Data-driven Molecular Dynamics Modeling

This project falls at the interface of mathematics, machine learning, and molecular dynamics. Molecular dynamics helps study properties of materials without actually synthesizing them, but by simulating the positions of atoms and molecules as a function of time using Newton's equations.

The work concerns a data-driven approach (equations from data) to forecast MD trajectories data so that the statistical properties of the forecasted data remain close to a correct evolution. The basis for the project is that long MD simulations can be potentially mathematically unsound, generating cumulative errors in numerical integration that we can avoid by using sound mathematically based methods to forecast data. The project aims to use learn a driven dynamical system and deep learning methods appropriately to forecast the data. The data is obtained through international collaborations. Success in this method is anticipated to yield in a research publication.

Skills needed:

1. A course in ordinary differential equations.
2. Appetite to understand (not necessarily prove) some mathematical results.
3. To be able to write computer programs in Python.
4. To work with big-data sets and use the CHPC computing resources at Cape Town.