Software installation for hands-on session I (Sunday)

For the first hands-on session which will be held on Sunday afternoon, you will be using the EON software (`https://theory.cm.utexas.edu/eon/`). EON consists of two parts, a 'server' and a 'client'. The latter performs simple calculations such as structural relaxation, nudged elastic band calculation and saddle point searches. The server performs more complex tasks such as adaptive kinetic Monte Carlo (AKMC) calculations of time evolution by sequential thermally activated events. The server repeatedly calls the client during such long time scale calculations. Both the server and client have to be installed on your computer.

Installation of EON
EON requires **python2.7**, **Numpy** and the **Atomistic Simulation Environment (ASE)** which can be installed via the python package manager (pip) (for ASE see: https://wiki.fysik.dtu.dk/ase/install.html)

To install EON:

- open the terminal and select a location to install EON

- clone the EON repository: $svn co http://theory.cm.utexas.edu/svn/eon

- Add the following lines to your $HOME/.bashrc (or $HOME/.bash_profile:) files
    export PYTHONPATH=your_path_to_EON/eon:$PYTHONPATH
    export PATH=your_path_to_EON/eon/bin:$PATH

- $source $HOME/.bashrc

- To install the EON server go into the downloaded EON folder (there should be a setup.py file in this folder) and execute the server install by: $sudo python setup.py install (**Note:** you will be asked to type in your sudo password)

- To install the EON client go into the client folder and execute make: $make. This should work without problems by using the standard GNU compilers.

- Copy the eonclient to the eon/bin: $cp eonclient ../bin/

- To make sure the path to the EON binaries were setup properly execute:
    $which eon
    $which eonclient
  Make sure the path corresponds to the path you expect.

- Now to test if both of the EON binaries *eon* and *eonclient* work. Go to directory
  your_path_to_eon/examples/akmc-al and execute eon. Then go to your_path_to_eon/examples/neb-al
  and execute the EON client