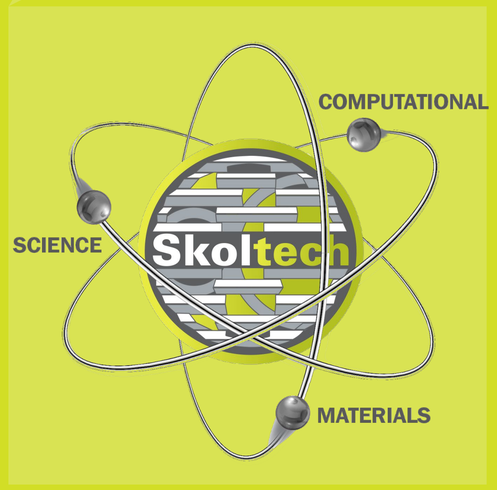
Tutorial 1: Command line and Lab 1



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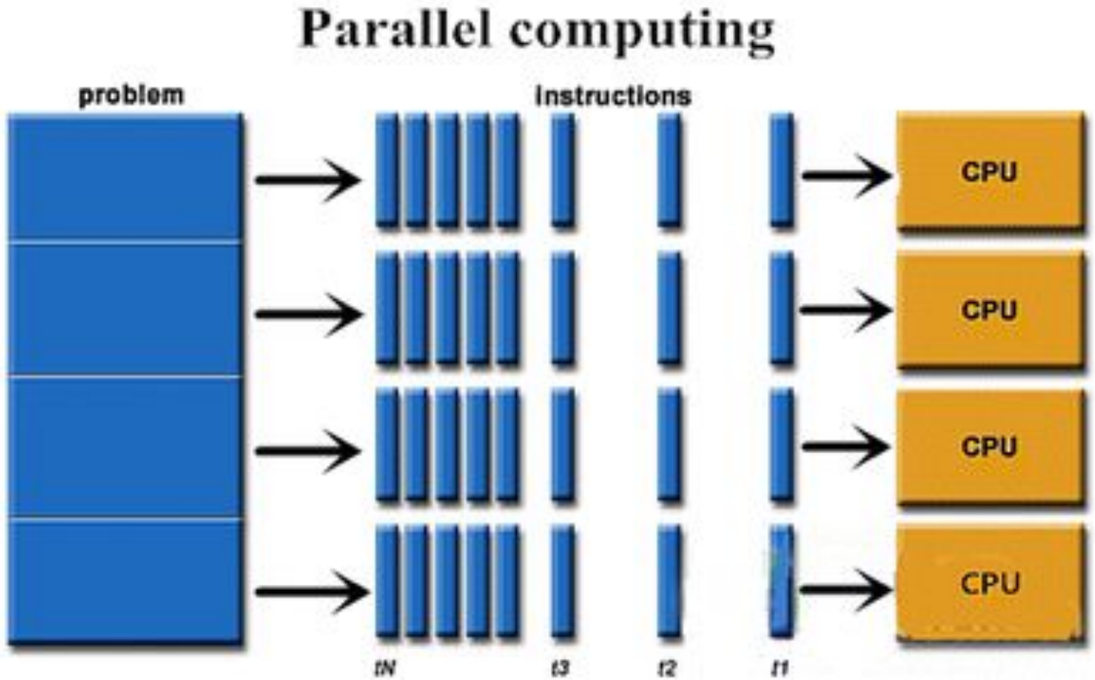
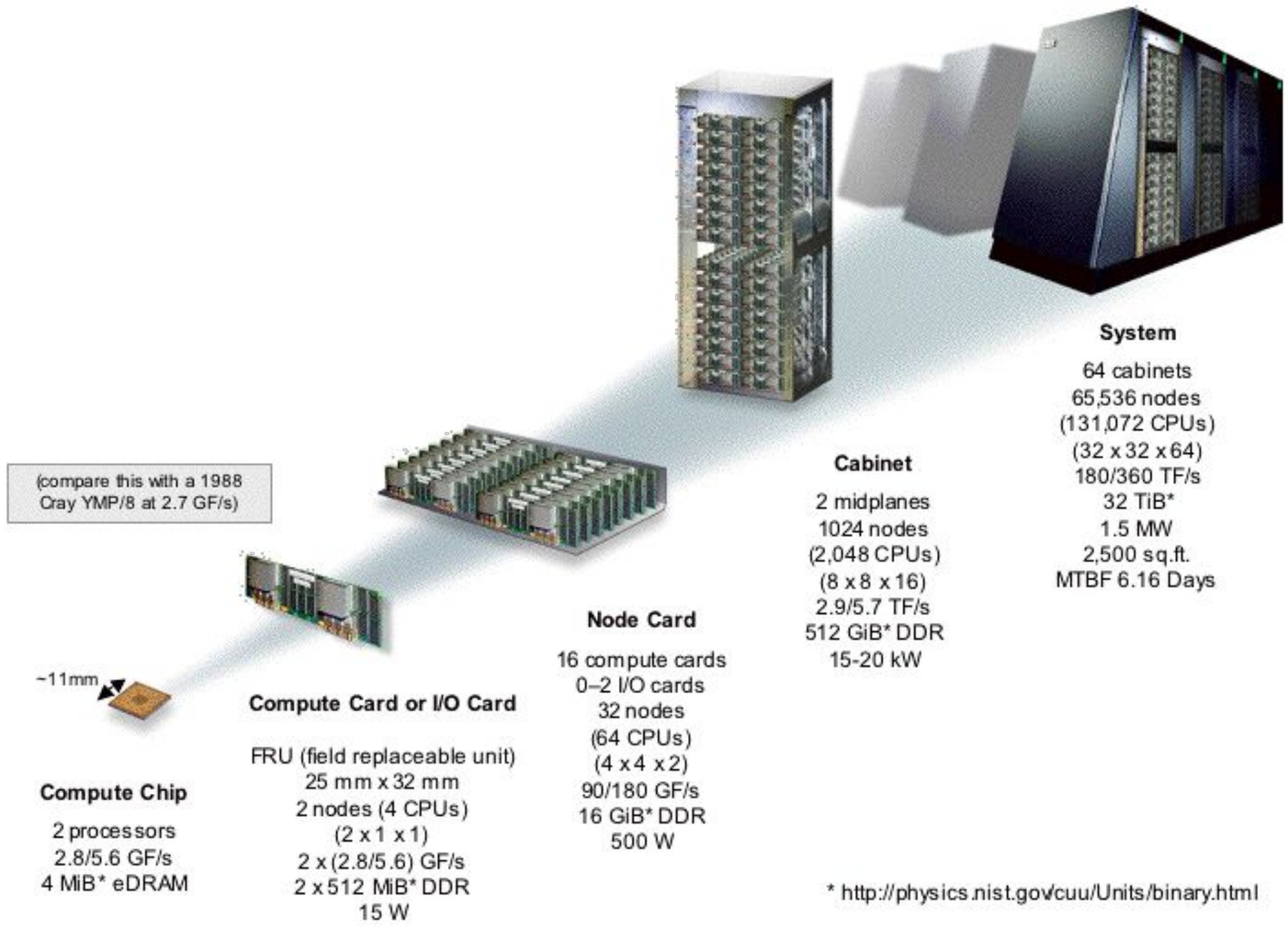
Presentation agenda

1. Computer clusters
2. How to connect to a remote machine?
3. What is Terminal in Linux and how to work with it?
4. Avogadro editor
5. Some reminders on semi-empirical methods
6. MOPAC program. Technical aspects
7. Lab 1 overview

What is a cluster for computing tasks?





