Quick Reference Guide - PBS

Job Submitting

- Submitting a job "jobname"
  [youraccount]$ qsub jobname
- Checking a job status "jobname"
  [youraccount]$ qstat jobname
- Checking all jobs of a user "usrname"
  [youraccount]$ qstat -u usrname
- Deleting a job, having a job ID "jobid"
  [youraccount]$ qdel jobid

Script Names

- Use text characters only, do not use blank spaces and special characters like %, $, ...
- Use two segment names, separated by a period. The name of the second segment is limited to maximum three characters
- Examples: aminoacid.pbs, dnabase.job, activesite1.sub

PBS Script running Q-Chem

```
#!/bin/tcsh
#PBS -S /bin/tcsh
#PBS -l nodes=4:ppn=2
#PBS -l walltime=72:00:00
#PBS -V
#PBS -o test.log
#PBS -N test
#PBS -j oe
#
set JOB = "test"
#
cd $PBS_O_WORKDIR
source $MODULESHOME/init/tcsh
module purge
module load modules
module load qchem
setenv ONEEXE -DONEEXE
setenv QCSCRATCH /scratch
setenv QCLOCALSCR $PBSTMPDIR
cat $PBS_NODEFILE | awk '{printf "%s.ccr.buffalo.edu\n",$1}'
       > tmp.$$
setenv PBS_NODEFILE tmp.$$
setenv P4_RSHCOMMAND /usr/bin/rsh
set NPROCS = `cat $PBS_NODEFILE | wc -l`
#
qchem -pbs -np $NPROCS $JOB.in $JOB.out
#
```

PBS Script running AMBER

```
#PBS -S /bin/tcsh
#PBS -l nodes=16:ppn=2
#PBS -l walltime=72:00:00
#PBS -m e
#PBS -j oe
#PBS -o test.out
#PBS -N test
#
source $MODULESHOME/init/tcsh
module load amber/8
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i min.in
    -o test.min.out  -c test.xyz -p test.top -r test.min.xyz
#
```

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Quick Reference Guide - Input Files

Q-Chem Input File

```
$molecule
 0 1
C      -2.413  -0.909  -0.196
C      -1.403  -1.328  -1.026
C      -0.387  -0.416  -1.414
C      -0.422   0.928  -0.952
C      -1.438   1.340  -0.125
C      -2.462   0.434   0.272
H      -3.197  -1.597   0.101
H      -1.375  -2.346  -1.396
H       0.365  -0.725  -2.126
H       0.346   1.622  -1.273
H      -1.479   2.367   0.223
C      -3.572   0.900   1.151
H      -4.292   0.113   1.371
H      -4.103   1.737   0.682
H      -3.179   1.291   2.097
O       0.631  -0.925  -0.599
C       0.363  -1.292   0.744
H      -0.421  -2.048   0.741
H       0.048  -0.434   1.352
H       1.266  -1.716   1.200
H       1.433  -0.327  -0.642
$end

$rem
jobtype                 opt
exchange                b3lyp
basis                   6-311+G*
geom_opt_max_cycles     200
mem_static              128
mem_total               2000
$end

$opt
CONSTRAINT
stre 3  16  1.4
ENDCONSTRAINT
$end
```

AMBER Input File

(Minimization)

```
2000 steps of minimization
 &cntrl
   imin=1, ntmin=2, drms=0.03,
   ntb=0, cut=12,
   ntc=1, ntf=1,
   ntpr=100,
   maxcyc=2000,
   ntr=1,
   restraint_wt=500.0,
   restraintmask=':WAT',
 /
```

(Heating)

```
100ps dynamics, heating 0-300K
 &cntr
  imin=0, irest=0, ntx=1,
  ntt=1, tempi=0.0, temp0=300.0, tautp=1.0,
  ntc=1, ntf=1, ntb=0, cut=12,
  ivcap=0, fcap=10.0,
  ntwe=200, ntwx=200, ntpr=200,
  nstlim=100000, dt=0.001,
  ntr=1,
  restraint_wt=1.0,
  restraintmask=':Cl-',
 /
```

(Dynamics)

```
100ps dynamics
 &cntrl
  imin=0, irest=1, ntx=5,
  ntt=1, temp0=300.0, tautp=1.0,
  ntc=1, ntf=1, ntb=0, cut=12,
  ivcap=0, fcap=10.0,
  ntwe=500, ntwx=500, ntpr=500,
  nstlim=100000, dt=0.001,
  ntr=1,
  restraint_wt=1.0,
  restraintmask=':Cl-',
 /
```

