In-Class Work: Molecular Dynamics Simulation

1. Numerical Integration

I will first give some short introduction.

1a. For $f(t, y) = Ax$ write a program which uses the Euler-step for integration (and therefore use the flowchart on the white board) to integrate

$$\frac{dx}{dt} = f(t, x) = Ax$$

Use $A = 0.3, t_0 = 0.0, x_0 = 0.6, \Delta t = 0.2, n_{\max} = 100$ (that means $t_{\max} = 20.0$). Print $t, x(t)$ for every time-step t. Save the data in a file, e.g. `out1sim0.2.dat`. To help you with the writing the data into a file of specified name, you may start with copying the following program into your working directory:
`~kvollmay/share.dir/inclass2019.dir/md1_start.py`

1b. What do you expect for $x(t)$ (we can solve the DE analytically).

1c. Add to your program that the exact solution for $t, x(t)$ is printed for every time-step into another file, e.g. named `out1theory.dat` Look at the comparison of the numerical solution and the theoretical solution with
`xmgrace out1theory.dat out1sim0.2.dat`
and if you would also like to use a logarithmic vertical axis and also set the x-range and y-range then you may use
`xmgrace out1theory.dat out1sim0.2.dat  -log y -world 0 0.6 20 300`
When you get to this, I can also show you how to set the y-axis and x-axis settings within xmgrace.

1d. Now rerun the program for $\Delta t = 0.1$ and adjust $n_{\max}$ to get the same $t_{\max} = 20.0$ and print into another file, e.g. `out1sim0.1.dat`. Then rerun the program again this time for $\Delta t = 0.01$ and $n_{\max}$ again adjusted. Look at your data with
`xmgrace out1theory.dat out1sim0.*.dat -log y -world 0 0.6 20 300 -legend load`
When you got this, please get me, I will show you a few tools with `xmgrace` I summarize here in footnote. [2]

2. Newton's Second Law

2a. Make sure to get me, before you continue. What are the Euler step updates for $x(t+\Delta t)$ and for $v_x(t + \Delta t)$?

2b. Numerically integrate for $F_x^{\text{net}} = -mg$. Use $g = 9.8, \Delta t = 0.2, t_{\max} = 20.0, x_0 = 5.0, v_{x0} = 2.3$. Print into a file $t, x(t), v_x(t)$. As above, also determine the analytical solution and rerun the numerical solution also for $\Delta t = 0.1$ and $\Delta t = 0.01$. Look at your comparison as in 1d.

[2] To save xmgrace session: `File` → `Save as` and in Selection entry give filename, for example `md1dfig.xmgr` To save eps-file `File` → `Print setup` then change `Postscript` to `EPS`. In case you had previously used Save as the eps-filename is already suggested and then click `Accept`. To get the eps-file printed use `File` → `Print`

3. Harmonic Oscillator & Surprise

3a. Numerically integrate this time for the harmonic oscillator, so $F_x^{\rm net} = -kx$. We can also analytically solve this equation. Let's choose $t_0 = 0.0, x_0 = 5.0, v_0 = 0.0$, then the theoretical solution is

$$x(t) = 5.0\cos(\omega_0 t) \qquad v_x(t) = -5.0\omega_0 \sin(\omega_0 t)$$

where $\omega_0 = \sqrt{(k/m)}$. So we know the period $T = 2\pi/\omega_0$. Let's choose $\Delta t = T/n_{\rm div}$. Integrate $F_x^{\rm net} = -kx$ for $k = m = 1$ and for $n_{\rm div} = 100$ and do $n_{\rm max} = 10n_{\rm div}$ MD steps. Print also the analytical solution and compare. **Note: Before you update $x(t)$, you need to copy the value of $x(t)$ into a temporary variable for example `xold=x` only then you can update x and then v. For v you need to use `xold`.** Try also with $n_{\rm div} = 1000$. What happens?

3b. Also determine the theoretical and numerical total energy

$$E_{\rm tot} = \frac{1}{2}kx^2 + \frac{1}{2}mv_x^2$$

as function of time, so $E_{\rm tot}(t)$. If you print for example into `out3sim100.dat` $t, x, v_x, E_{\rm tot}$ and similarly into the other files, you can compare the $E(t)$ results with

```
xmgrace -block out3theory.dat -bxy 1:4 -block out3sim100.dat -bxy 1:4 -block out3sim1000.dat  -bxy 1:4
```

Get me, when you have the results.

4. Euler-Cromer

Read in the Gould & Tobochnik's book the first page of chapter 3. Change your program from 3b to use the Euler-Cromer step instead of the Euler step. Repeat the integration and compare again with the theoretical solution.

5. Integration Methods

If time is left, start reading the Appendix 3A which is near the end (page 30 out of 41 pages) of Chapter 3 of the Gould & Tobochnik book.