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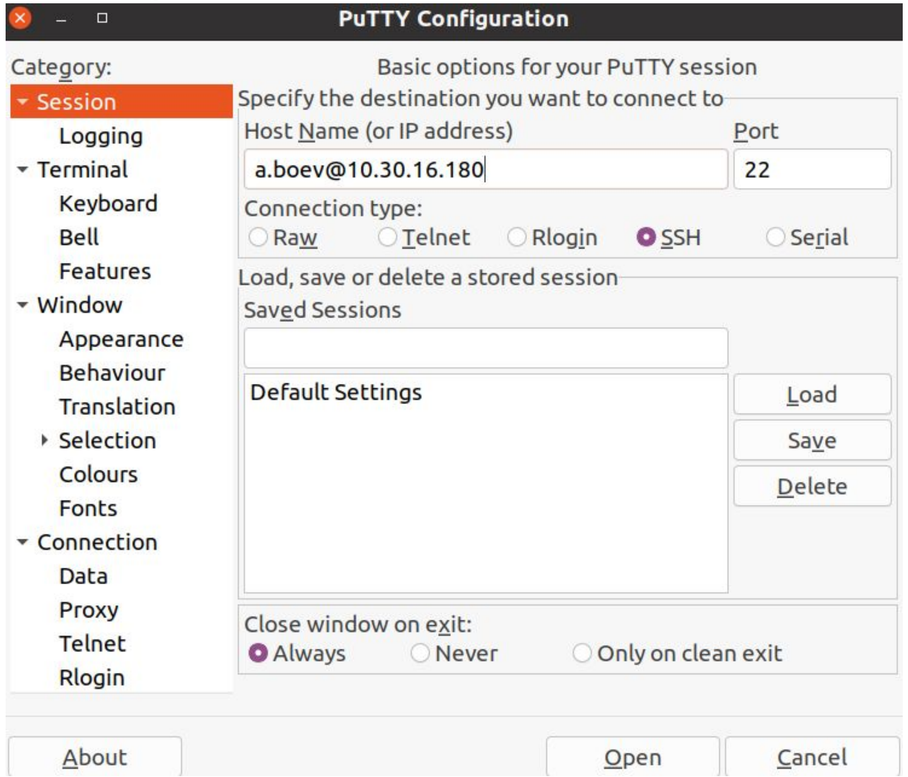
Settings for your laptop

How to connect to Virtual Machine (cluster) via SSH?

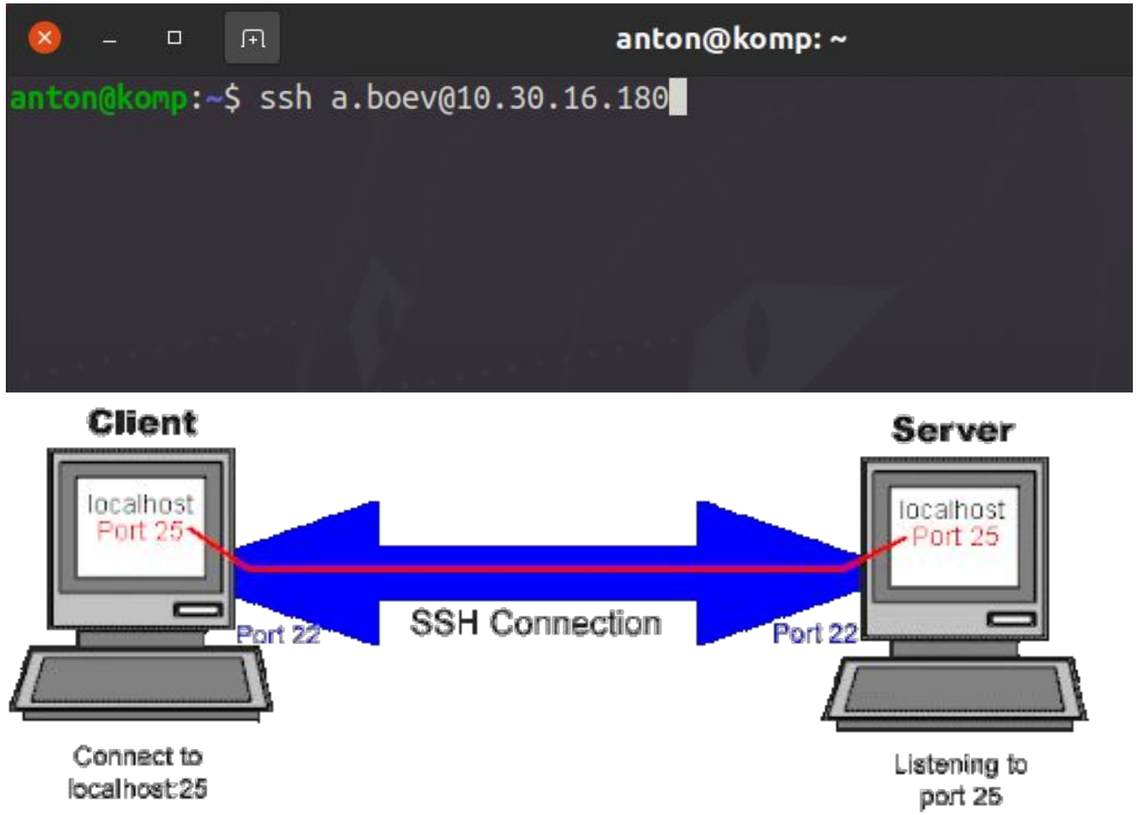
Windows: via [PuTTY](#) (portable version is enough)

‘your_login’@10.30.16.180
‘your_password’



Linux/Mac: via Terminal

ssh ‘your_login’@10.30.16.180
‘your_password’



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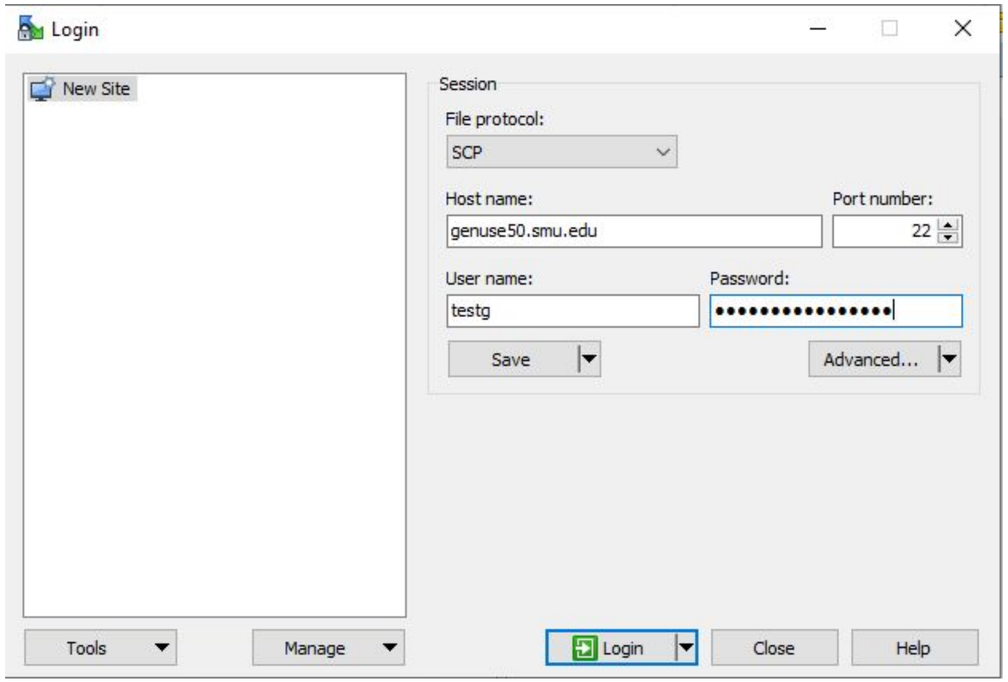
How to copy files b/t laptop and VM?