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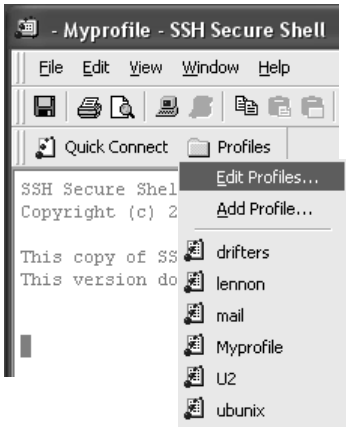
Quick Reference Guide - SSH (Telnet)

Adding a new profile

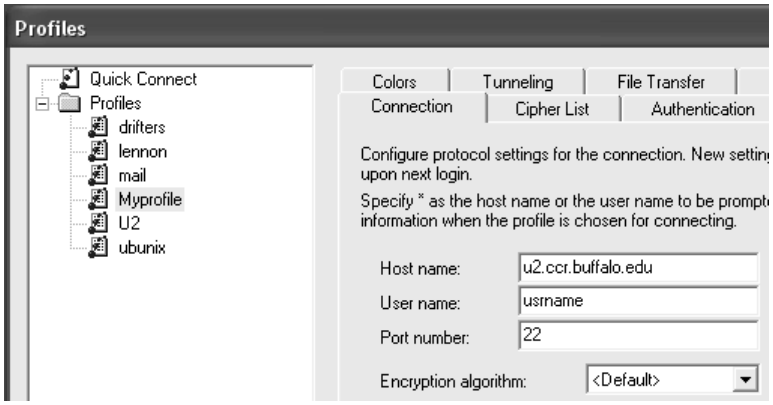
- Click "Profiles" and then "Add Profile..."

- In the Profile window type the profile name, the click "Add to Profiles"



Editing a profile

- Click "Profiles" and then "Edit Profiles..."
- From the profiles menu select the profile to edit
- In the "Host name" window type the internet address of the server
- In the "User name" window type your user name
- Click "OK"



Login into your profile

- Click "Profiles" in the main SSH window, and then select your profile
- Type your password

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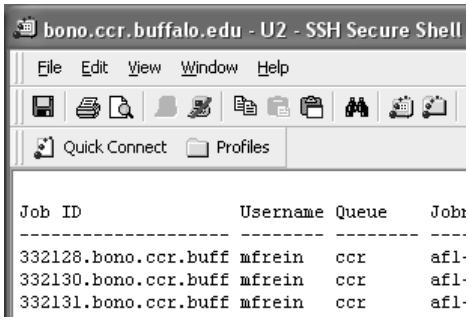
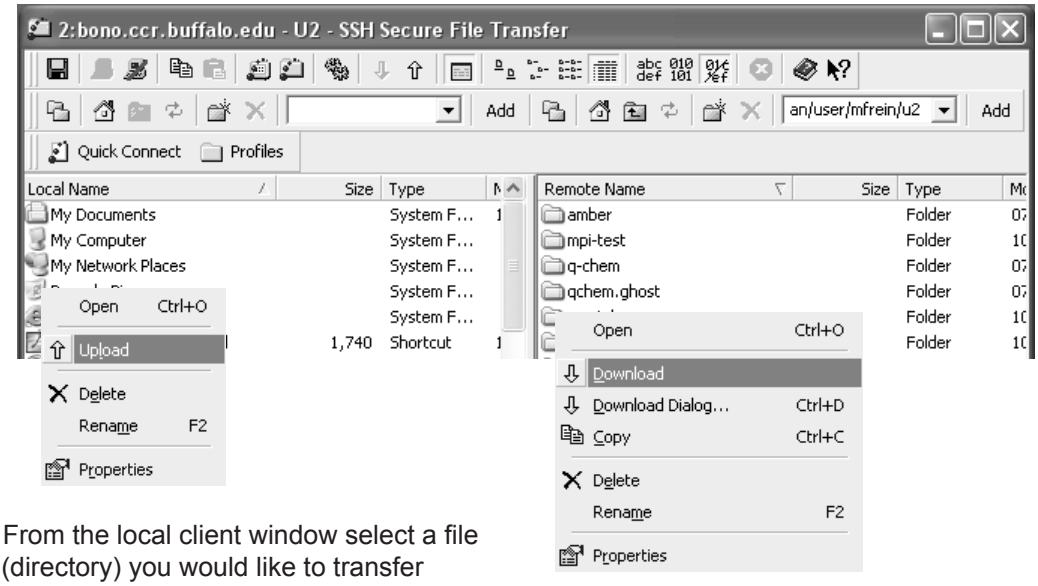
Quick Reference Guide - SSH (FTP)



