mdspass2 Tutorial and Exercises

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Introduction

- When starting up, **mdspass2** reads a configuration file **CONFIG** (atomic structure) and a condition-setting file **SETDAT**.
- If you press the **Write Config** button near the bottom of the *Control* panel, the current structure is written out to a file named CONFIG.OUT. Similarly, if you press the **Write Setdat** button near the bottom of the popup window opened by **Set param**, the current calculation settings are written out to SETDAT.OUT. It is convenient to rename these files (e.g., remove the extension) and use them as input files when starting mdspass2.
- The default SETDAT file included in the downloaded package may contain somewhat complicated settings. It is safer to download SETDAT.SIMPLE from https://github.com/yoshiumeno/mdspass2/tree/main/sample_files
  rename it to SETDAT, and then proceed with the following exercises.
- Please note that clicking the "×" button at the top-right corner of any window does **not** close only that window; it terminates the entire mdspass2 application. This behavior seems to be a limitation of the GLUI library used by mdspass2 and cannot be avoided. Be careful not to click the "×" button when you only intend to close a popup window.

Part I: Ideal Crystal Structures

1. Creating Crystal Structure Models
   1. Near the bottom of the Control panel, inside the frame titled File control and config creation, you will find three buttons: Read Config, Write Config, and Create Config. (If these buttons are not visible, click on "File control and config creation" to roll out that section.)
      Click Create Config to open the Create config popup panel.
   2. First, let us create an aluminum crystal structure. Near the top of this panel, there is a label Atom with a text field to its right. Make sure that Al is entered there. If not, type Al and press Enter.
      If there is another field labeled Atom(2) below it, set that one to Al as well.
   3. Next, change the Potential setting. Left-click in the input field and a selection

bar will appear. Choose EAM.

Note: There are several variants of EAM; GEAM and Mishin can be selected. We will select the specific variant later from the Control panel.

4. Below that, you will see radio buttons specifying the crystal structure. Aluminum has an fcc structure, so select FCC.
5. Now look at the upper right part of the panel. The fields labeled # of rep in x/y/z indicate how many unit cells (for fcc, a cubic cell containing 4 atoms is the unit cell) are replicated in the x, y, and z directions. Enter 3 for each of x, y, and z. You can change the values either by typing them or by clicking the up/down arrows. This will create a cell containing a total of 108 atoms.
6. A bit further down, you will find Lattice const. a. Enter the lattice constant in Å. For aluminum, set this to 4.04.

   The field Lattice const. c below it is ignored when generating an FCC lattice.
7. At the bottom of the panel there are three buttons. Click Create. Once the structure appears in the MD viewer window, click Close at the bottom of the Create config panel to close it.
8. In the upper part of the Control panel, confirm that EAM is displayed next to Potential:. Click the ARG/FILE button to the right, and a popup window for selecting the ARG will appear. Select Mishin, then close the popup.

2. Finite-Temperature MD

Using the 108-atom aluminum cell created above, we will perform a simple MD simulation.

1. At the very top of the Control panel, there are check boxes labeled PBC x/y/z. These determine whether periodic boundary conditions are applied in the x, y, and z directions. Since we are simulating a crystal, make sure that all three boxes are checked.
2. In the Temp set field, enter the target temperature in K. Choose an appropriate value in the range of about 100–500 K.
3. If you click on Algorithm, a selection bar appears allowing you to choose the statistical ensemble. Here we will perform a constant-temperature simulation using the velocity-scaling method (an NVT ensemble), so select NVT. (More specifically, select NVT (Scaling).)
4. In the Status area near the bottom, there is a field labeled dt (fs). This is the MD time step in femtoseconds. Enter a suitable value such as 1.0–2.0. If the

value is too large, the simulation may diverge; if it is too small, the atomic motion will be very slow.

5. Click the Set param button near the top of the Control panel to open the Set parameters panel. This panel is used to configure visualization options and various calculation settings. Click on the Deformation settings bar near the bottom to roll it out. The fields ex, ey, and ez are used to contract the cell size in the x, y, and z directions. Make sure they are all set to 0. After confirming this, click Close at the bottom of the Set parameters panel to close it.
6. On the Control panel, there is a button labeled MD on/off near the top. Click it once to start MD. Check in the MD viewer window that the atoms are vibrating. Click MD on/off again to pause the MD simulation.