Windows: via **WinSCP**

‘your_login’@10.30.16.180
‘your_password’



Linux/Mac: via Terminal

scp -r ‘your_local_file’
‘your_login’@10.30.16.180:’path_to_folder_on_VM’

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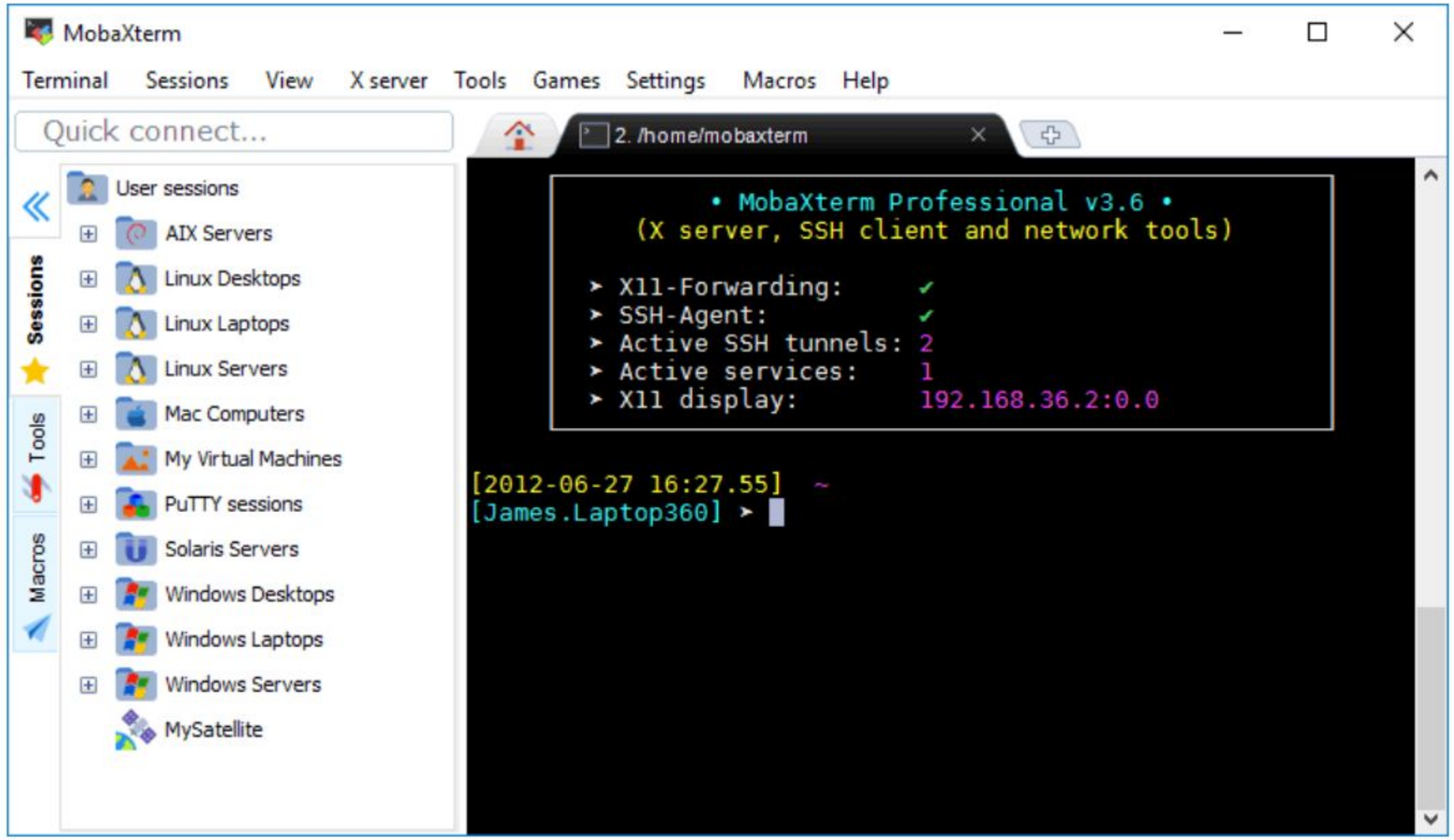
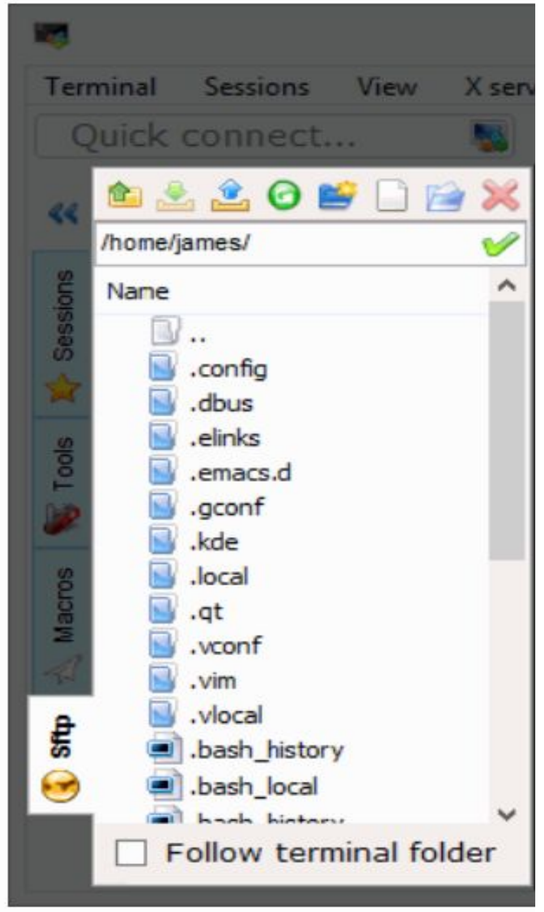
An alternative for Windows: Mobaxterm

SSH session with terminal:

