MOLECULAR AND BUSINESS MODELLING IN SCIENCE
AN INNOVATION LAB 2020 PROJECT

by

Lau Pak To
Marcel Mordarski
Lukas Supragonas
Maja Walnik

July - August 2020

Natural Sciences Department

The Faculty of Mathematical & Physical Sciences

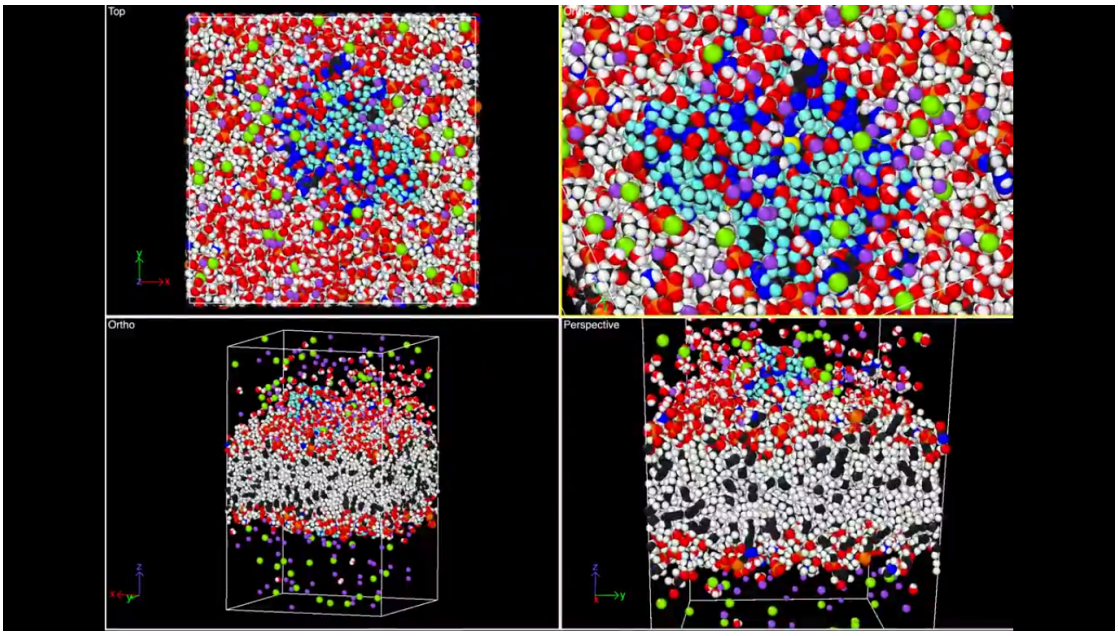
University College London

For any enquires, questions, cooperation proposals, or amendments suggestions (which are very welcome), please email the leader of MM Team, Marcel Mordarski:
marcel.mordarski.19@ucl.ac.uk.

ABSTRACT

A survey conducted within the UCL Natural Sciences community revealed that despite the students interest in the subject, academic experience often provides only an insufficient knowledge and understanding of molecular modelling. Moreover, according to most of the respondents, the only existing resources on MM neither extensively nor accessibly cover the topic, leaving many at a loss in attempting any simulation tasks at hand. In an attempt to improve this situation, our team created an introductory course revolving around the molecular modelling software LAMMPS. Beginning with installation and progressing to generating ones own simulations, we believe to have created a reasonably-sized course in the basics of operating the LAMMPS software. Another feature of this project is a tutorial on Supply Chain Analytics simulations in PuLP[1], as well as some advice on comprehensive data collection by the means of conducting surveys.

Keywords: LAMMPS, PuLP, Python, Molecular Modelling, Business Modelling, Supply Chain Analytics, Simulations, Avogadro.



Case Study: Remdesivir analog GS-441524 and model human cell membrane

THE PROJECT

While our teams mission is to teach and encourage similar endeavours, by no means are we denying having experienced some challenges along our way in this project. Struggle with the initial choice of the case study proved to be the first difficulty. Having little idea of what the project might entice exactly, the agreement was that the attempt to simulate any biological system might be too overbearing, given the relatively small processing power of our desktop computers available. This idea was quickly overturned by the newfound motivation to cover, at least to some extent, the interaction of a possible COVID-19 treatment drug with a model lung cell.

Often caught in a somewhat of a Catch-22 situation of needing resources to continue with the project though having to create the resources ourselves, it was a challenge to find enough information to proceed at times. Working as a team, however, definitely facilitated the problem-solving every step of the way, allowing us to create the tutorials on running LAMMPS simulations.

[1]The course on Supply Chain Analytics available at DataCamp was the inspiration for this part of the project

The result of our efforts are not only the tutorials, though also visualising the simulation of the interaction of a Remdesivir metabolite with a cell membrane. Obtaining a tangible final result is a moment of great satisfaction, through which struggling with the installation of the software itself or operating Ovito or Avogadro seem only distant unpleasant memories.

TUTORIALS

The step-by-step tutorials begin by covering very simple tasks such as installing LAMMPS, they then go onto more complicated actions such as creating data and input files. Later on, they finally explain how to run a simulation. Since once is prone to making syntax errors in the LAMMPS code, there is also a tutorial dedicated precisely to avoiding and fixing them. Other tutorials created in this project cover aspects of business modelling, namely exploring supply chain analytics, the idea of dictionary function, as well as price sensitivity shadowing. Guides on conducting comprehensive surveys for similar project undertakings have also been made available.

NAVIGATION OF THE WEBSITE

1. Introduction
    - About this project
    - About LAMMPS and its applications
2. Molecular Modelling
    - The LAMMPS installation guide
    - Creating data files
    - More notes on data files
    - Pre & post processing tools for LAMMPS
    - Our LAMMPS code
    - Automating the LAMMPS data file writing
    - Building a LAMMPS input file: a tutorial
    - Running a LAMMPS simulation: a guide
    - Errors and troubleshooting
3. Case Study
    - Case study description and simulation - visualised
    - Simulation files for the case study
4. Business Modelling
    - Supply chain analytics, dictionary function and shadowing prices
5. Surveys
    - Summary of our survey and honest advice on surveys