   In MD simulations, one often wants to stop the simulation automatically when certain conditions are met. These stopping conditions can be specified in the middle right area of the Set parameters panel. If you check Stop MD by Fmax, MD is turned off when the maximum force on any atom reaches the specified value (entered in the box below). If you check Stop MD by step, MD stops after the specified number of steps. It is also possible to stop when the stress components fall within ±(given value) MPa of the target stress.
7. ~~If MD is stopped, you can temporarily switch Algorithm to NVE and then immediately switch back to NVT. This assigns initial atomic velocities according to the target temperature using random numbers.~~

   (Note added in Dec. 2020: this functionality has now been removed.)
8. In the Status area of the Control panel, the following are displayed: elapsed MD step number, average potential energy per atom, current temperature, maximum force on atoms, cell size, and so on.

3. Changing Visualization Settings

1. Click the Set param button on the Control panel to open the Set parameters panel.
2. Click Setup for drawing to roll it out. Here you can adjust visualization-related settings. For example, the Ortho check box toggles between perspective and orthographic projection. Sphere radius and Sphere segment control the size of the atomic spheres and the smoothness of their surfaces. Try changing these values to see the effect.
3. If Draw bond is checked, atoms within the distance specified by Bond length (in Å) are connected by lines. For the aluminum crystal above, if you enter a value

like 3.2, nearest-neighbor atoms should be connected. If Bond-PBC is checked, bonds to atoms in adjacent (image) cells across the periodic boundaries are also calculated and displayed for atoms near the cell edges.

Below that, there are radio buttons to choose between Line and Cylinder. If you choose Cylinder, bonds are drawn as 3D cylinders (this is recommended here). Line is intended for cases with a very large number of atoms to reduce drawing cost. You can also select the color of the bonds according to your preference.

4. Draw force displays the force vectors on atoms as arrows. The arrow length is scaled by F-arw length. This parameter is just a scaling factor without physical units.
5. Redraw interval specifies how many MD steps elapse between redraws of the atomic configuration. Smaller values make the MD calculation itself slower but produce smoother apparent motion. Try values such as 2 or 10 and compare.
6. During MD, the energy and temperature changes are written to files energy.d and temp.d, respectively. In energy.d, the columns are: step number / potential energy (per atom, in eV) / kinetic energy / total energy. In temp.d, the columns are: step number / temperature (K). Plot these using your favorite graphing software and examine the behavior.
7. If you press the Capture button in the middle of the Control panel, the current viewer image is captured and written as a PNG file. Each time you press the button, the number in Cap-file# below it increases by one. For example, if the number is 10, the output file will be SNAPSHOT0010.png. You can also manually change the value of Cap-file#. If you check Auto capture near the center of the Set parameters panel, snapshots are taken automatically during MD at intervals of CONF Wr itvl steps. For example, if you set CONF Wr itvl to 100, an image is generated every 100 steps.

   In Auto capture mode, in addition to the PNG files, configuration files config****.cfg and config****.cfge (in a format readable by AtomEye) are also written. AtomEye has a function where pressing the Delete key increments the numerical part of the filename it reads. By using this feature, you can visualize the time evolution of atomic configurations.

[Exercises]

1. Comparison of Ensembles

1) Create a cubic crystal of Cu atoms replicated 3×3×3 unit cells, set an appropriate temperature, and run the NVT ensemble to observe the thermal motion of atoms

(thermal fluctuations). The lattice constant of Cu is approximately 3.61 Å.

2) Switch to the NVE ensemble and run MD for a while. Plot the time evolution of each energy component and the temperature. Confirm that the total energy is conserved.

3) Next, switch to the NVT (thermostat) ensemble (temperature control using the Nose–Hoover method). Set an appropriate target temperature and observe how the temperature is controlled. Vary the virtual mass of the thermostat and examine how the temperature response changes.