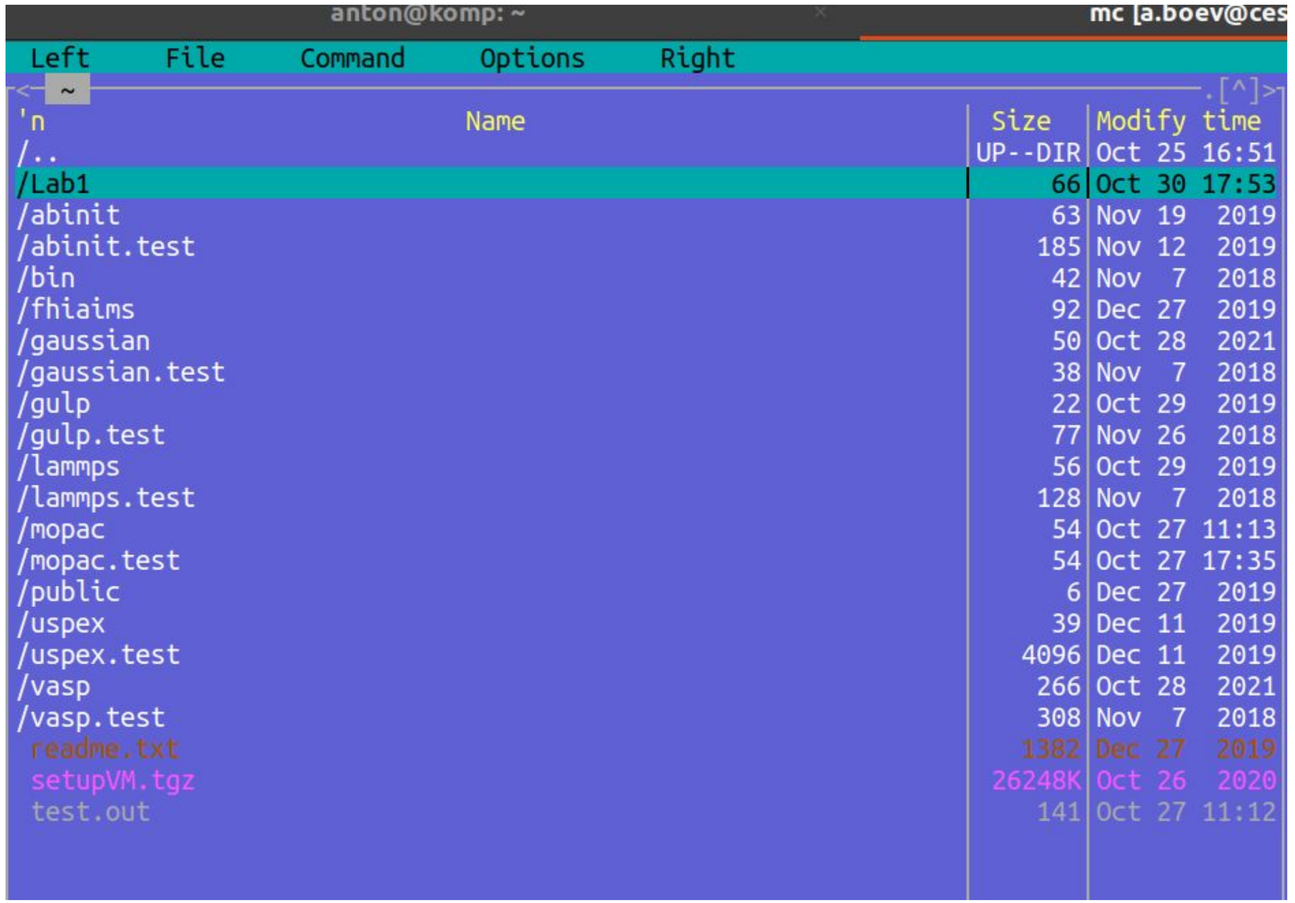
Transferring files from your PC on the remote cluster; Transferring files from one directory to another on the remote machine.





Midnight commander (MC) file manager

```
anton@komp:~$ mc
```



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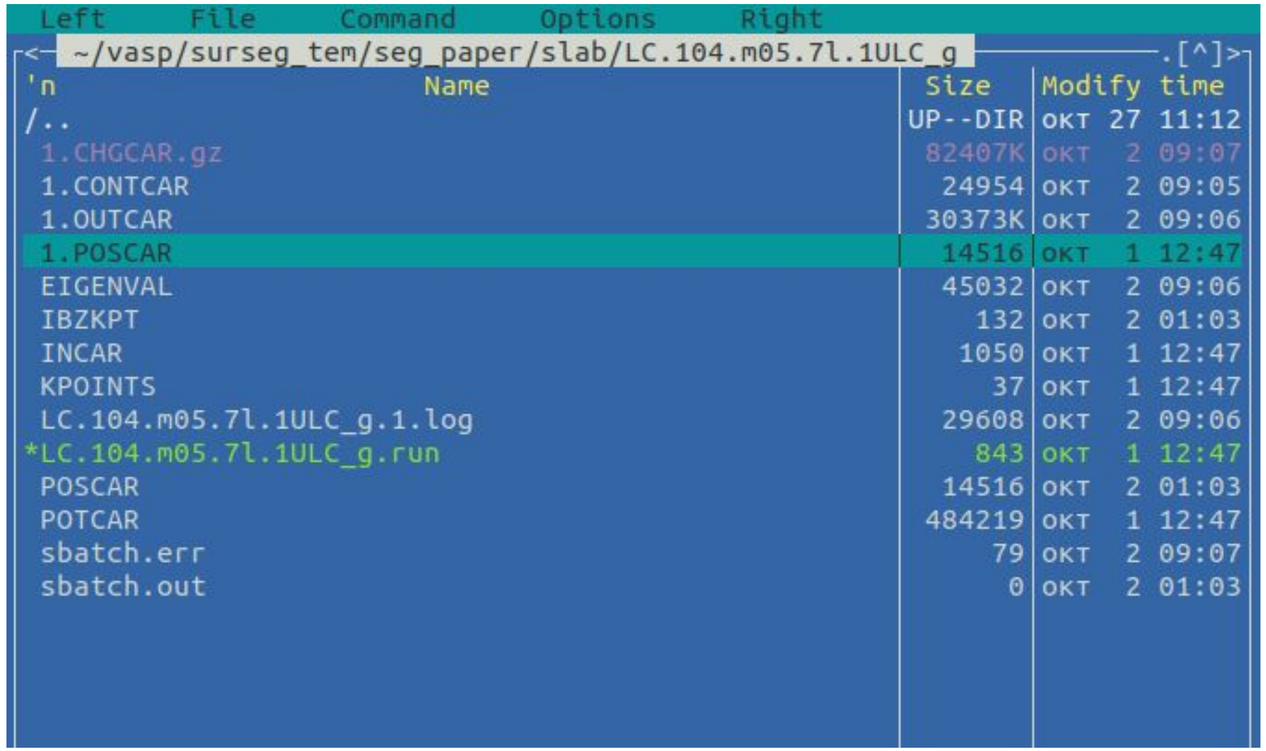
Hotkeys in MC

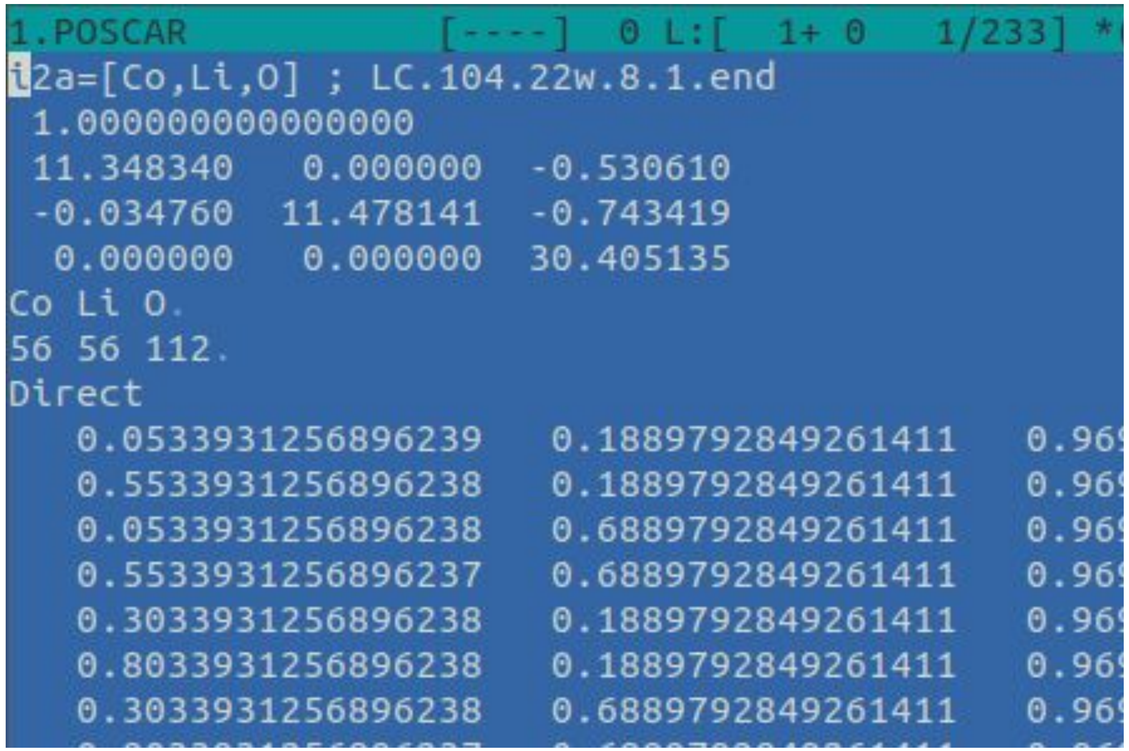
- ***TAB*** – switch active panel.
- ***F***<1-10>

