Contribution ID: **145** Type: **Workshop/BoF proposal**

Setting Up Basic Molecular Dynamics (MD) Calculations at CHPC Using DL_POLY Code”

Thursday, 7 December 2017 13:30 (20 minutes)

Proposal for a Tutorial at 2017 CHPC National Meeting

Title: “Setting Up Basic Molecular Dynamics (MD) Calculations at CHPC Using DL_POLY Code”

Lecturer(s): 1. Sylvia Ledwaba, University of Limpopo, raesibe.ledwaba@ul.ac.za

1. Cliffton Masedi, University of Limpopo/CSIR, cmasedi@csir.co.za Description: 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.

Duration: 1 day (6 hours)

Size: (max number of available seats)

Target Audience:
This one day workshop is intended for undergraduate project students, postgraduate students, postdoctoral researchers and researchers who are familiar with the field and want to employ state-of-the art methodology based on the density functional theory to understand bulk materials properties, surface science and heterogeneous catalysis phenomena.
Prerequisites: Familiarity with UNIX or Linux environment.

Type of tutorial: Mix of tutorials and hands-on (mostly practical)

Special requirements:

Attendees need access to a laptop or workstation, active CHPC user account cluster with access to DL_POLY software.
Open source spreadsheet such as Microsoft Excel with graphing capabilities is required for post-processing of output data.
Free visualization softwares (e.g. VMD, VESTA, etc.), necessary for structure visualization.
Outline of full syllabus:
Introduction to Molecular Dynamics
Properties of Molecular Dynamics
Simulation code (DL_POLY)
Fitting and validation of interatomic potentials
Setting up molecular dynamic simulations
Force Field Models/ Interatomic Potentials
General Description
Potential Models (Buckingham + Three-Body)
Compatibility of Interatomic Potentials

Validation
Hands-on exercises on:
Construction of Structure File
Validation of Interatomic Potentials
Generation of DL_POLY input files
Submission of Calculations at CHPC_Lengau

HPC content

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.

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Session Classification: Thursday Workshop: Basic Molecular Dynamics Using DL_POLY

Track Classification: Workshops