MSE 317 Modelling Lecture 9: Current Research – Exercises

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In the exercises, we are going to use VPN, Linux server and Python. One needs to connect College VPN to get access to Linux machines. Simulations will be carried out in Linux operating system. A MATLAB script will be used for post analysis.

Part 1 Use Linux operation system and set up the program

The KMC code is written in Fortran programming language and compiled for Linux operating system. We are going to use virtual machine of Linux operating system in this course.

(1) Connect the College VPN using your usual College credentials. (https://www.imperial.ac.uk/admin-services/ict/self-service/connect-communicate/remote-access/virtual-private-network-vpn/)

(2) You can log onto one of two student Linux machines using **ssh** in a terminal with your Imperial username and password. (https://www.imperial.ac.uk/admin-services/ict/self-service/research-support/rcs/support/getting-started/using-ssh/)

For Windows user, pleases feel free to use your preferred way. If you do not have one, MobaXterm is recommended, which is a collection of graphical user interface and an enhanced terminal. (see the step-by-step instruction at the end of this file)

```
ssh username@mt-studentx.mt.ic.ac.uk
```

or

```
ssh username@mt-studenty.mt.ic.ac.uk
```

(3) Open a terminal and navigate to where you would like to run your KMC code. Each user should have a folder called **homedir** that is the College H: drive. This is probably the easiest way to copy files over. To go to **homedir** folder, you type

```
cd homedir
```

(4) Get a Git repository by typing

```
git clone https://github.com/dreamslink51/MSE317.git
```

To go to KMC folder, you type

cd MSE317/KMC

The executable file is called *snapshot_KMC.x* and the input file is *input.inp*.

(5) To run *snapshot_KMC.x* you type

./snapshot_KMC.x input.inp

(6) Output files will be generated in the same folder including *distance.dat* and *tcheck.dat*. Those two files will be read by *AnalyseDistance.py*, a Python script, to compute mobilities.

./AnalyseDistance.py -nsample <your #KMC> -temp <your temerature>

nsample: number of KMC runs (Default: 10)

temp: temperature (K) (Default: 283)

For example ./AnalyseDistance.py -nsample 10 -temp 283

The charge mobility μ can be generally derived from the Einstein-Smoluchowski equation with the diffusion coefficient *D*.

$$\mu_{ij} = qD_{ij} / (k_B T) \qquad (1)$$

where q is the electron charge, k_B is the Boltzmann constant, and T is the temperature.

The diffusion coefficient *D* in the three dimensional system can be obtained from the mean square displacements (MSD):

$$2D_{ij}t = \left\langle \left(R_i(t) - R_i(0)\right)\left(R_j(t) - R_j(0)\right) \right\rangle \qquad (2)$$

where t is the time, $R_i(t)$, $i = x,y,z,$ is the successive Cartesian coordinates for the centre of mass of the molecule carrying the excess charge that were monitored along a kinetic Monte Carlo trajectory.

Part 2 The simulations

1. Check the convergence of a random sample.

(1) The default *input.inp* is to run 10 KMC simulations on a static crystal structure (a single molecular dynamics trajectory). You can check *input_comment.inp* file to check the explanations of the input parameters. To read and edit a file, you

can nano filename or vim filename . Run the simulation and compute the mobilities using the MATLAB script. It is noted that in the MATLAB script, there are changeable two parameters, one is the number of KMC runs and the other is temperature. Repeat 5 times and see whether you get the same values.

(2) Repeat the above simulations using bigger number of KMC runs, such as 100 times, 1000 times. The bigger the number, the longer the simulation will take. Remember to use the right parameters in MATLAB script. What differences do you see with different number of KMC runs? How many KMC runs do you need to get a reliable mobility?

2. The effect of dynamic disorder.

   The crystal is not frozen at a finite temperature. Molecular dynamics (MD) is a computer simulation method that allows the physical movements of atoms and molecules, giving a view of the dynamic "evolution" of the system. Run the simulations with a bigger number (start from 1 to 10 and 99) of MD trajectories, i.e. with a smaller step of choosing snapshot from a MD trajectory (change the second from last parameter in *input.inp* from 99 to 10 and 1) and compare the mobility tensors (mobility values and directions).

3. The effect of temperature.

   The default temperature is 283K i.e. room temperature. We want to explore the temperature dependency of mobility. Run the simulation at 100K, 200K, 400K and 500K. Compare the difference and plot a temperature-mobility figure. Explain.

4. Advanced tasks (to be done if you have time)

(1) Repeat the simulations with difference KMC time cutoff.

(2) Repeat the simulations with difference distance cutoff.

(3) Repeat the simulations with difference reorganization energy.

Appendix

For windows users:

1. Download MobaXterm: https://mobaxterm.mobatek.net/download-home-edition.html
2. Double click downloaded item and click extract all, set the destination to your preferred folder.
3. Open MobaXterm by double click "MobaXterm_Personal_xx.x.exe" (xx.x is the version infomation).
4. In the welcome page, click "session" button on the top left corner, then, click SSH in the window titled "Session settings" at the top left.
5. Type in the following information then hit enter:
   Remote Host: mt-studentx.mt.ic.ac.uk
   Specify username: Your college username
   Type in your password and hit enter. (Note: what you type will not display on screen due to safety reasons.)
6. Here is your terminal connected to the college provided remote machine on the right hand side of the screen with black background and white command lines.
   Follow the on-screen guide to save your password(optional).