- **Ctrl+O** – switch between MC window and command line.

Open file in MC

- ***F3/F4*** - read only/edit mode





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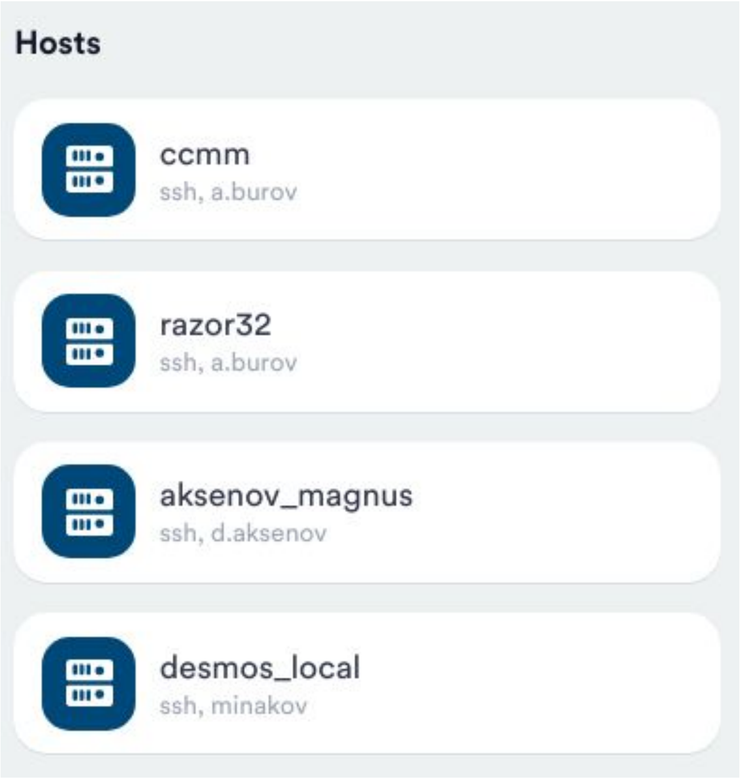
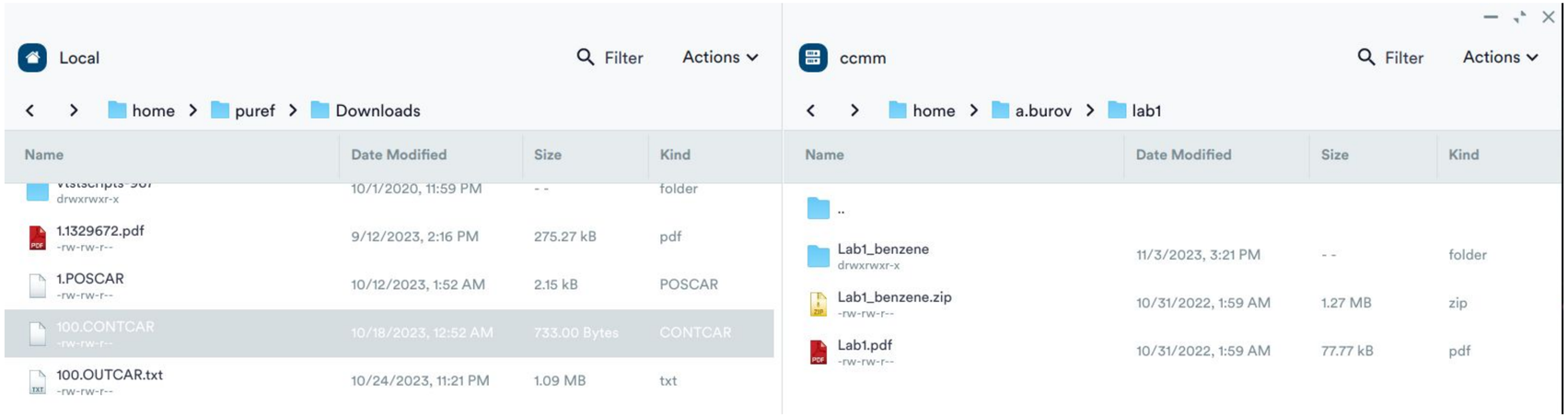
An alternative for Linux: Termius

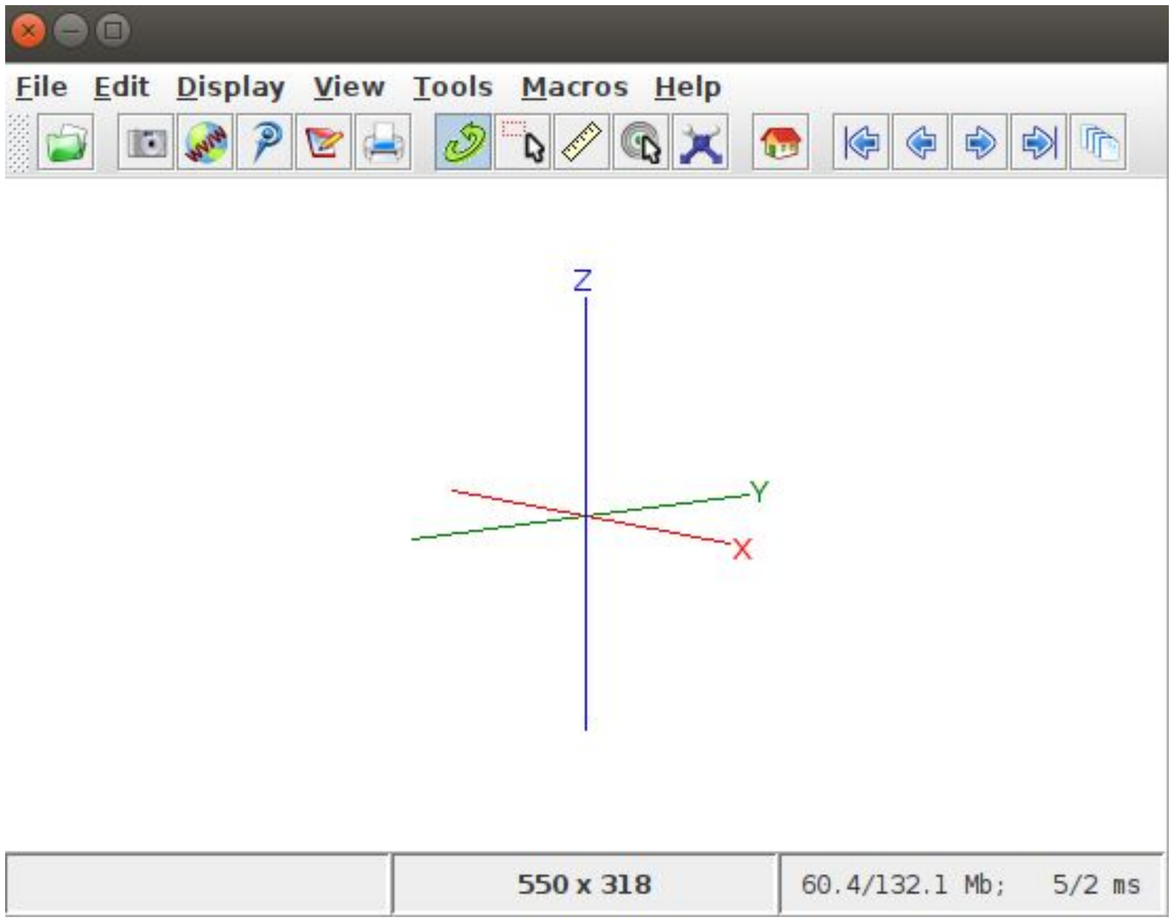
SSH sessions with terminal:



