

basics

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1 Basics pre-requisites molecular modeling

1.1 New to HPC & Sigma2?

Read https://documentation.sigma2.no/getting_started/getting_started.html

1.2 TigerVNC

Remote desktop (mac/win) - tigerVNC (https://documentation.sigma2.no/getting_started/remote-desktop.html) - Download & install TigerVNC: <https://tigervnc.org/> - Start TigerVNC and enter as **server to connect to**: - `desktop.saga.sigma2.no:5901` - Right click the desktop window and choose Open Terminal Here

1.3 Maneuvering the command line (cmd)

In short, bash is a command processor that runs in a text window where the user (you) types **commands** that causes **actions**. Since bash also can read and execute commands from files, it can be used to write scripts.

1.3.1 Some basic commands

ls — List directory contents

```
ls -ltr
```

cd — Change directory

```
cd path/to/some/place  
cd ../
```

. and **..** . means here where I am now

```
cp somestuff/from/somewhere/foo.txt .
```

.. means the previous directory. One level up.

```
cd ../
```

pwd — Print working directory Where am I? > pwd

echo — Prints text to the terminal window echo Hello world

touch — Creates a file touch readme.txt

less — view the contents of a text file

```
touch readme.txt
echo hello world >> readme.txt
less readme.txt
```

grep — search

```
grep hello readme.txt
```

mkdir — Create a directory

rmdir — Remove directory

1.4 Git

1.4.1 clone

```
git clone https://github.com/....
```

1.4.2 Update repo

```
git pull
```

1.4.3 Add changes (add - commit - push)

```
git add filename
git commit -m "did some changes in filename"
git push
```

1.5 REACT on Saga

```
module load chemREACT/REACT
REACT.py
```

1.6 Qgui on Saga

```
module load Qgui/Qgui
```

The Qgui module automatically loads Q6.

1.7 Gaussian on SAGA

A job scrip, g16run.sh, is in bin.

```
g16run.sh $inputfile $nodes $hours
```

[]: