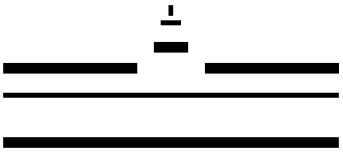

Westfälische
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Linux und Simpson

Cheatsheet

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1 Introduction

This will be a short summary of the various, self programmed tools and aliases that can be used inside the Linux virtual machine (VM). Some of these tools also work under Windows, but the main focus of this summary is Unix, especially Ubuntu 16.04.
These tools were developed by many different people and no comprehensive summary existed until now.
The summary will be divided into a part about the technical aspects, a part for the various *SIMPSON* plugins and *TCL* scripts and a third part about *BASH* scripts and Linux aliases.

2 Installation under *UNIX*

New tools should be accessible for every user, from every path on the virtual system, without requiring knowledge of the correct physical path of the programm. This can be achieved by either copying the tools to the systems */usr/bin* path, or copying the code directly to the *~/.bashrc*. Using the */usr/bin* folder is the preferred method for TCL scripts, or larger programs.
Small, user-defined aliases can be in placed into the *~/.bashrc*. If many aliases are used, or the user wants to sync his aliases across multiple system an additional file, containing only the aliases can be defined. This file should be *~/.bash_aliases* and needs to be placed along the *~/.bashrc*.

3 *SIMPSON* and *TCL*

3.1 ascii2spe

Converts *ascii* files to *.spe* files normally generated by *SIMPSON*.

3.2 bruk2simpson

Converts *Bruker* 1D spectra (1r and 1i) to *.spe* files normally generated by *SIMPSON*

3.3 dipole

Calculates the dipole-dipole coupling strength based on user input. The user can define a pair of nuclei and the distance between them in Angstroem.
Example: *dipole 1H 11B 2.0*

3.4 dist

Calculates the distance between two nuclei based on the given dipolar coupling strength (in Hz).
Example: *dist 1H 1H -20000*

3.5 fphase

Fixes the phase settings of a *SIMPSON* file (*.spe*).

3.6 fref

Fixes the reference settings of a *SIMPSON* file (*.spe*).

3.7 pipe2spe

Converts *pipe* files to *.spe* files normally generated by *SIMPSON*.

3.8 protonfreq

Calculates the proton frequency of a given nuclei based on the resonance frequency (in MHz)
Example: *protonfreq 13C 125.0*

3.9 pwcalc

Caclulates the pulselength for a 90ř-pulse based on the given nutationfrequency (in kHz).
Example: *pwcalc 83.3*

3.10 resfreq

Calculates the resonance frequency of a given nuclei based on the proton frequency (in MHz)
Example: *protonfreq 13C 500.0*

3.11 rfcalc

Caclulates the nutationfrequency for a 90ř-pulse based on the given pulselength (in μs).
Example: *pwcalc 3.0*

3.12 spe2ascii

Converts *.spe* files normally generated by *SIMPSON* to *ascii*.

4 *BASH* and *ALIAS*

4.1 quickplot

Minimalistic command to plot an *ascii* (e.g. *.xy*) file from the terminal. It utilises *gnuplot* to plot the first and second line as the x- and y-column respectively.
Example: *quickplot filename.xy*

4.2 quickplot_folder

This alias executes the quickplot command for every *.xy* file in the current folder.
Note: Very limited! No color difference and legend.

4.3 share_link

Opens the hardcoded shared folder from the terminal.
Standard setting: */mnt/hgfs/sciebo/*.

4.4 Useful aliases for the *~/.bash_aliases*

The following code can be placed into the *~/.bash_aliases* or the *~/.bashrc* file and is available at the next restart. The examples will be listed by categories and gradually extended.

Control the *ls* command:

```
## Colorize the ls output ##
alias ls='ls --color=auto'
## Use a long listing format ##
alias ll='ls -la'
## Show hidden files ##
alias l.='ls -d .* --color=auto'
```

Control *cd* behaviour:

```
## get rid of command not found ##
alias cd..='cd ..'
## a quick way to get out of current directory ##
alias ..='cd ..'
alias ...='cd ../../../'
alias ....='cd ../../../../'
alias .....='cd ../../../../'
alias .4='cd ../../../../'
alias .5='cd ../../../../..'
```

Set *vim* as default:

```
alias vi=vim
alias svi='sudo vi'
alias vis='vim "+set si"'
alias edit='vim'
```

Shorten *apt-get* and *update*:

```
## installation and removal shortcut
alias install='sudo apt-get install'
alias remove='sudo apt-get remove'
alias purge='sudo apt-get purge'
alias autoremove='sudo apt-get autoremove'
## update on one command
alias update='sudo apt-get update && sudo apt-get upgrade'
```

Get system information:

```
## graphical taskmanagerlike top command
alias gtop='/usr/bin/gnome-system-monitor'
## pass options to free ##
alias meminfo='free -m -l -t'
## get top process eating memory
alias psmem='ps auxf | sort -nr -k 4'
alias psmem10='ps auxf | sort -nr -k 4 | head -10'
## get top process eating cpu ##
alias pscpu='ps auxf | sort -nr -k 3'
alias pscpu10='ps auxf | sort -nr -k 3 | head -10'
## Get server cpu info ##
alias cpuinfo='lscpu'
```

This list is not finished. If you have own useful aliases, please send them to me and I will add them.