Technical info

- Using Google find MobaXterm, download the Home version (for free), Portable edition.
- Connect to the “free” network called Hotspot (no password). Note that your access to the Internet will be interrupted.
- Start MobaXterm and select “Start new terminal”. After a prompt (>), type command
  ```
  > ssh -X guest@10.42.0.1
  ```
  You will be given the password to login.

Notes:

- Write case-sensitively! “`-X`” is hyphen and uppercase X
- Sometimes, backspace does not work. Try ctrl-h instead.

The shell

The traditional style of work in linux/unix is based on writing commands to a command interpreter called a **shell**; the command is executed after Enter is pressed. Your shell is called bash.

- The line start (e.g., `guest@403-as67-03:~/VY$ `) is called **prompt**.
- A window with a prompt and command interpreter is a **terminal**.
- To fix/repeat previous command(s), use cursor arrows.

Test of connection:

```
guest@403-as67-03:~/VY$ xeyes
```

A pair of eyes should appear. Kill it by clicking × , or by ctrl-c in the terminal.

NOTE: ctrl-c in a terminal = interrupt, not Copy!

Do not see the eyes?

- They may be iconized, look at the bottom bar.
- Restart MobaXterm.
- Restart Windows.

Some shell commands

You likely will not need this:

exit	logout (also ctrl-d)
cd FOLDER	change directory (folder)
cd ..	parent directory (back one level)
cd -	previous directory
cd	home directory
ls	list files
ls -l a*.g	list details selected files
cat FILE	print (a short ASCII) file
history	show previous commands
rm FILE	remove file (lost forever!)
cp FILE NEWFILE	copy file
cp FILE DIRECTORY	copy file
mv FILE NEWFILE	rename file
mv FILE DIRECTORY	move file

Hints

But there may be surprizes, so read this:

- – If a terminal gets covered by text (and no program is runing), type Enter.
  – If it does not help, type (as if to invisible prompt): `reset` Enter.
  – But in Midnight Commander (see below), type ctrl-o.
- ctrl-c in a terminal is not “Copy”, but it interrupts the runing program.
- To copy/paste in a terminal, use:
  ctrl-shift-c = Copy to clipboard,
  ctrl-shift-v = Paste.
- In the native X environment, a marked text is pasted by the middle mouse button (a wheel). This is much faster than ctrl-shift-c/ctrl-shift-v.
- The system is case-sensitive!

Midnight Commander

The Midnight Commander is similar to the Windows/Total Commander. Start it by:
`guest@403-as67-03:~/VY$ mc`
Both mouse operations and many keyboard shortcuts (hot keys) are accepted.

Most important hot keys:

- ctrl-o Toggle screen output / file list panels.
  In addition, a (mc-internal) command prompt is available.
- F3 View text file (or run the associated application).
- Enter Run a script or open (= run the associated application),
  the same as doubleclick.
- F4 Edit text file (= `mcedit FILE` from the command prompt)
- F9 Open the menu.
- F10 End/Quit (function, editor, Midnight Commander. . .).

Our Midnight Commander is configured to show one wide window, use Tab to access the other panel.

Symbol * in front of file name denotes a **script**, a set of commands in bash.
Symbol / in front of name denotes a directory (folder).
Symbol /.. is the previous (parent) folder.

Viewing the trajectory (`show`)

The usage is intuitive:

- clicking any button by the right mouse = help
- left mouse = rotate
  wheel = zooms out/in
  middle mouse = move
  right mouse = rotate around center
- button proj or hot key = toggles parallel/central projection
- button std or hot key Tab brings back the original orientation
- control the “movie” by the `----  playback  ----` panel
- get a raytraced picture by NFF, then one frame+render
- get a stereogram (parallel-eyes-type) by ZBUF, then one frame+render
  (remove the box by box first)
- useful hot keys: PgUp and PgDn: go by 1 frame
  i play from start

Graphs (plot)

- Several plots started from the same application (as convergence profiles) can be killed by button kill all or hot key K.
- You can show the file info by the right mouse button.
- To zoom, select a rectangle by the left mouse.
- Undo the zoom by undo or hot key k.

Task A: Melting point of a model of NaCl

Aim: Determine the melting point of a model of NaCl by direct equlibrium in the slab geometry ("zone melting").

Model: Lennard Jones + charges*.

Simulation details: Verlet/leap-frog integrator, Andersen thermostat, Ewald summation, Berendsen barostat, linked-cell list.