Transferring files from your PC on the remote cluster; Transferring files from one directory to another on the remote machine.



How to visualize atoms?



http://jmol.sourceforge.net/ web_version

Jmol supports lots of structure file formats (~100)

The most commonly used are XYZ and Crystallographic Information File (cif) formats.

```
24
Caffeine
H       -3.3804130    -1.1272367     0.5733036
N        0.9668296    -1.0737425    -0.8198227
C        0.0567293     0.8527195     0.3923156
N       -1.3751742    -1.0212243    -0.0570552
C       -1.2615018     0.2590713     0.5234135
C       -0.3068337    -1.6836331    -0.7169344
C        1.1394235     0.1874122    -0.2700900
N        0.5602627     2.0839095     0.8251589
O       -0.4926797    -2.8180554    -1.2094732
C       -2.6328073    -1.7303959    -0.0060953
O       -2.2301338     0.7988624     1.0899730
H        2.5496990     2.9734977     0.6229590
C        2.0527432    -1.7360887    -1.4931279
H       -2.4807715    -2.7269528     0.4882631
H       -3.0089039    -1.9025254    -1.0498023
H        2.9176101    -1.8481516    -0.7857866
H        2.3787863    -1.1211917    -2.3743655
H        1.7189877    -2.7489920    -1.8439205
C       -0.1518450     3.0970046     1.5348347
C        1.8934096     2.1181245     0.4193193
N        2.2861252     0.9968439    -0.2440298
H       -0.1687028     4.0436553     0.9301094
H        0.3535322     3.2979060     2.5177747
H       -1.2074498     2.7537592     1.7203047
```

```
# generated using pymatgen
data_LiCoO2
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   2.84289827
_cell_length_b   2.84289827
_cell_length_c   14.14561550
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   120.00000000
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Li  Li0  1  0.00000000  0.00000000  0.00000000  1.0
  Li  Li1  1  0.66666667  0.33333333  0.33333333  1.0
  Li  Li2  1  0.33333333  0.66666667  0.66666667  1.0
  Co  Co3  1  0.33333333  0.66666667  0.16666667  1.0
  Co  Co4  1  0.00000000  0.00000000  0.50000000  1.0
  Co  Co5  1  0.66666667  0.33333333  0.83333333  1.0
  O  O6  1  0.00000000  0.00000000  0.23958700  1.0
  O  O7  1  0.66666667  0.33333333  0.09374633  1.0
  O  O8  1  0.66666667  0.33333333  0.57292033  1.0
  O  O9  1  0.33333333  0.66666667  0.42707967  1.0
  O  O10  1  0.33333333  0.66666667  0.90625367  1.0
  O  O11  1  0.00000000  0.00000000  0.76041300  1.0
```

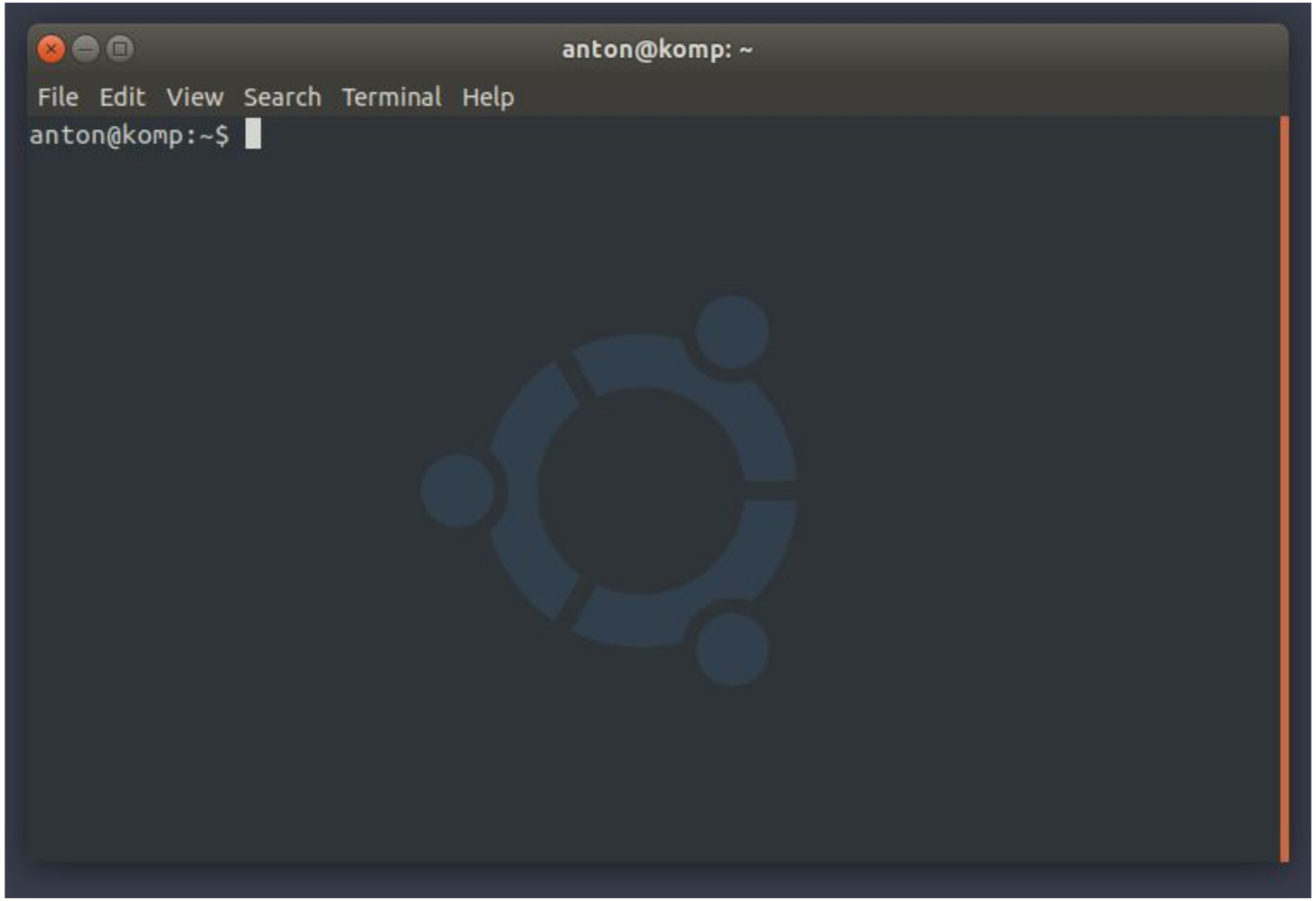
Command line basics

What is the Terminal in Linux?

