In-Class Work: Mini-Project II

Today you will work in groups of two or three on assigned mini-projects (see below to which group and project you belong). You will work today more with molecular dynamics simulations of the Lennard-Jones system and their analysis. You will work from 9:30-10:00 on your analysis, from 10:00-10:20 on your slides (one or two) and 10:20-10:52 each group will present for 5min their results to the class.

Mini-Project II.1 (Andy and Damon)

II1a. You will determine the radial distribution function for several densities. Start with the program
`~kvollmay/classes.dir/phys338.dir/phys338_s2015.dir/md.dir/mdprojII1_start.py`
The program has a loop over density. For each density the program rescales the particle positions to the desired density $\rho = N/L^3$ and equilibrates first with a very small Δt and then continues with a larger Δt. The program also determines the radial pair distribution function:

$$g(r) = \frac{1}{\rho} \frac{h(r_{\text{bin}})}{N_{\text{meas}}(N-1)(\text{shellvolume})} \tag{14}$$

where N is the number of particles, r is the distance between two particles, $h(r_{\text{bin}})$ is the histogram for the distances between pairs i, j and N_{meas} is the number of measurements. Read the program and find out what $g(r)$ measures physically.

II1b. Now run the program for one density (adjust the program), so that you can test the program. Look at the resulting $g(r)$

II1c. Run the program for several densities in the range $0.3 \leq \rho \leq 0.9$. Make one figure with $g(r)$ for the different ρ (your result figure). Think about the interpretation of your results.

II1d. Make one or two slides for your 5 min long talk. You will have to start with defining $g(r)$ and you will have to explain that you varied ρ and kept the temperature the same ($T=?$). Plan the words for your 5 min talk.

II1e Put your slide and program in your `~/share.dir/` and give me read-permission.

Mini-Project II.2 (Jonathan, Ian and Joe)

II2a. You will determine the radial distribution function for several temperatures. Start with the program
`~kvollmay/classes.dir/phys338.dir/phys338_s2015.dir/md.dir/mdprojII2_start.py`
The program has a loop over temperature. For each temperature the program equilibrates first and then determines the radial pair distribution function:

$$g(r) = \frac{1}{\rho} \frac{h(r_{\text{bin}})}{N_{\text{meas}}(N-1)(\text{shellvolume})} \tag{15}$$

where N is the number of particles, r is the distance between two particles, $h(r_{\text{bin}})$ is the histogram for the distances between pairs i, j and N_{meas} is the number of measurements. Read the program and find out what $g(r)$ measures physically.

II2b. Now run the program for one temperature (adjust the program), so that you can test the program. Look at the resulting $g(r)$

II2c. Run the program for several temperatures in the range $0.5 \leq T \leq 2.0$. Make one figure with $g(r)$ for the different T (your result figure). Think about the interpretation of your results.

II2d. Make one or two slides for your 5 min long talk. You will have to start with defining $g(r)$ and you will have to explain that you varied T and kept the density the same ($\rho = N/V =?$). Plan the words for your 5 min talk.

II2e Put your slide and program in your `~/share.dir/` and give me read-permission.

Mini-Project II.3 (Sean and Sarah)

II3a. You will determine the equilibrium potential energy $\langle E_{\rm pot}\rangle$ as function of temperature. Start with the program
`~kvollmay/classes.dir/phys338.dir/phys338_s2015.dir/md.dir/mdprojII3_start.py`
The program has a loop over temperature. For each temperature the program already measures $E_{\rm pot}(t)$. Look at the program, so that you can adjust the wanted parameters and can include the desired measurement of $\langle E_{\rm pot}\rangle(T)$

II3b. Now run the program for one temperature (adjust the program), so that you can test the program. Look at the resulting $E_{\rm pot}(t)$, so first at the potential energy as it equilibrates over time. Now add at line 211 (indicated) the measurement of `Vpotequil`. Note that the program already has the normalization and the printing into a file for $\langle E_{\rm pot}\rangle(T)$ in the last two lines of the program.

II3c. Run the program for several temperatures in the range $0.5 \leq T \leq 2.0$. Make one figure with $\langle E_{\rm pot}\rangle(T)$. (your result figure). Think about the interpretation of your result. If you have time, try if you find a specific dependence.

