Implementation of time series forecasting in openMM

Description:

Implementation

Create Interface with DFT

Test on simple system

Time series forecasting is a way to predict the state of a system at a certain point in the future based on information on its past states. In molecular simulation, time series forecasting can skip time steps by predicting the state of the molecule in a future time step. If these time steps are computationally expensive skipping them can lead to a computational speed up. In this project time series forecasting will be implemented in openMM and interfaced with common quantum chemistry programs capable of doing DFT (such as, TURBOMOLE). The implementation will be tested on a simple system to evaluate the implementation's performance.

Meetings with main supervisor every other week.