The **terminal** is the GUI window that you see on the screen. It takes commands and shows output.

The **shell** is the software that interprets and executes the various commands that we type in the terminal.

Bash is a particular shell. It stands for **Bourne Again Shell.**



Basic bash commands

- ***ls*** – show the content of the current directory
- ***cd*** <directory> – change directory
- ***cd*** .. – change current directory to parent directory
- ***pwd*** – show the path to the current directory
- ***touch*** <name.ext> – create a new file with extension *.ext*
- ***mkdir*** <name> – create a new directory
- ***rm*** <name.ext> – remove file
- **rm -r** <name> – remove the directory
- ***cat*** <file> – show a file

[Cheat sheet with Linux commands]

List of useful terminal commands

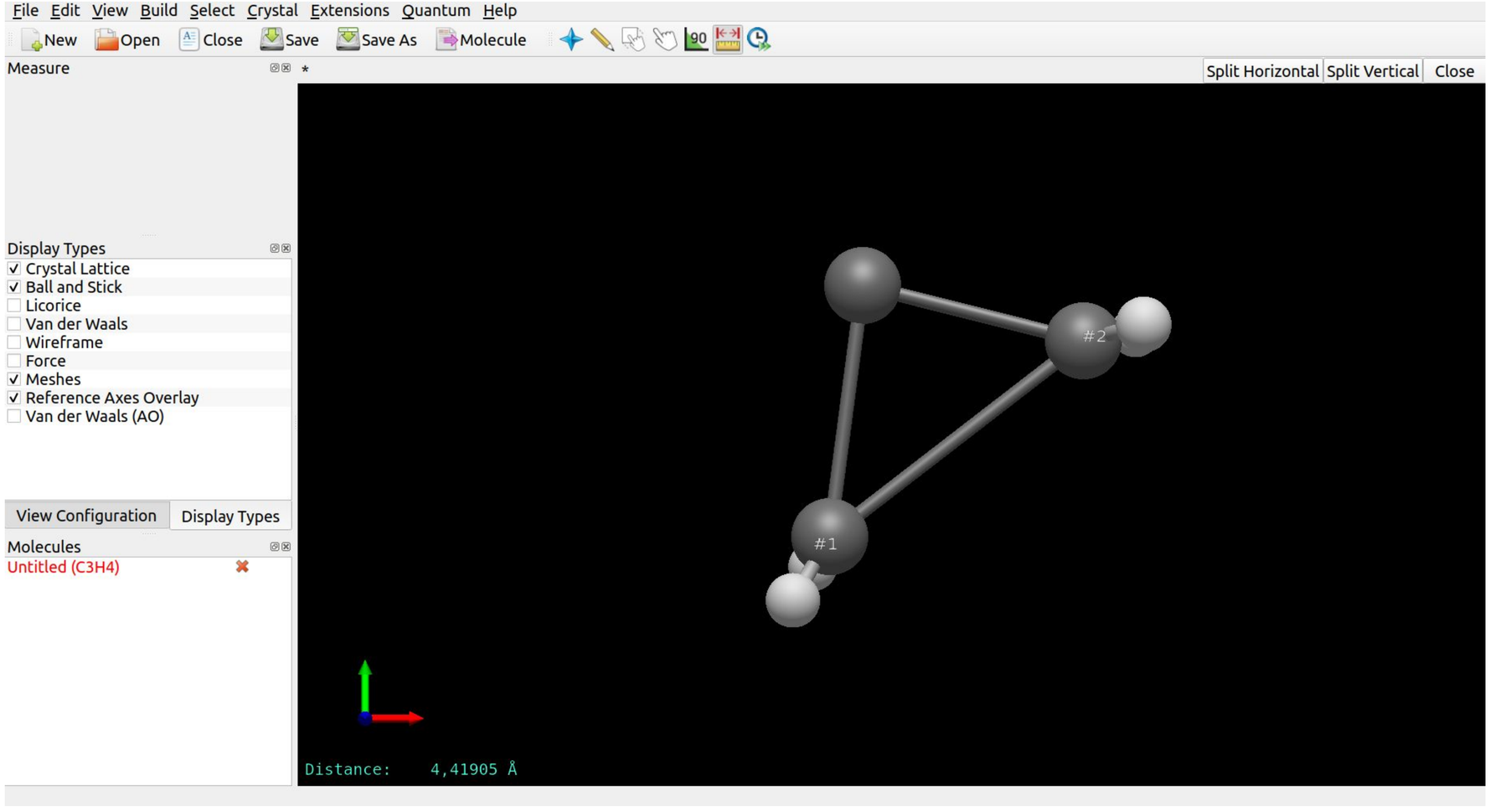
- ***ssh username@10.30.16.180*** – access to the cluster
- ***mc*** – run file manager
- **Ctrl+O** – switch between MC and command line
- **Tab** – switch between MC panels (left - right)
- ***squeue*** – show job schedule on cluster
- ***unzip name.zip*** – unzip archive
- ***zip -r <name_of_new_archive>.zip <folder_name>*** – compress a folder into zip archive

[Cheat sheet with Linux commands]

Construction of molecules (Avogadro)

Avogadro editor

Avogadro is an advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible high quality rendering and a powerful plugin architecture.



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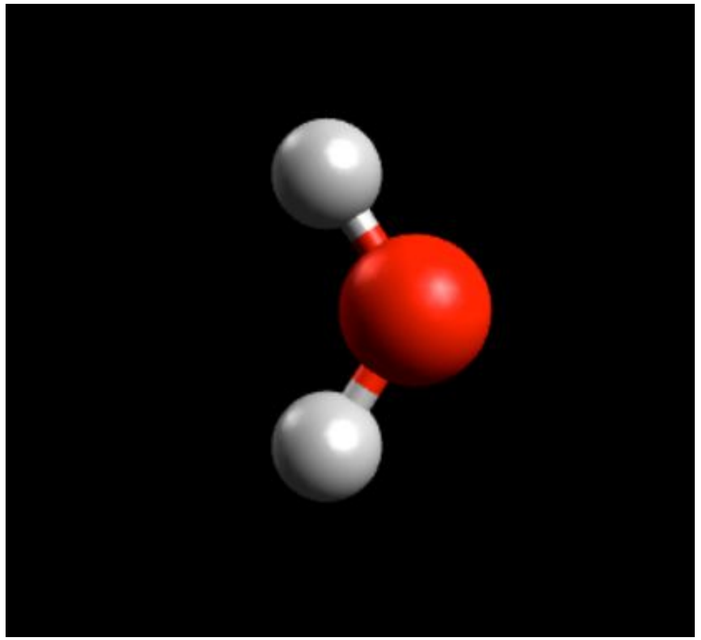
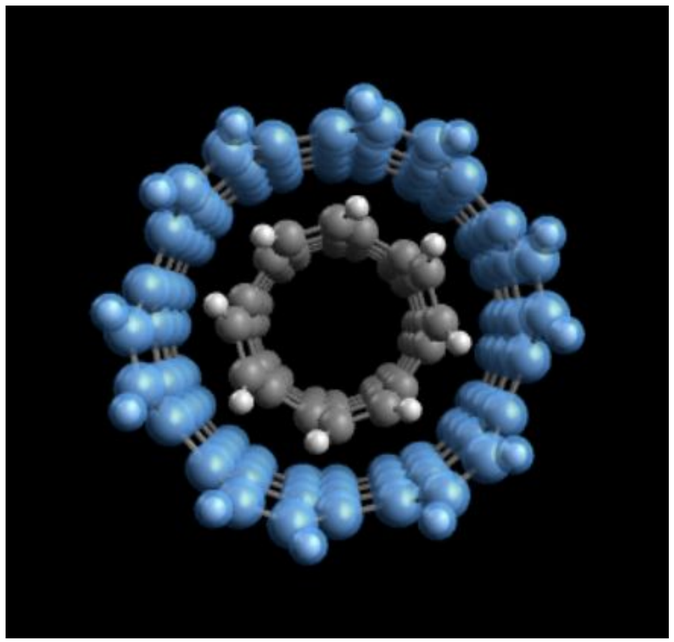
Avogadro can build:

