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Automating Desmond MD Report Generation on the Lengau CHPC Cluster

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Fri, 21 November 2025 | 12h00-12h30 SAST

Attend online

ABSTRACT

For many users, generating Schrödinger's Desmond molecular dynamics reports often requires downloading large trajectory and CMS files, sometimes creating data transfer overhead for CHPC users, depending on system size and simulation time. This tutorial introduces `easy_desmond_mds_report`, a Bash script that automates report generation directly on the Lengau CHPC cluster. The tool streamlines workflows, reduces data movement, and produces compact, ready-to-download report folders. It also gives control to analyse any part of the system (such as specific domains on proteins). Participants will learn how the script works and how to use it for their MD data.

BIOGRAPHY

Adeshina Odugbemi is a postdoctoral research fellow in the Biochemistry Department at Stellenbosch University, specialising in computational drug discovery. His current research focuses on structure-guided identification of inhibitors of antimalarial targets. He completed his PhD in Bioinformatics at the University of the Western Cape and has developed capacity in machine learning applications in Quantitative Structure-Activity Relationship, molecular dynamics simulations, AI-assisted docking and deep learning approach for cancer drug response prediction.

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