Opening file transfer

- Click the icon on the main window of SSH

- Left window is a local client, right window is a remote server



- From the local client window select a file (directory) you would like to transfer

- Use the right mouse button to see the menu

- Select and click "Upload" to transfer a file from the local client to the server

- From the server window select a file (directory) you would like to transfer

- Use the right mouse button to see the menu

- Select and click "Download" to transfer a file from the remote server to the local client

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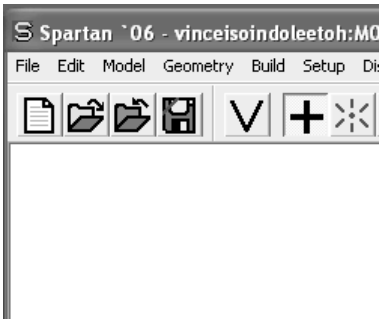
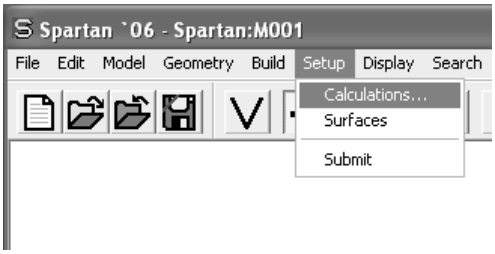
Quick Reference Guide - Spartan



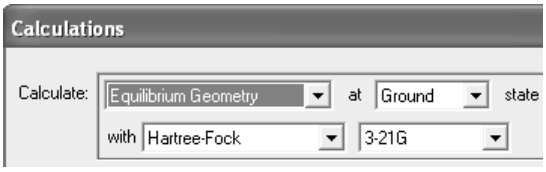
Building a molecule

- Click the  icon to go into the "add mode"
- Click a chemical symbol of the menu
- To place a chemical symbol in the main window, click at any place of the main window
- Connect atoms by clicking the  icon



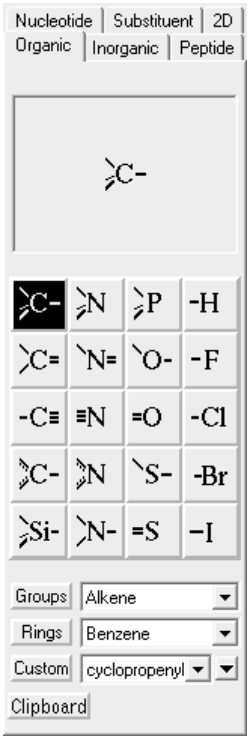
Calculations

- Click the "Setup" and "Calculations" on the main menu
- Select a level of theory and a type of calculations, then press OK
- Click the "Setup" and "Submit" to run calculations



Opening a molecule

- Click the  icon to open a molecule
- Select from the menu "Spartan" or "All" format



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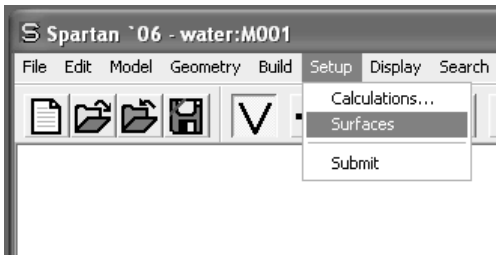
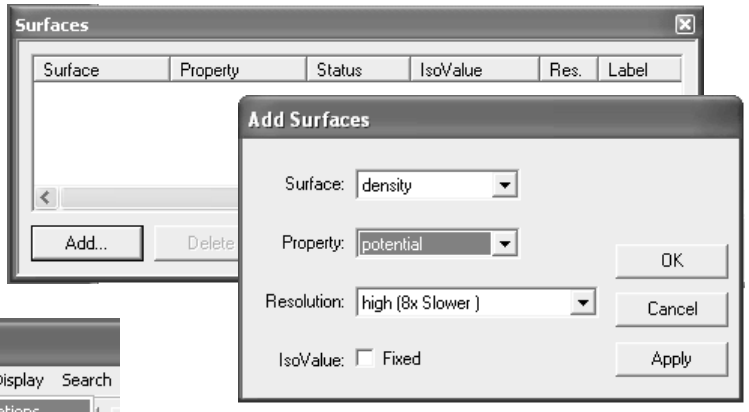
Quick Reference Guide - Spartan

