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Role of High Performance Computing in the Applications of Bio-economically Important Proteins

Tuesday, 4 December 2018 13:30 (20 minutes)

The main research interest of the Research Unit in Bioinformatics (RUBi) at Rhodes University is in structural bioinformatics and its applications to bio-economically important research questions, i.e. to drug discovery projects for diseases related to Africa, and to biodiversity and bioprocessing. Centre for High Performance Computing (CHPC), South Africa, is regularly used for accelerating computer intensive methods including drug virtual screening, molecular modelling, quantum mechanics, molecular mechanics, molecular dynamics (MD) and combinations of these techniques. RUBi's research is computationally highly expensive; i.e. within 3 months (February – April 2018) a total of 7.2 million cpu hours was used. Hence, CHPC has a great impact on RUBi's research, international collaborations and human capacity development. This talk focuses on the application of HPC to RUBi's research projects with some specific examples including analysis of drug resistance of HIV, identification of new drug targeting sites for cancer, and investigation of proteins related to the production of biofuels. Further, computational details, e.g. benchmarking, compute time, details of software used and/or developed will also be given to demonstrate the need for HPC resources.

Presenter Biography

Primary author: Prof. TASTAN BISHOP, Ozlem (Rhodes University)

Presenter: Prof. TASTAN BISHOP, Ozlem (Rhodes University)

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