   Note: In the Set parameters panel, around the middle left, there is a field NH mass that controls the virtual mass for temperature control. It is specified in powers of ten; increasing the value by 1 multiplies the virtual mass by 10. Choose an appropriate virtual mass, run MD, and examine the temperature evolution in temp.d. You should verify that a larger virtual mass leads to a slower temperature response.

4) Using NσH ensemble, perform a stress-controlled simulation. Set target stress components and confirm that the stress is properly controlled.

   Note #1: In this software, the stress-controlled ensemble is labeled NPH, not NσH. Selecting NPH or NPH+PR damper in Algorithm enables stress control. NPH corresponds to the original Parrinello–Rahman method, while NPH+PR damper introduces a damping term to suppress oscillations of the cell.

   Note #2: If you press the Stress button, a popup window appears. The stress acting on the cell is shown at the top. In the middle region of the popup, under PR Setting, you can enter target stress components (set them all to zero here).

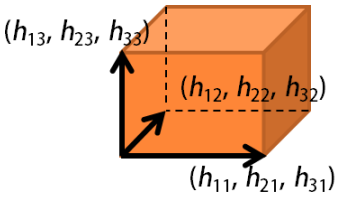
   Note #3: The virtual mass for stress control is set in the same way as in 3) above. The time evolution of the stress components is output to stress.d. The fluctuations of the stress components are quite large, but this is normal (you need to take averages over an appropriate time window).

２. Determination of Lattice Constants and Heating Analysis

1) Create a crystal model of appropriate size, and perform MD under zero-stress and constant-temperature conditions. Set a suitable (rather low) temperature, run MD for a sufficient number of steps, and determine the lattice constant at that temperature (and pressure).

   Note: The crystal structure may be fcc. Available atomic species depend on the chosen potential function. You can also try a diamond structure such as Si by using Tersoff or Stillinger–Weber (SW) potentials.

The time evolution of the cell size is written to cell.d. The meaning of each column is described in the first line, and the cell matrix components are defined as shown in the right-hand figure. Dividing the cell size along a given direction by the number of unit cells in that direction gives the lattice constant. In stress-control methods without damping, the cell size continues to oscillate, so you may need to take a time average over a suitable interval.



2) Next, increase the temperature somewhat and repeat the same procedure. By repeating this for several temperatures, determine the relationship between lattice constant and temperature (the slope of this relation yields the linear thermal expansion coefficient).

3) If you continue to raise the temperature further, the crystal eventually melts. Even after melting, you can still determine an effective lattice constant by the same procedure. Check that the lattice-constant–temperature curve bends near the melting point (a very rough estimate of the melting temperature).

３. Structural Relaxation and Elastic Constant Calculation

1) Create a crystal model of appropriate size. Press the Stress button to open the popup window and examine the stress acting on the cell shown at the top. If you have entered a lattice constant somewhat arbitrarily, the stress will likely not be zero; record its value.

2) Perform a relaxation calculation under zero-stress conditions and confirm that the stress converges toward zero.

Note: In the middle region of the Stress popup, under PR Setting, you can enter target stress components. After confirming that all target stresses are set to zero, choose Full relaxation (static) in Algorithm and run MD. In this mode, both atomic structure relaxation and cell relaxation (to reach the target stress) are carried out simultaneously.

3) Next, apply a small strain and, under fixed cell size conditions, perform an atomic structural relaxation calculation to obtain the stress components. From these results, determine the elastic constants of the crystal.

Note #1: To apply a uniaxial tension or compression along x, y, or z, you can simply enter the desired cell size in the Cell fields of the Status area in the Control window. To apply shear strain, use the Cell dimension entries in the window that appears when you press Create Config. The three vectors (1, 2, 3) correspond to the three cell vectors shown in the figure below.

Note #2: In this case, only atomic structural relaxation is performed, so choose Relaxation (atom) in Algorithm. In this mode, the equations of motion are integrated as in NVE, and structural relaxation is carried out according to the method specified by Relax algo. Open the Set parameters panel via Set param, and set Relax algo to GLOC, a relaxation method that "applies a brake when $\sum_i \vec{v_i} \cdot \vec{F_i}$ is negative".

You can also choose Relax algo = FIRE, which accelerates relaxation by adjusting the time step and other parameters, but the stability is reduced (the structure may diverge and collapse).