II3d. Make one or two slides for your 5 min long talk. To be able to define $\langle E_{\rm pot}\rangle(T)$ you might want to start with an example figure of $E_{\rm pot}(t)$ and then define $\langle E_{\rm pot}\rangle(T)$. Then you will have to explain that you varied T and kept the density the same ($\rho = N/V =?$). Plan the words for your 5 min talk.

II3e Put your slide and program in your `~/share.dir/` and give me read-permission.

Mini-Project II.4 (Andrew, Akim and Narayan)

II4a. You will determine the equilibrium potential energy $\langle E_{\rm pot}\rangle$ as function of density of your system. Start with the program
`~kvollmay/classes.dir/phys338.dir/phys338_s2015.dir/md.dir/mdprojII4_start.py`
The program has a loop over density. For each density the program rescales the particle positions to the desired density $\rho = N/L^3$ and equilibrates first with a very small Δt and then continues with a larger Δt. For each density the program already measures $E_{\rm pot}(t)$. Look at the program, so that you can adjust the wanted parameters and can include the desired measurement of $\langle E_{\rm pot}\rangle(\rho)$

II4b. Now run the program for one density (adjust the program), so that you can test the program. Look at the resulting $E_{\rm pot}(t)$, so first at the potential energy as it equilibrates over time. Now add at line 236 (indicated) the measurement of `Vpotequil`. Note that the program already has the normalization and the printing into a file for $\langle E_{\rm pot}\rangle(\rho)$ in the last two lines of the program.

II4c. Run the program for several densities in the range $0.3 \le \rho \le 0.9$. Make one figure with $\langle E_{\rm pot}\rangle(\rho)$. (your result figure). Think about the interpretation of your result. If you have time, try if you find a specific dependence.

II4d. Make one or two slides for your 5 min long talk. To be able to define $\langle E_{\rm pot}\rangle(\rho)$ you might want to start with an example figure of $E_{\rm pot}(t)$ and then define $\langle E_{\rm pot}\rangle(\rho)$. Then you will have to explain that you varied ρ, that you first equilibrated with smaller Δt and that you kept the temperature the same ($T =?$). Plan the words for your 5 min talk.

II4e Put your slide and program in your `~/share.dir/` and give me read-permission.

Mini-Project II.5 (Pete, Chris and Gus)

II5a. You will determine the equilibration time $t_{\rm eq}$ of the potential energy $E_{\rm pot}(t)$ as function of temperature. Start with the program
`~kvollmay/classes.dir/phys338.dir/phys338_s2015.dir/md.dir/mdprojII5_start.py`
The program has a loop over temperature. For each temperature the program already measures $t_{\rm equ}(T)$. Look at the program, so that you can adjust the wanted parameters. The program already measures $t_{\rm eq}(T)$ [2]

II5b. Now run the program for one temperature (adjust the program), so that you can test the program. Look at the resulting $E_{\rm pot}(t)$, so first at the potential energy as it equilibrates over time. Also look at $t_{\rm eq}$.

II5c. Run the program for several temperatures in the range $0.5 \le T \le 2.0$. Make one figure with $t_{\rm eq}(T)$. (your result figure). Think about the interpretation of your result. If you have time, try if you find a specific dependence.

II5d. Make one or two slides for your 5 min long talk. To be able to define $t_{\rm eq}(T)$ you might want to start with an example figure of $E_{\rm pot}(t)$ and then define $t_{\rm eq}(T)$. Then you will have to explain that you varied T and kept the density the same ($\rho = N/V =?$). Plan the words for your 5 min talk.

II5e Put your slide and program in your `~/share.dir/` and give me read-permission.

[2] The program also determines $E_{\rm pot}(t)$ and even $\langle E_{\rm pot}\rangle(T)$ under the condition that you comment out the `break` command for the $t_{\rm eq}$ measurement.

Upcoming Deadlines:

- April 14 (today): Mini-Project II (in class & graded)
  and title and abstract of main projectpaper
- April 21, 23, 28: 5, 5, 3 Talks
- April 21: First Version of Second Main Project Paper
- May 6 (our final): Final Version of Second Main Project Paper