Contribution ID: **137** Type: **Workshop**

Different Techniques of Force-field Derivation and Setting Up Molecular Dynamics (MD) Calculations at CHPC Using DL_POLY Code

Sunday, 30 November 2025 09:00 (1h 30m)

Molecular dynamics (MD) is a computer simulation method for studying the physical movements of atoms and molecules. The MD method can assist one in obtaining the static quantities and dynamic quantities. This method gives a route to dynamical properties of the system: transport coefficients, time-dependent responses to perturbations, rheological properties and spectra. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic evolution of the system. The DL_POLY Code parallel molecular dynamics simulation package will be utilised for exploration of such properties of molecular systems.

Presenting Author

Email

Student or Postdoc?

Institute

Registered for the conference?

CHPC User

CHPC Research Programme

Workshop Duration

Half-day

Primary authors: MASEDI, Cliffton (University of Limpopo); KGATWANE, Kenneth (University of Limpopo); Dr PHAAHLA, Tshegofatso (Materials Modelling Centre); HLUNGWANI, Donald (University of Limpopo)

Presenter: MASEDI, Cliffton (University of Limpopo)

Session Classification: Workshop