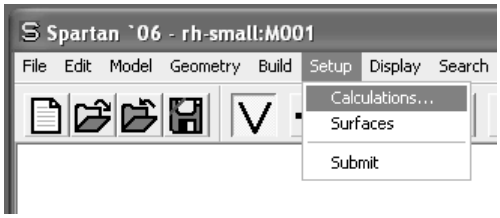


Electrostatic potential

- Click "Setup" and "Surfaces" on the main menu

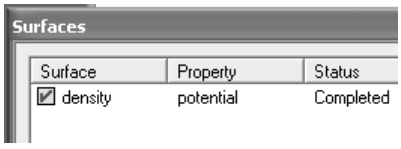
- Click "Add" and select "density" and "potential" from the menu
- Click "OK"
- Close the "Surface" window

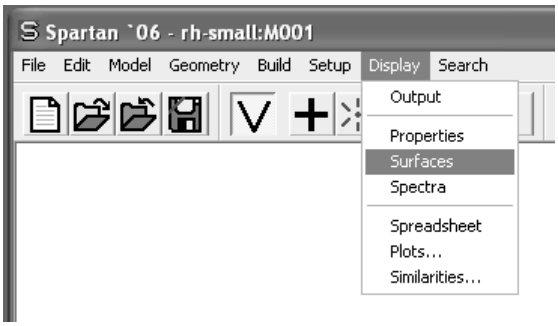




- Click "Setup" and "Submit"

- After the calculations are completed click "Display" and "Surfaces"
- Click the yellow box ☑





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Quick Reference Guide - UNIX

Directories

- Making a new directory "dirname"
  [youraccount]$ mkdir dirname
- Removing the directory "dirname"
  [youraccount]$ rmdir dirname
- Going into the directory "dirname"
  [youraccount]$ cd dirname
- Going back from the directory "dirname"
  [youraccount]$ cd ..
- Showing the name of the current directory
  [youraccount]$ pwd
- Listing the current directory
  [youraccount]$ ls

Directory Names

- Use text characters only, do not use blank spaces and special characters like %, $, ...
- Examples: proteins, dna12, active1site

Files

- Copying a file "oldname" into a "newname"
  [youraccount]$ cp oldname newname
- Removing the file "filname"
  [youraccount]$ rm filname
- Removing all files from the current directory
  [youraccount]$ rm *
- Copying the file "filname" from a current directory into a directory "dirname"
- Copying all files from a directory "dirname" into a current directory

File Names

- Use text characters only, do not use blank spaces and special characters like %, $, ...
- Use two segment names, separated by a period, the name of the second segment should be limited to
- Examples: base.pdb, acid.out, dna1.in

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Quick Reference Guide - UNIX

vi Editor

- Opening a file "filname.ext"
  [youraccount]$ vi filname.ext

Edition Mode
(after opening the file, press "Esc" key)

- Move the cursor to go to different places in the "filname.ext"
- Ctrl f - moving forward
- Ctrl b - moving backward
- 1G - going to the beginning of the file
- G - going to the end of the file
- x - deleting a character at the cursor position
- dd - deleting a line at the cursor position
- ma - marking a line with a mark "a"
- /w - finding a character "w" in the file

Insert Mode
(after opening the file, press "i" key)

- Type anything from the keyboard
- Press "Enter" to go to the next line

(press "Esc" key to come back to the edition mode)

Command Mode
(after opening the file, press ":" key)

- w! filname.ext - saving the file with a name "filname.ext"
- q! - quitting the editor
- 'a,'b d - deleting a text between a mark "a" and a mark "b"
- 'a,'b w! newname.ext - writing a text between a mark "a" and a mark "b" into a new file "newname.ext"
- r oldname.ext - reading (inserting) the contest of the file "oldname.ext", from the cursor position
- 'a,'b s/old/new/g - replacing the text "old" by the text "new" in the file between the marks "a" and "b"

(press "Esc" key to come back to the edition mode)

