scale to make use of the full machine and be able to perform larger computations, providing possible drug targets in a fraction of the current timeline.

This is the 25th in a series of online e-Seminars organised by CompBioMed.

Watch the full series at www.compbiomed.eu/training!

Agastya Bhati is currently a postdoctoral research associate in the department of Chemistry at University College London (UCL), UK. Before this he worked as a scientific consultant at CBK Sci Con Ltd based in UK for over a year after completing my PhD from UCL in 2018. His area of expertise is developing computational methods for accurate, precise and reproducible free energy predictions for biomolecules that are based on performing ensembles of molecular dynamics simulations. The methods he developed are equipped with statistically robust techniques for proper uncertainty quantification of results. Currently, he is active in developing a novel drug discovery workflow called "IMPECCABLE" that couples physics-based methods with machine learning techniques to accelerate the traditional process of drug discovery. It is a complex workflow with several implementation challenges that require specialised workflow managers to overcome. Agastya has substantial experience of performing large-scale jobs on a number of supercomputers across the globe including several within the worlds top 10.

Moderated by Tim Weaving, **UCL**

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