Please read this compendium before the lab session.

Practical Lab Session in Computational Physics:
TFYA92

Molecular dynamics simulations I

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1. Introduction

In the next two lab sessions, you will get hands on experience in using the Molecular Dynamics (MD) simulations technique. As you know from the lectures, MD is a tool that is widely used in materials science, as well as in other physics fields and/or chemistry and biology. The main aim of these lab sessions is to learn how to correctly setup and run a MD simulation, to understand the advantages and limitations of the method, but above all, to understand the meaning, or the actual physics, behind the actual numbers you will obtain at the end of each simulation.

As always, when using computer simulations, a trade-off has to be made between the accuracy of the model and the complexity of the simulation. In addition, don't forget that the size scale of the system to be simulated and time scale chosen will generally dictate the type of problem that can studied using MD simulations. Consequently, during the lab session, and whenever you use computer simulations, **you should always think of the approximations made, the limitations of the model, the accuracy expected, and the reasonable conclusions that can be drawn based on all of the above arguments.**

We start out by introducing the tools needed to do the lab, which is the MD program used. We will use an MD code called **MDSinecura**. Many programs used for computer modeling are difficult to use and require quite some time to learn. **MDSinecura** is, however, designed to be easy to use and can be controlled completely via the GUI. It has been developed here at the university and the version you will run is a beta version, so please be patient as there might be a few bugs left…

2. Computer Tools

Setting up the necessary files & directories

The simulations will be run in a UNIX environment on PCs using the Linux Operating system. You should login in one of the PCs using the student username and password you received upon starting your studies at the university (**bring this password to the lab if you do not remember it**). After the successful login, you need to do several operations necessary for the proper setup of your working environment, especially for those not used with the Unix/Linux operating system. Here they are:

1. Right click the mouse, and from the menu choose with the mouse pointer **OPEN TERMINAL**. A smaller window should now open on the monitor after this selection.

2. Point the mouse cursor in the newly open window and type:
mkdir mdlab and press **Enter**. This will create a new directory in your so-called home directory. Notice that there should a SPACE (highlighted in RED) between the command **mkdir** and the name of the new directory **mdlab**. Nevertheless you can use whatever directory name you want, but in this compendium, the newly created directory will be referred to as **mdlab**.

3. Now type **cd mdlab** and press **Enter**. This command will take you in the newly created **mdlab** directory.

4. Move the mouse cursor out of the terminal window towards the upper left corner of the Linux desktop window and choose the **APPLICATIONS** tab. From here you should select **Firefox** and start the browser.

5. Use the browser to go to the following site:
http://www.ifm.liu.se/theomod/theophys/scientific_software/mdsinecura/

6. Once there, download **MDSinecura Linux** (double click) into the newly created directory in your home directory (**mdlab**). When this operation is completed, **CLOSE** the Firefox window.

7. Now move the mouse pointer on top of the Linux terminal window and left click. This should take you back in the **mdlab** directory (you can check this by typing in the command **pwd**, followed by **Enter**; you should see something like edu/student_name/mdlab). Just make sure you are in the **mdlab** directory.

8. Now type in the following command: **tar zxvf MDSinecura.tar.gz** and press **Enter**. Notice the SPACE after **tar** and the SPACE after **zxvf**. This command will unzip the MDSinecura code you just downloaded and create a new directory, named **MDSinecura**, containing all the program files required for the lab session.

9. As you still are/should be in the MDLAB directory, at the command prompt type the following command: **mkdir lab1** then press **Enter**. The command creates a new directory in which all the results from this lab session will be stored.
OBS: PLEASE DO NOT STORE THE LAB RESULTS IN THE MDSinecura directory!!!

10. We now need to change directory in order to start the MDSinecura program. To do that, at the command prompt type **cd MDSinecura** then press Enter.

11. Now, you can start the MD program. At the command prompt type the following command: **./MDSinecura**, then press **Enter**. Notice that this time there is NO SPACE between the **.** the **/** and **MDSinecura**.

