Computational Physics and Biology

Date: Sunday, December 8th, 2019 to Monday, December 9th, 2019

Venue: Nelson Mandela African Institution of Science and Technology (NMAIST)

An introduction

Computational simulations of materials and bimolecular systems based on physical principles are becoming more important, and sometimes crucial, to shed light on microscopic mechanisms of a variety of chemical and physical processes. This workshop aims at providing an introduction to the field, with practical exercises to empower the attendants to perform calculations on their own. The workshop also will relate how quantum mechanics and classical mechanics together can be used to answer question of interest in biology and chemistry.

Facilitators:

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Programme of activities

Day 1

Time	Activity
0800-0830	Introductions and purpose of the workshop
0830-0930	Introduction to computational physics/Linux operations
0930-1030	**Break**
1030-1230	Introduction to computational physics
1230-1330	**Lunch**
1330-1430	Introduction to Density Functional Theory (DFT)
1430-1530	Introduction to Molecular dynamics (MD) simulation
1530-1600	**Break**
1600-1700	Discussion and reflection

Day 2

Time	Activity
0800-0830	Practical sessions DFT/MD
0930-1030	**Break**
1030-1230	Practical sessions DFT/MD
1230-1330	**Lunch**
1330-1430	Practical sessions DFT/MD
1430-1530	Practical sessions DFT/MD
1530-1600	**Break**
1600-1700	Discussion and reflection

Outline

1. Computational Physics
2. Linux operations
3. DFT
4. MD simulation
5. Practical sessions

Outline description:
Minimum course of Linux operations is provided as a hands-on tutorial. The course starts with very elemental explanations about the directory/file operations etc.

Taking DFT simulations, the course also includes to teach 'script works', 'text handlings with sed, awk and grep', 'graphic plots using gnuplot' etc.

Participants are quite strictly trained for efficient and fast blind-typing with Tab-completions.

Participants will also learn on how to simulate a real system. For example, simulation of a natural products to understand its conformational changes in solvents such as water.