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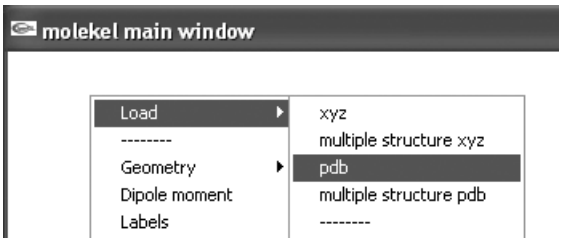
Quick Reference Guide - Molekel

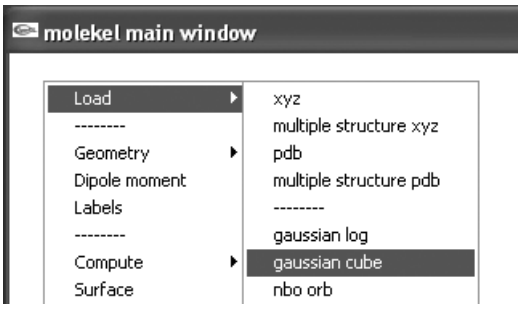


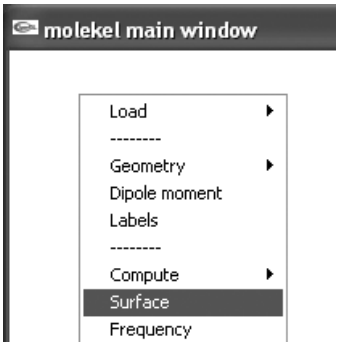
Opening a molecule

- Click the right mouse button, and select "Load"
- Select the "pdb" format
- In the "file browser" window, select the pdb file

Electrostatic Potential

- Click the right mouse button, and select "Load"
- Select the "gaussian cube" format
- In the "file browser" window, select the cube file





- Click the right mouse button again, and select "Surface"
- In the "file browser" window, select the same cube file

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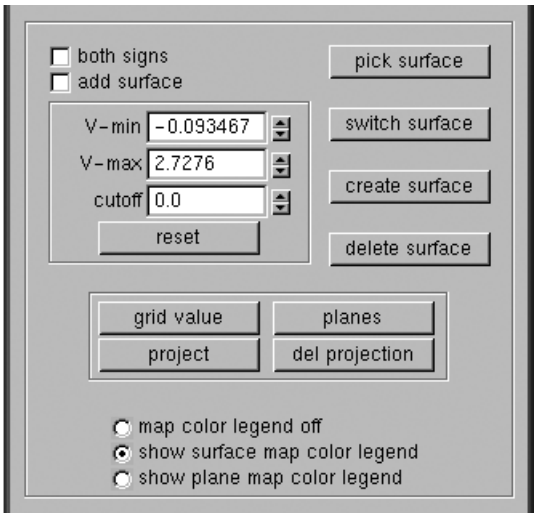
Quick Reference Guide - Molekel

- Select "gaussian cube" from the "surface" window
- Click "load" button of the "surface" window

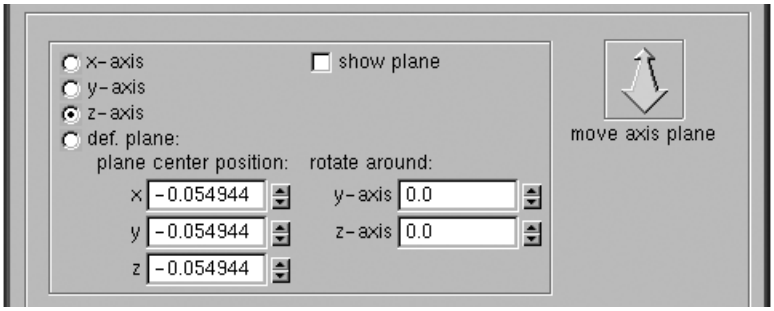
Surface

- Click "create surface" button
- Click "grid value" button
- Check "show surface map color legend"



Plane

- Click "planes" button on the "surface" window
- Check "show plane" on the "planes" window
- Use the mouse on the "move axis plane" button of the "planes" window, to move the plane



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Quick Reference Guide - Q-Chem

Geometry Optimization

- Simple geometry optimization without any constraints

```
$molecule
 0 1
 H     -6.572   4.048  -0.066
 O     -5.695   4.501   0.014
 H     -5.561   5.099  -0.764
$end

$rem
jobtype                 opt
exchange                b3lyp
basis                   6-31+G*
mem_static              256
mem_total               2000
$end
```