12. The MDSinecura window should pop up now and welcome you to the wonderful world of MD simulations. You can of course enlarge it to suit your needs.

At this point, the following instructions should also be completed:

13. Minimize the previously used terminal window as it should not be needed anymore. **ATTENTION: DO NOT CLOSE the window, just MINIMIZE it, this is important!!!**

14. Open up a new terminal window (right click on the Linux desktop and choose Terminal Window), it might be useful to locate certain files created by MDSinecura.

OBS: All students attending the lab should arrive at this point at approximately the same time, since this is also an interactive lab session, in which one might have to compare many sets of results, to make the most of the lab session. The students with Linux expertise are kindly requested to assist those who may get lost in the sequence of the above operations. I will of course do it myself, but if you help me, the lab session will progress in a smooth manner with no delays. Thank you!

3. The MD Program

MDSinecura uses the following classes in the approach. When you first run the program, you will be asked to **Choose a Workspace**. This is the place where all files created by MDSinecura will be stored. You have already created this Workspace, it is the **lab1** directory in your **mdlab** directory. At this time, you should then select this directory following the prompts on the MDSinecura window.

Every time you start a new session with MDSinecura, you will be asked to create a ***New Project*** and/or a ***New Simulation*** within the project. Both these classes can be created from within MDSinecura. You create ***New Projects*** and ***New Simulations*** using the two tabs on the upper left of the MDSinecura window, or using the ***File*** menu. Typically, the project will contain all the work related to a certain chemical element, material or specific surface, for example *Argon*, *Platinum*, or *Silver_Surface*. In each project you can then create new simulations related to the particular material. The name given to each simulation is of course entirely up to you, but the suggestion here is that the name reflects to some extent the purpose of the simulation. For Argon, you can use for example *Ar_1*, *Ar_2*, *Ar_3*, or, *Ar_relax*, *Ar_Bulk*, *Ar_3D*, *Ar_2D*, *Ar_MSD*, *Ar_Debye* etc. The choice is yours as long as you remember what simulation does what.

All settings and output data in MDSinecura can be selected, accessed, controlled and/or visualized by ***(left) double-clicking*** on the different **Tabs** displayed in the left-hand part of the project and/or simulation window. Each time you select and double-click on one of the tabs, a new window will open giving you further options in terms of selecting/modifying the different parameters available under the particular tab. To close any of the newly open windows, you must ***left-click on the cross*** on the upper right part of the screen. Here's a quick summary of the choices available:

BEFORE THE MD RUN

CONFIG - Here you set up your simulation. To the right you will see three more tabs:

SIMULATION: - typically, under this tab you can select the ***size*** of the MD time step, ***number*** of time steps to be executed, the ***temperature*** of the simulation, the ***thermostat*** type (including none), settings for periodic boundary conditions (PBC), and a number of other MD runs parameters such as plot frequency, back-up and sampling intervals, etc. Under this tab, note the ***VISUALIZATION*** settings, which you can use to set the storage/frequency parameters required for the production of MD movies, which can be viewed at the end of the MD run.

POTENTIAL: - useful to modify the interaction potential parameters for each chemical element, potential cut-off, and potential tabulation settings.

CALCULATION: - use the options available under this tab to select to quantities you want to be calculated in a particular MD run. You can choose to calculate the specific heat, mean square displacement (MSD), the radial distribution function, pressure, energies and a number of other properties. Make sure you GIVE CONSIDERABLE THOUGHT to ***what, when*** and ***how*** you calculate. Simply by TICKING the boxes for **ALL** properties to be calculated will not be very useful or instructive….

GEOMETRY - Here you set up the geometry of the system to be simulated.

The default settings will take you to a so-called ***Groups*** tab (on the right of the window). A number of crystallographic lattice types can be used (primarily fcc and diamond-like). You can choose to create bulk unit cells (3-D simulations), surfaces (2-D simulations), and more complex arrangements such as adatoms

on surfaces. In each case, you must click on the respective tab (***Bulk***, ***Surface***, etc) and you just specify the number of unit cells to be created in X, Y and Z. When you are finished with your settings, press the ***Edit*** button. You can also ***Export*** and/or ***Import*** and existing atomic configuration by using the respective tabs.