Steps:

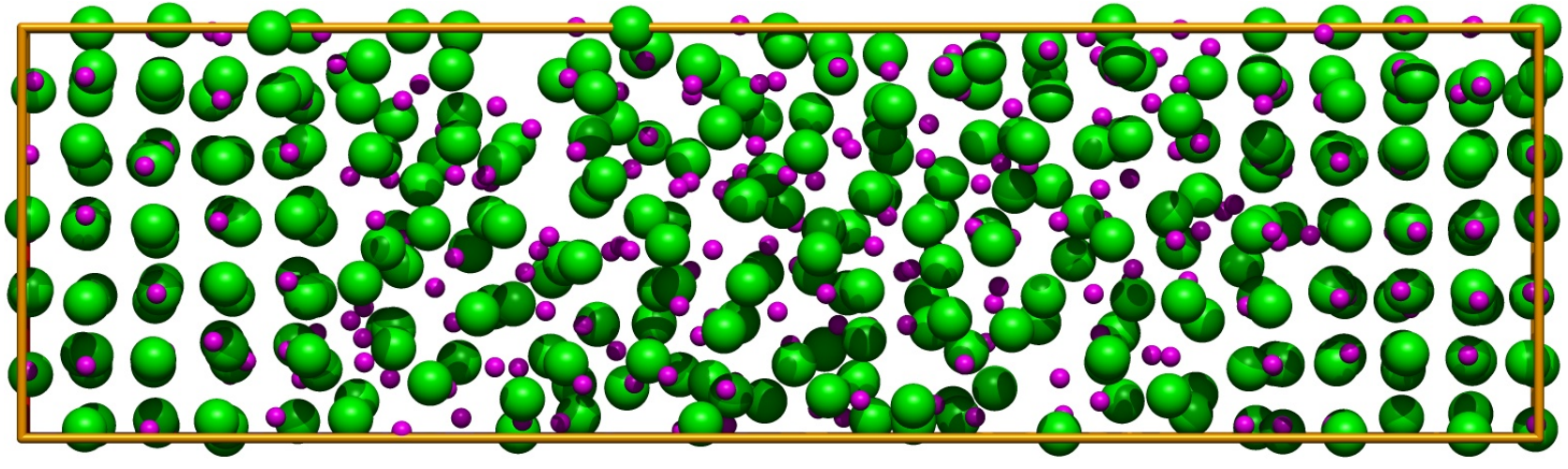
- Replicate Na_4Cl_4 $3 \times 3 \times 3$ times and simulate the crystal $Na_{108}Cl_{108}$ in the periodic boundary conditions.
- Determine the equilibrium box size, radial distribution function, and running coordination numbers.
- Melt and analyze the same quantities.
- Replicate crystal $Na_{108}Cl_{108}$ $1 \times 1 \times 3$ times and melt half of the box.
- Simulate at given temperature and determine whether the crystal melts or grows.

*In Suk Joung and Thomas E. Cheatham, III: Determination of Alkali and Halide Monovalent Ion Parameters for Use in Explicitly Solvated Biomolecular Simulations, *J. Phys. Chem. B* **112**, 9020–9041 (2008)

Start (using Midnight Commander)

- Click (or select and Enter) `START.sh` and follow the instructions.
- Find the folder you have created in the previous step.
- Click or select (by cursor arrows + Enter) the first script to run:
  `A01-prepare-Na4Cl4.sh`.
  and **carefully read and follow the instructions**.
- Then, continue by script `A02-replicate.sh`, etc.

In the A03 step, you should select temperature. Negotiate this with your colleagues so that the interval of 1200–1400 K is uniformly covered.



Task B: Structure around a solute in water

Aim: Study the stucture of water around a solute molecule.

Models: water: SPC/E (classical model, Simple Point Charge/Extended)
solute: Lennard-Jones (+ charge, fulleren: CHARMM21)
(Na^+, Cl^-, Li^+, Ca^{2+}, noble gases, endofullerenes)
Warning: the simulations with endofullerenes are slower!

Simulation details: Verlet/leap-frog integrator, SHAKE, Berendsen thermostat, smoothed cutoff electrostatics to 10–12 Å, Berendsen barostat, direct pair sum.

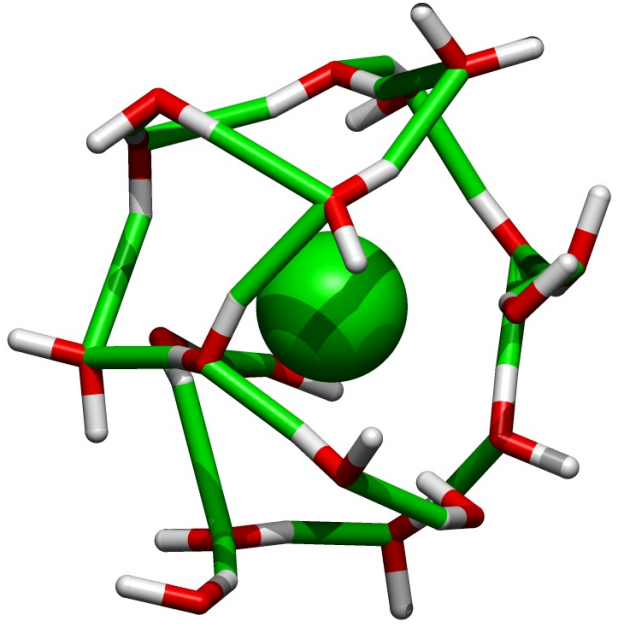
Steps:

- Prepare (by random shooting) a configuration of the solute in about 200 waters.
- Equilibrate.
- Simulate at constant T, p.
- Show the radial distribution function and the running coordination number.
- Observe the orientation of the water molecules around the solute.
- Observe the hydrogen bond network in the solvation shell.