- Geometry optimization with constraints (interatomic distance, angle and torsion angle)

```
$opt
CONSTRAINT
stre   2  5         1.8
bend  2  7  8      120.0
tors   3  4  8  9   140.0
ENDCONSTRAINT
$end
```

- Geometry optimization with constraints (absolute position of an atom)

```
$opt
FIXED
  4    xyz
ENDFIXED
$end
```

Oscillation Frequencies

- Oscillation hessian calculations, normal mode analysis

```
$rem
jobtype                 freq
exchange                b3lyp
basis                   6-31+G*
mem_static              512
mem_total               2000
$end
```

Electrostatic Potential

- Electrostatic potential calculations on a grid around the molecule

```
$rem
jobtype                 sp
exchange                b3lyp
basis                   6-31+G*
ianlty                  200
igdesp                  -1
mem_static              256
mem_total               2000
$end

$plots
  Electrostatic potential on a grid
 10  -5.0   5.0
 10  -3.0   3.0
 10  -2.0   2.0
  0   0   0   0
  0
$end
```

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Quick Reference Guide - Q-Chem

Anharmonic Frequencies

- Oscillation hessian calculations and anharmonic corrections

```
$rem
jobtype          freq
exchange         hf
basis            aug-cc-pVDZ
anhar            true
vci              4
mem_static       512
mem_total        2000
$end
```

Natural Bond Orbital

- Natural bond orbital analysis for coupled cluster calculations

```
$rem
jobtype          sp
exchange         hf
correlation      ccsd
basis            cc-pVDZ
nbo              true
mem_static       128
mem_total        2000
$end
```

MP2 Correction

- HF calculations with MP2 correction

```
$rem
jobtype          opt
exchange         hf
correlation      mp2
basis            cc-pVDZ
mem_static       256
mem_total        2000
$end
```

Excited Electronic States

- Time depended DFT calculations of excited electronic states

```
$rem
jobtype          sp
exchange         b
correlation      lyp
basis            cc-pVTZ
cis_n_roots      5
rpa              true
mem_static       128
mem_total        2000
$end
```

Effective Core Potential

- Pseudopotential calculations

```
$rem
jobtype          opt
exchange         b3lyp
ecp              gen
basis            gen
mem_static       512
mem_total        2000
$end

$ecp
  Rh
  lanl2dz
  ****
$end

$basis
  Rh
  lanl2dz
  ****
  C
  6-31G*
  ****
$end
```

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Quick Reference Guide - tleap

Loading AMBER module

- Before running "tleap" program, load AMBER module
  [youraccount]$ module load amber/9

- Run "tleap" program, using a command
  [youraccount]$ tleap

Using "tleap" program

- Loading the AMBER parameter file "name.par"
  > loadAmberParams name.par

- Loading the AMBER preparation file "name.in"
  > loadAmberPrep name.in

- Loading the PDB file "name.pdb" to the unit "P"
  > P = loadPdb name.pdb

- Adding counter ions "IM" to the system "P"
  > addIons P IM 0

- Printing a center of the system "P"
  > center P

- Printing information about the atom number "2" of the residue number "34" in the system "P"
  > desc P.34.2

- Creating a chemical bond between the atom number "4" of the residue number "12", and the atom number "7" of the residue number "34" in the system "P"
  > bond P.12.4 P.34.7

- Deleting a chemical bond between the atom number "3" of the residue number "10", and the atom number "2" of the residue number "44" in the system "P"
  > deleteBond P.10.3 P.44.2

- Removing the atom number "12" from the residue number "26" of the system "P"
  > remove P.26.12

- Solvating the system "P" by a box of water molecules
  > solvateBox P TIP3PBOX 10

- Solvating the system "P" by a sphere of water molecules of a radius 20A, centered at the position (7., 3., 2.)
  > solvateCap P TIP3PBOX { 7. 3. 2. } 20.0

- Saving the coordinates of the system "P" in the file name "name.pdb"
  > savePdb P name.pdb

- Saving the topology file of the name "name.top" and the coordinate file of the name "name.xyz" of the system "P"
  > saveAmberParm P name.top name.xyz

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Quick Reference Guide - antechamber

Loading AMBER module

- Before running "antechamber" program, load AMBER module
  [youraccount]$ module load amber/9

- Run "antechamber" program, in this example the program takes the pdb file "name.pdb" and generates the preparation file "name.in", using the AM1 charges

