

NITheCS Mini-school

Wednesday 6, 13 and 20 April 2022, 14h00 – 15h00

Dr Krishna Govender (Centre for High Performance Computing (CHPC))

‘An introduction to computer aided drug design’



ABSTRACT

During the time of COVID-19 when lockdown regulations were at their worst, the use of computational methods were imperative to speed up the development of COVID-19 vaccinations. Were it not for computational methods, conventional vaccine development would take up to 10 years and the world would not have had a vaccination for COVID-19, let alone the booster shots that are currently available.

In this course we will look at the various methods that can be used during the computer-aided drug design process and conduct hands-on exercises such as protein-ligand preparation, grid generation, setting up virtual screening, setting up molecular dynamics of possible hit ligands and running some of these workflows in a high-performance computing environment. This will all be done with the aid of the software package, Schrödinger.

BIOGRAPHY

Dr Krishna Govender is a Senior Research Scientist at the Centre for High Performance Computing (CHPC), specialising in Computational Chemistry and Material Science. He currently supports the largest number of high-performance computing (HPC) users in the cluster.

He is the lead lecturer for the various human capital development (HCD) events that are run by the CHPC, including the CHPC-NITheCS Coding Summer School, CHPC Winter School and various CHPC outreach events with high school learners from Grade 10 – 11. He is a Y2 rated

NRF researcher who holds a Senior Research Associate position within the Department of Chemical Sciences at the University of Johannesburg. Further, he has graduated 2 MSc students with distinction and 3 PhD students.

Since joining the CHPC in 2015, he has published over 30 peer reviewed papers in high impact journals. He also has ongoing collaborations with the University of KwaZulu-Natal, Durban University of Technology, University of Fort Hare, University of Cape Town, Cape Peninsular University of Technology, University of Ghana and University of Sri Jayewardenepura.

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