CHL Lab

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**Software Installation Instructions for Desktop Computers:**

(If you do not yet know Unix commands, do this first: [http://tldp.org/HOWTO/Bash-Prog-Intro-HOWTO.html](http://tldp.org/HOWTO/Bash-Prog-Intro-HOWTO.html" \t "_blank))

You need access to a desktop that runs gmx / solefp for visualization, easy file access, and preparation for gmx run, etc.

You can use either the Work Station computers, or your own Mac/Linux computer.

To Install MD, SolEFP and lineshape conversion softwares on your desktop, do:

**1.** **Gromacs**

If using Work Station computers: Gromacs is already installed.

If using your own Mac/Linux computer: Go to <http://www.gromacs.org/Downloads>

In addition, put MD/forcefields folder in a certain location on your desktop.

Take note of the file path in which gmx is installed and forcefields is put.

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You will need these two documentations very, very often:

Gromacs command line reference: <http://manual.gromacs.org/documentation/5.1/user-guide/cmdline.html> 🡪 reference guide for gmx commands

Gromacs .mdp file options: <http://manual.gromacs.org/online/mdp_opt.html> 🡪 reference guide for md parameter file options

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You might also need the Gromacs manual at some point (etc. to understand the force field function types for making new parameters):

<http://manual.gromacs.org/documentation/2016-current/manual-2016.5.pdf>

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There is no need for you to refer to an external tutorial. See my MD/protocols/ gromacs\_general\_protocol.txt to get started. Job submission scripts can be found in “Submission scripts”.

**2. SolEFP**

Put folders anaconda and slv\_util in a certain directory on your desktop.

Take note of the file path in which these two directories are installed.

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The solefp fragments live in anaconda/lib/python2.7/site-packages/solvshift-dat/frg. Once you have made a new fragment, this is where you should put it so that slv can read the fragment properly.

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The solefp programs (as well as lineshape conversion, interhelical angles, cyanylation programs, etc.) are written in python.You will need to learn some basic python to better understand / modify these scripts. See [https://www.learnpython.org/](https://www.learnpython.org/" \t "_blank) Just do the "Learn the Basics" part.

**3. ~/.bashrc (Linux) or ~/.bash\_profile (Mac)**

You will need to add something in your bash start up file so that md and solefp packages can be run properly. Type in commad line “nano ~/.bashrc” or “nano ~/.bash\_profile”. Then add the following lines:

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source /[where you installed gromacs]/gromacs/bin/GMXRC

export GMXLIB=/[where you put forcefields]/forcefields

export PATH="/[where you put anaconda]/anaconda/bin:$PATH"

export SLV\_DATA="/[where you put anaconda]/anaconda/lib/python2.7/site-packages/solvshift-dat

export PATH=$PATH:/[where you put slv\_util]/slv\_util

export PATH=$PATH:/[where you put slv\_util]/slv\_util/lib

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Then, type “source ~/.bashrc” or “source ~/.bash\_profile”.

**4. Text Editors**

You will need to learn either nano or vi.

In addition, install TextWrangler: <https://www.barebones.com/products/textwrangler/>

TextWrangler is an alternative to TextEdit but has a much clearer layout. You will want to use it to look at data files or write input files, etc. You might also want to use it to write/modify awk scripts (see below).

For Mac users: Xcode is a good editor for writing shell scripts.

**5. Awk**

Awk is an excellent software for processing program input / outputs. It is currently used for gathering solefp results (see ir-md-solefp.sh), rewriting time points (see rewrite\_time.awk), and cleaning up the numbering of residues (see rewrite\_residue\_index.sh), switching hydrogen names so gmx can read them (SwitchHydrogenNames.awk), etc. It is like the C languages, but with additional features that allow you to process lines and strings.

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Awk comes with Linux operation systems.

To install gawk on Mac: See [http://macappstore.org/gawk/](http://macappstore.org/gawk/" \t "_blank)

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Awk tutorials:

There is an excellent (2 hours) Lynda.com class called “AWK-Essential-Training”. Haverford furnishes free Lynda.com licenses.

You can also read my notes from that class: awk\_essential\_training-notes-rjx.pdf.

**6. Xmgrace**

You will need to install xmgrace, and use it for visualizing md rms, gyrate, sasa, dihedral trajectories and solefp lineshapes, etc. Xmgrace can produce Origin-like plots on your computer with a simple command "xmgrace [filename]”. If your data file has one x- column but multiple y-column, type "xmgrace –nxy [filename]”.

Install xmgrace here: [https://nokyotsu.com/qscripts/2011/05/installing-xmgrace-on-snow-lepoard.html](https://nokyotsu.com/qscripts/2011/05/installing-xmgrace-on-snow-lepoard.html" \t "_blank) .

**7. Chimera**

You will need to install Chimera for visualizing .pdb files: either single structures or md trajectories (such as \*-trj.pdb and \*-protein.pdb generated at the end of md trimming), and pre-processing the .pdb files for gromacs simulation. Download Chimera here: <http://www.cgl.ucsf.edu/chimera/download.html> .

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To make a movie out of a multi-frame .pdb file, do:

Tools/MD-Ensemble Analysis/MD Movie. Configure the input as "single" "pdb file". Then, open the .pdb files you have got.

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You will want to change the appearance of plots, etc. so you might also want to refer to the Chimera user guide: <http://www.cgl.ucsf.edu/chimera/docs/UsersGuide/>

If having trouble with Chimera, ask Casey to train you.