[youraccount]$ **antechamber -i name.pdb -fi pdb -o name.in -fo prepi -c bcc**

Program parameters

-help print these instructions
-i input file name
-fi input file format
-o output file name
-fo output file format
-c charge method
-nc net molecular charge (int)
-m mulitiplicity (2S+1), default is 1

Charge methods

RESP	resp
AM1-BCC	bcc
CM1	cm1
CM2	cm2
ESP (Kollman)	esp
Mulliken	mul
Gasteiger	gas
Read in charge	rc
Write out charge	wc

File format tyes

Antechamber	ac
Sybyl Mol2	mol2
PDB	pdb
Modifiled PDB	mpdb
AMBER PREP (int)	prepi
AMBER PREP (car)	prepc
Gaussian Z-Matrix	gzmat
Gaussian Cartesian	gcrt
Mopac Internal	mopint
Mopac Cartesian	mopcrt
Gaussian Output	gout
Mopac Output	mopout
Alchemy	alc
CSD	csd
MDL	mdl
Hyper	hin
AMBER Restart	rst
Jaguar Cartesian	jcrt
Jaguar Z-Matrix	jzmat
Jaguar Output	jout
Divcon Input	divcrt
Divcon Output	divout

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Quick Reference Guide - sander

Minimization

2000 steps of minimization

```
 &cntrl
    imin=1, ntmin=2, drms=0.05,
    ntb=0, cut=12,
    ntc=1, ntf=1,
    ntpr=100,
    maxcyc=2000,
 /
```

Heating

100ps dynamics, heating 0-300K

```
 &cntrl
   imin=0, irest=0, ntx=1,
   ntt=1, tempi=0.0, temp0=300.0, tautp=1.0,
   ntc=1, ntf=1, ntb=0, cut=12,
   ntwe=200, ntwx=200, ntpr=200,
   nstlim=100000, dt=0.001,
 /
```

Dynamics

100ps dynamics

```
 &cntrl
   imin=0, irest=1, ntx=5,
   ntt=1, temp0=300.0, tautp=1.0,
   ntc=1, ntf=1, ntb=0, cut=12,
   ntwe=500, ntwx=500, ntpr=500,
   nstlim=100000, dt=0.001,
 /
```

Cartesian restraints

```
ntr=1,                  (Cartesian restraints)
restraint_wt=1.0,       (force constant)
restraintmask=':1-58',  (atoms in residues 1-58
                         restrained)
```

Internal restraints

```
nmropt=1,               (Internal restraints)
/
&wt type='END' /
DISANG=name.rst         (File with restraints)
```

File of internal restraints

```
 # interatomic constraints
  &rst iat=9618,9824, r1=1.20, r2=3.20,
       r3=3.20, r4=5.20, rk2=200.0, rk3=200.0, /
```

Water sphere potential

```
ivcap=0, fcap=10.0,     (harmonic potential)
```

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Quick Reference Guide - ptraj/rdparm

Loading AMBER module

- Before running "ptraj/rdparm" program, load AMBER module
  [youraccount]$ module load amber/9

Ptraj - program

- Run "ptraj" program, using the "name.top" topology file, and "name.in" ptraj input file
  [youraccount]$ ptraj name.top name.in

Rdparm - program

- Run "rdparm" program, using the "name.top" topology file
  [youraccount]$ rdparm name.top

Extracting coordinates

```
trajin  traj.md100.crd.Z 1 999
trajout traj.md100.xyz restart
go
```

Manipulating coordinates

```
trajin traj1.Z 1 20 1
trajin traj2.Z 1 100 1
trajin restrt.Z
trajout fixed.traj nobox
rms first out rms @CA,C,N
center :1-20
image origin center
radial rdf 0.5 10.0 :WAT@O
strip :WAT
average avg.pdb pdb
atomicfluct out bfactor.dat byatom bfactor
go
```

Program parameters

```
help □ □ □ (help)
atoms □□ □ (print atoms)
bonds □□ □ (print bonds)
angles □□ □ (print angles)
dihedrals □ □ (print dihedrals)
printLennardJones □ (print L-J parameters)
printTypes□ □ (print atom types)
checkcoords□ □ (check coordinates)□
delete  <bond || angle || dihedral> <number>
□ □ □ (delete bond, ...)
restrain <bond || angle || dihedral>
□ □ □ (apply constraints)
writeparm <filename> □ (saving new parm. file)
analyze <trajectory || coordinates>
□ □ □ (analyze trajectory)
transform <trajectory>□ (transform trajectory)
stripwater□ □ (remove water)
```