IMPORTANT: you **must** use the **list of available chemical elements** for the respective interaction potential (displayed above the Bulk, Surface, tabs) to **CORRECTLY SELECT THE CHEMICAL ELEMENT** you want to simulate.

SIMULATION - Double-click on this tab when you are finished with a particular setup. Start the simulation by pressing the ***Simulate*** button.

AFTER THE MD RUN

PLOTS - When the MD run has finished, the results for a number of properties (total, potential, cohesive energies, temperature, pressure etc), can be viewed under this tab.

RESULTS - Final average values for a number of properties are tabulated here.

VISUALIZATION - Movies of the entire MD run can be accessed and viewed under this tab. Animations can be controlled using the controls displayed in the movie window.

LAB EXERCISES

Exercise 1.

Start a ***New Project*** named ***argon***. In the New Project start a New Simulation which should be called ***bulk_40K***. Click on the **CONFIG** tab, then under SIMULATION make sure the following settings are set correctly (you can simply tick below on your notes to make sure of this):

Time step = 1 fs (default)
Timesteps = 20000 (default 1000)
Temperature = 40 K (default 300 K)
Scaling Time = 50 fs (default 300 fs)
Thermostat = None (default)
On the right side, under Visualization, set Store Frequency at 100 (default value is 25).

You can now inspect the values under the POTENTIAL tab. Move on to the CALCULATION tab to the right and make sure YOU **DON'T** CALCULATE the following properties (un-tick the respective boxes): Specific Heat (C_V), Mean Square Displacement (MSD), Radial Distribution Function (RDF).

Now click on the **GEOMETRY** tab to set-up your simulation atomic slab. The ***Groups*** tab will show up to the right, make sure you click on the ***Bulk*** tab to the right. Here you MUST select the chemical element to be simulated from the available list:

- select Argon
- change the number of unit cells to 15 (default is 8) in each Cartesian direction.
- click on ***Save*** to actually generate your starting atomic configuration.

To start the simulation, double-click on the **SIMULATION** tab, then press the ***Simulate*** button. Closely follow the information displayed. Upon the completion of the simulation, you can use the ***Results*** and/or ***Plots*** tabs to inspect the final results. Use **Visualization** the tab to view a movie of the MD run.

OBS: There is **BUG** in the program which is very difficult to find & fix. To view the MD movie under double-click on **Visualization**, then open (double-click) one of graphs available under Plots, then close the graph displayed. The same sequence should be followed to view the atomic slab under **GEOMETRY**.

Comment the results (WRITE DOWN on your notes), what you observe. Is the system in equilibrium? What happens to the temperature? Write down all values for E_{kin}, E_{pot}, E_{tot}, E_{coh}, as well as other important values. How does the cohesive energy of your system compare with the tabulated/text book value of 0.08 eV/atom? What is the reason for what you observe?

Exercise 2.

Within the same project (***argon***), point the mouse cursor to the ***bulk_40K*** simulation and right-click on it. You see the option the ***Copy to a New Simulation***. Do that, and at the prompt use the name ***cutoff*** for this new simulation (it will immediately be displayed under ***bulk_40K***). In the new simulation, ***cutoff***, make the following changes:

- under SIMULATION TURN OFF ***Visualization*** (un-tick the respective box).
- under POTENTIAL examine carefully the lattice constant value for Argon (5.31) and compare it with the cutoff value displayed above. These are the parameters used in Exercise 1, so write down how many neighbor shells have been included in the previous Exercise.