Start (using Midnight Commander)

- Click (or select and Enter) `START.sh` and follow the instructions.
- Find the folder you have created in the previous step.
- Click or select (by cursor arrows + Enter) the first script to run:
  `B01-NVT-start.sh.`
  and **carefully read and follow the instructions**.
- Then, continue by script `B02-NPT-equilibrate.sh`, etc.

} already done



Task C: Coealescence of small water droplets

Aim: Prepare two small water droplets and let them coalesce. Observe a possible increase of temperature caused by decreasing the surface energy.

Water model: SPC/E (classical model, Simple Point Charge/Extended).

Simulation details: Verlet/leap-frog integrator, SHAKE, Berendsen thermostat, smoothed cutoff electrostatics to 12 Å, direct pair sum.

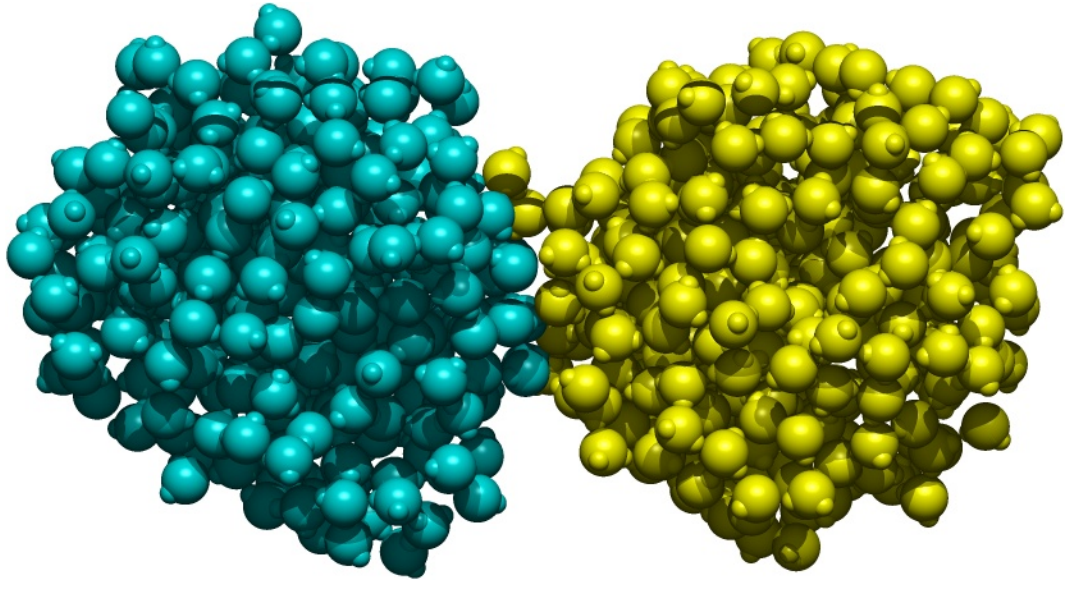
Steps:

- Prepare a box of $N = 200$ to 400 water molecules and equilibrate a bit.
- Place it into a large box and simulate: a spherical droplet will be created.
- Replicate twice and add small velocity to both droplets so that they will meet.
- Simulate in the microcanonical ensemble and observe the coalescence.
- Try to determine the potential energy and temperature increase during the coalescence from the temperature convergence profile.
- Calculate the increases theoretically (you will need the surface tension, density, and heat capacity; use the data for real water).

Task C: Start (using Midnight Commander)

- Click (or select and Enter) `START.sh` and follow the instructions.
- Find the folder you have created in the previous step.
- Click or select (by cursor arrows + Enter) the first script to run:
  `C01-box-of-water.sh`
  and **carefully read and follow the instructions**.
- Then, continue by script `C02-one-droplet.sh`, etc.

} already done



Appendix: MACSIMUS file types

Some MACSIMUS file types and associated applications in Midnight Commander and command `start`

type	contents	application	action
.che	chemical formula	blend	edit, optimize from start (F3=vibrations)
.mol	mol. topology	blend	edit, optimize
.plb	trajectory	show	show (and edit) trajectory
.cp	convergence profile	showcp	show graphs
.cfg	configuration	showcfg	show configuration
.sta	statistics	staprt	averages, errors, etc. (F3=detailed)
.rdf	pair histograms	rdfg	show RDF (F3=running coord. #)
.g	RDF	plot	show RDF
.cn	running coord. #	plot	plot running coordination number
.def	default parameters	go	run the 1st line
.get	simulation param.	go	run the 1st line
.nff	scene data	ray	raytrace and show