LINUX QUICKSTART

- *NOTE:* These instructions apply only for the Linux computers at Aalto. See further information at the project home page if you wish to install the tools on other Unix-based computers.
- *Terminal* is a text-based tool for interacting with the computer. Open the terminal with *Ctrl+Alt+t*, or by left-clicking a desired folder and selecting "Open Terminal".
- We run commands in the terminal by typing them in and executing them with enter. The history of latest commands is preserved and can be retrieved with the keyboard up and down arrows. Pasting text into the terminal happens with *Ctrl+Shift+v*. You can also use auto-completion for commands and filepaths by pressing *Tab*.

BASIC TERMINAL COMMANDS

- Here is a list of relevant terminal commands for this project. Some of them can be also executed with GUI+mouse, others cannot.

`pwd`	Print path of current directory
`ls`	List files and folders in current directory
`cd path`	Change directory to given path
`cd ..`	Change directory to parent directory
`cd ~`	Change directory to home folder
`mkdir dirname`	Make a new directory
`python filename.py`	Execute the given python file.
`vmd filename.xyz`	Visualize the given xyz-trajectory.
`touch filename`	Creates a new file if it does not exist

SETUP SIMULATION ENVIRONMENT

- See detailed instructions at the project home page
- To download and install the simulation libraries at your home folder, run the following commands in the terminal:

```
cd ~
wget http://users.aalto.fi/~asf/teaching/aalto_physics/_downloads/linux_tools.zip
unzip linux_tools.zip
cd linux_tools
wget http://users.aalto.fi/~asf/teaching/aalto_physics/_downloads/friction_tools.py
touch ~/.zshenv
echo "export PYTHONPATH=$HOME/linux_tools:$PYTHONPATH" >> ~/.zshenv
source ~/.zshenv
```

RUN FIRST TUTORIAL

- The project home page has an extensive set of tutorial simulations. Here we run the first one.
- Run the following commands to create a new folder ("tutorial1") for the simulation, and to create a new file ("tutorial1.py") in that folder:

```
cd ~
mkdir tutorial1
cd tutorial1
touch tutorial1.py
```

RUN FIRST TUTORIAL

- Use your favourite text editor to copy the following python code to the file tutorial1.py.:

```
#! /usr/bin/env python
import friction_tools as ft

# create the simulation containing two atoms
simu = ft.FrictionSimulation()
simu.create_atoms(element='C',positions=[[0, 0, 0],
                                         [6, 0, 0]])

# create an interaction between the two atoms
#simu.create_interaction(['C','C'],strength=10.0,equilibrium_distance=5.0)

# give the atoms some initial velocities
vs = [[0.1, 0, 0],[-0.1, 0, 0]]
#simu.set_velocities(indices=range(2), velocity=vs)

# tell that we want to run the simulation with default settings
simu.create_dynamics()

# tell that we want to record the movement of the atoms
simu.save_trajectory_during_simulation(interval=5)

# run the simulation for 1000 fs
print "starting simulation"
simu.run_simulation(time=1000.0)
print "finished simulation"

# after finishing, create an xyz-file for viewing what happened
ft.trajectory_to_xyz()
```

RUN FIRST TUTORIAL

- Execute this python code with

```
python tutorial1.py
```

- To visualize the simulation trajectory with VMD, run the following command

```
vmd simulation.xyz
```