Nr. of neighbor shells in Exercise 1: _____

- modify the value of the cutoff to include FOUR neighbors in your new calculation (Enter the value in the respective field and press **Enter**. Make sure the new value is properly entered, otherwise you just repeat the previous MD run.
- under **GEOMETRY**, MAKE SURE you double-click on the atomic slab displayed under Groups, then press Bulk -- > Save, to make sure the new parameters in POTENTIAL have been updated.
- double-click on **SIMULATION**, then press ***Simulate*** to start the new MD run.

At the conclusion of the MD run, write down all values of interest and everything else you observe. How long it took to complete this MD run? How does that compare with the previous run (you can still access this information under SIMULATION window under the ***bulk_40K*** run. What should happen to energy, accuracy etc.

Exercise 3.

As in Exercise 2, copy the ***bulk_40K*** run to a new simulation named ***tabulation***. We'll keep using this initial MD run for a while, as it has all settings in it, so please DO NOT DELETE IT! In the new simulation, ***tabulation***, insert the following changes/settings:

- under SIMULATION TURN OFF ***Visualization*** (as before, un-tick the respective box).
- under POTENTIAL change the value for ***Potential Tabulation*** to 0.5 Å.
- use the same procedure under **GEOMETRY** as in the previous exercise to make sure the new parameters are loaded in the new run.
- double-click on **SIMULATION**, then press ***Simulate*** to start the new MD run.

Write down again all relevant values and describe what you observe.

Exercise 4.

Copy the ***bulk_40K*** run to a new simulation named ***epsilon_1***. In the new simulation, ***epsilon_1***, insert the following changes/settings:

- under SIMULATION TURN OFF ***Visualization*** (as before, un-tick the respective box).
- under POTENTIAL change the value of EPSILON for Argon by **+10%.**
- use the same procedure under **GEOMETRY** as in the previous exercise to make sure the new parameters are loaded in the new run.
- double-click on **SIMULATION**, then press ***Simulate*** to start the new MD run.

Upon completion of the MD run, repeat the entire procedure and create New simulations named ***epsilon_2*** and ***epsilon_3***, in which you chance the value of EPSILON by **-50%** (in ***epsilon_2***) and **+100%** (in ***epsilon_3***).

In each case, write down all relevant values and describe what you observe. Note in particular changes in the ***Potential*** graph under ***Plots***.

Exercise 5.

Copy the ***bulk_40K*** run to a new simulation named ***sigma_1***. In the new simulation, ***sigma_1***, insert the following changes/settings:

- under SIMULATION TURN OFF ***Visualization*** (as before, un-tick the respective box).
- under POTENTIAL change the value of SIGMA for Argon by **+10%**.
- use the same procedure under **GEOMETRY** as in the previous exercise to make sure the new parameters are loaded in the new run.
- double-click on **SIMULATION**, then press ***Simulate*** to start the new MD run.

Upon completion of the MD run, repeat the entire procedure and create New simulations named ***sigma_2*** and ***sigma_3***, in which you chance the value of SIGMA by **-50%** (in ***sigma_2***) and **+100%** (in ***sigma_3***).

In each case, write down all relevant values and describe what you observe. Again, note in particular changes in the ***Potential*** graph under ***Plots***.

Exercise 6.

Copy the ***bulk_40K*** run to a new simulation named ***atoms***. In the new simulation, ***atoms***, insert the following changes/settings:

- under **GEOMETRY**, change the number of unit cells to **20** in each Cartesian direction. Use the **Groups -- > Bulk -- > Save** buttons and make sure you have generated a new atomic slab.
- double-click on **SIMULATION**, then press ***Simulate*** to start the new MD run.

Write down again all relevant values and describe what you observe. How long did it take to complete this MD run (compare with ***bulk_40K***)? You can watch the MD movie of this run, what do you observe?

Exercise 7.

Start a **NEW** simulation named ***thermostat_1***. In the new simulation, ***thermostat_1***, make exactly the same inputs as in **Exercise 1**, but with the following changes/settings:

- select ***No Initial Scaling***
- select ***Thermostat -- > Scaling*** (default None)
- input ***Scaling Activity*** as 2000
- TURN OFF Visualization (un-tick the box on the upper right-hand side).
- double-click on **SIMULATION** and press ***Simulate*** to start the new MD run.