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Quick Reference Guide - QM/MM (no bonds between QM and MM)

- Generate the pdb structure of the QM system, using any graphic program, the name of the QM residue should be "QMM" :

```
ATOM      1  NZ  QMM     1     -14.748  -3.998   7.037  1.00  0.00
ATOM      2  HNZ QMM     1     -15.003  -3.032   6.989  1.00  0.00
ATOM      3  H49 QMM     1     -13.849  -4.084   7.466  1.00  0.00
ATOM      4  CA  QMM     1     -14.700  -4.569   5.662  1.00  0.00
ATOM      5 1HA  QMM     1     -14.426  -5.611   5.703  1.00  0.00
ATOM      6 2HA  QMM     1     -15.653  -4.450   5.169  1.00  0.00
```

- Run "antechamber" program to generate the preparation file of the QM residue

```
This is a remark line
molecule.res
QMM     INT  0
CORRECT     OMIT DU   BEG
  0.0000
   1  DUMM  DU    M    0  -1  -2     0.000      .0        .0      .00000
   2  DUMM  DU    M    1   0  -1     1.449      .0        .0      .00000
   3  DUMM  DU    M    2   1   0     1.522   111.1        .0      .00000
   4  NZ    NT    M    3   2   1     1.540   111.208   180.000  -0.90547
   5  HNZ   H     E    4   3   2     1.000    75.230   177.155   0.34244
   6  H49   H     E    4   3   2     1.000   154.048   -78.664   0.34298
   7  CA    CT    M    4   3   2     1.490    91.847    67.448   0.14996
   8  HA1   H1    E    7   4   3     1.078   110.093  -105.007   0.05265
```

- Merge the pdb structure of the ligand and the pdb structure of the protein. Run the "tleap" program to generate one topology file and the pdb file of the protein and ligand together. The topology file should have name "prt.top" and the pdb file should have name "prt.pdb".

- Run "qmmm_setup" script, using a command
[youraccount]$ ./qmmm_setup.pl

- The "qmmm_setup" script will generate the q-chem input file for the QM/MM calculations including charges and Lennard-Jones parameters of the protein:

```
$external_charges
  25.450    1.169    9.488    0.294   0.000271   6.141614
  25.499    2.156    9.280    0.164   0.000023   2.034136
  25.931    0.997   10.360    0.164   0.000023   2.034136
  24.496    0.859    9.367    0.164   0.000023   2.034136
  26.236    0.438    8.454   -0.010   0.000174   6.424450
  27.048   -0.115    8.926    0.089   0.000025   3.703833
```

- and Lennard-Jones parameters of the ligand:

```
$lj_parameters
1 0.00020 7.40
2 0.00005 4.20
3 0.00005 4.20
4 0.00010 7.60
```

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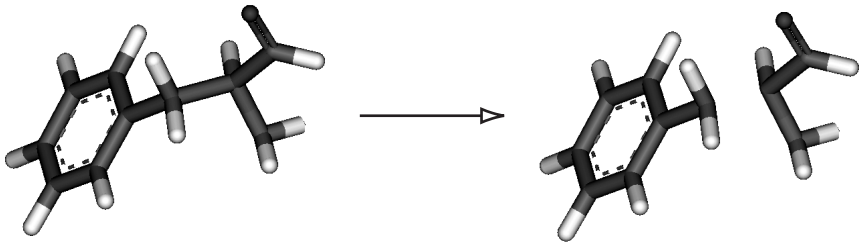
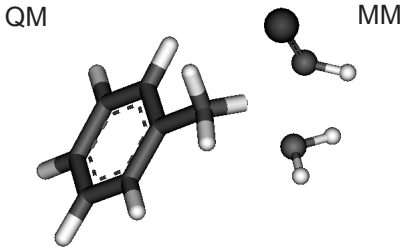
Quick Reference Guide - QM/MM (linking atom approximation)

- Separate the ligand from the protein using any graphic program, cutting the chemical bonds between them



- Place a hydrogen atom on the ligand, and remove a close laying atom from the protein. Remove also hydrogen atoms which are connected to the close laying atom of the protein

- Replace the atoms of the protein by point charges and Lennard-Jones spheres



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