Upon completion of the MD run, repeat the entire procedure and create New simulations named ***thermostat_2*** and ***thermostat_3***, in which you chance the value for Scaling Activity to **500** (in ***thermostat_2***) and **50** (in ***thermostat_3***). Write down again all relevant values and describe what you observe. What happens to temperature, to all energies (compare with values in ***bulk_40K***).

Exercise 8.

Start a **NEW** simulation named ***andersen_1***. In the new simulation, ***andersen_1***, make exactly the same inputs as in **Exercise 1**, but with the following changes/settings:

- select ***No Initial Scaling***
- select ***Thermostat -- > Andersen*** (default None)
- input ***Scaling Activity*** as 0.01% (make sure you choose the %-tile option here)
- TURN OFF Visualization (un-tick the box on the upper right-hand side).
- double-click on **SIMULATION** and press ***Simulate*** to start the new MD run.

Upon completion of the MD run, repeat the entire procedure and create New simulations named ***andersen_2*** and ***andersen_3***, in which you chance the value for Scaling Activity to **1%** (in ***andersen_2***) and **25%** (in ***andersen_3***). Write down again all relevant values and describe what you observe. What happens to temperature, to all energies (compare with values in ***bulk_40K*** and ***thermostat_1/2/3***).

Exercise 9.

Start a **NEW** project named ***ideal_lattice***. In the new project, you'll have to create at least **six** new simulations, each at a different lattice constant value, in order to determine the ideal lattice constant for Argon as obtained using MDSinecura. You can use the procedure detailed in Exercise 1 to set-up, ***each time***, a new simulation with the following parameters:

Under SIMULATION

Time step = 1 fs (default)
Timesteps = 20000 (default 1000)
Temperature = 40 K (default 300 K)
Scaling Time = No Initial Scaling
TURN OFF Visualization
Thermostat = Choose what you think is best suited from your previous exercises.

Under POTENTIAL

Change the tabulated value for lattice constant (**5.31 Å**) for **Argon** by +1% (run1), 2% (run2), 3% (run3), then by -1% (run4), -2% (run5), -3% (run6). Remember to USE IN EACH RUN the procedure under **GEOMETRY** (Exercises 2-5), to make sure the lattice parameter values are updated. Write down in each case all energies values. These, in combination use those calculated in Exercise 1 for 5.31 Å (simulation bulk_40K) should be enough to sketch the Energy vs. Distance dependence, curve from which you can determine the ideal lattice constant.

Exercise 10.

Start a **NEW** project named ***melting***. In the new project, you'll have to create at least **six** new simulations, each at a ***different temperature***, in order to determine whether Argon is melting when using MDSinecura. The easiest way to proceed is to copy ***bulk_40K*** run from project argon in this project, then start the new simulation from the last MD time step in bulk_40K (call me for assistance). You can use this procedure to continue each new run, at a higher temperature, from the previous run. Here are the basic inputs:

Under SIMULATION

Time step = 1 fs (default)
Timesteps = 20000 (default 1000)
Temperature = 60K (run2), 80K (run3), 100K (run3), 120K (run4), 140K (run5), 160K (run6)
Scaling Time = No Initial Scaling
TURN OFF Visualization (for the first 3 runs)
Thermostat = Choose what you think is best suited from your previous exercises.

Under POTENTIAL

Choose the lattice constant value determined in Exercise 9.

Under CALCULATION

- TICK ALL boxes for CV, MSD and RDF (to calculate all these properties)
- select Start Time for sampling as 5000 fs
- select Time between Samples as 100 fs

At the completion of the run at each temperature, write down all relevant values and inspect all graphs under Plots. Use the MSD values to calculate the diffusion constant, Lindeman criteria (constant) and Debye temperature. What happens with the CV as the temperature increases? Determine, based on these calculations, the approximate temperature interval in which Argon is melting.