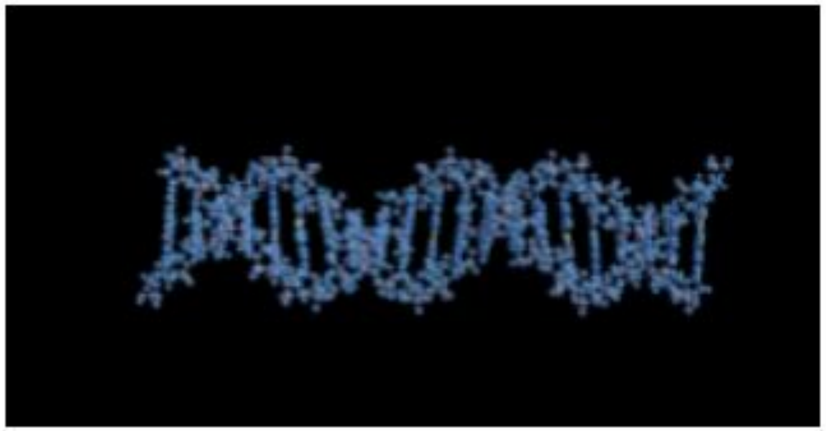
Molecules



Nanotubes



DNA/RNA



A little of theoretical information

Some images are taken from: http://openmopac.net/

Semi-empirical methods

Ignore core electrons: only consider valence electrons
Replace many costly two-electron integrals in HF theory with parameters

Parameters from experimental and high-level calculations
Good parameters can give solutions with accuracy of HF theory

DFT and post-HF methods include more electron correlation, so are more accurate

Semi-empirical good for:

- Quick geometry screening
  Big systems before DFT
- Compromise: properties instead of DFT for big molecules

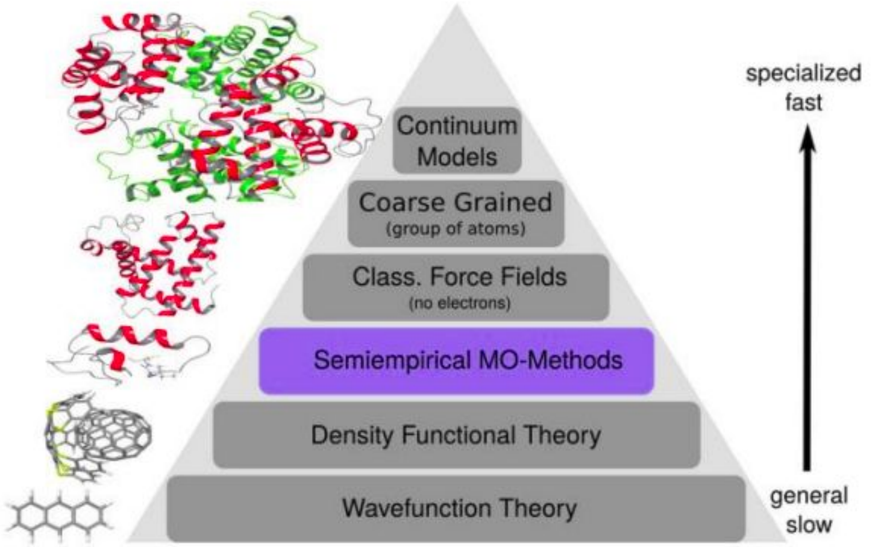
Semi-empirical bad for:

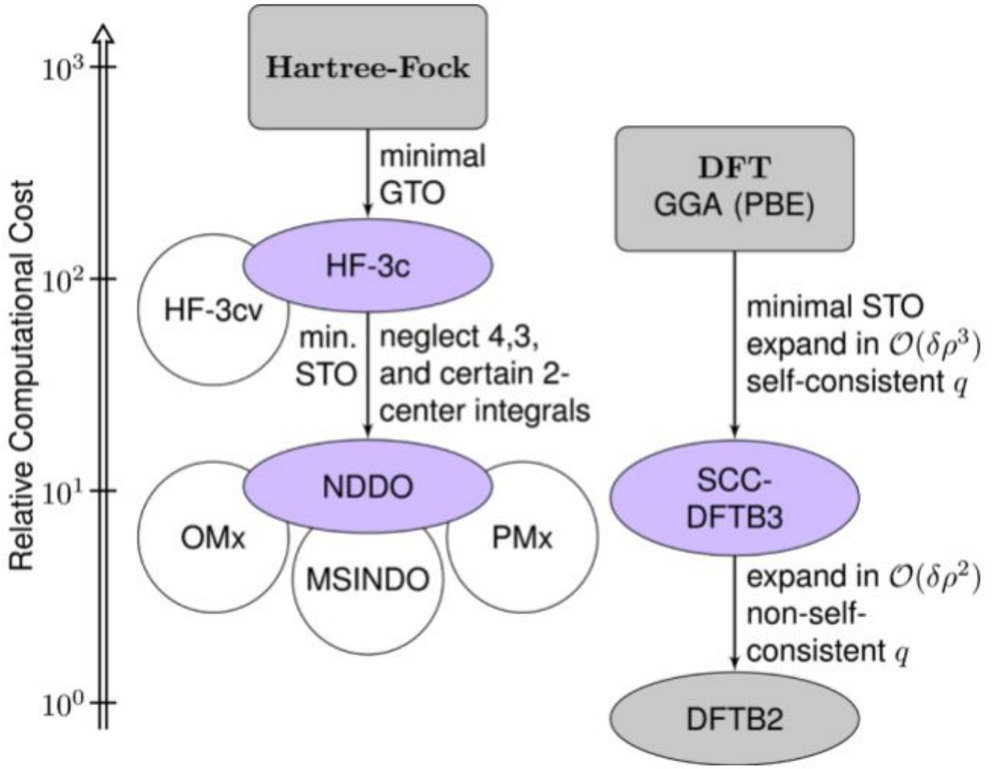
- Heavy atoms Transition metals (generally)
- Open-shell systems
- Small systems (DFT cheap)
  (Intermolecular interactions)

MOPAC. Parameterizations

AM1 (Austin)	Earliest model
	Superseded by PM3 (then 6,7)
RM1 (Recife)	Good for organics
	Lacks heavier atoms (e.g. Si)
PM6 (Parameterisation)	Heavily parameterised model. Wide applicability. Includes TMs Has dispersion and H-bond optimised versions
	Bad for sp2 nitrogen planarity
PM7	Improvement on PM6
	Nitrogens in amino acids still bad
ZINDO/S (Zerner's intermediate neglect of differential overlap) (Hyperchem)	Good for electronic spectra: may beat B3LYP in many cases!
	Bad for geometries Often good to add empirical parameters for π and s overlap.

Semi-empirical methods





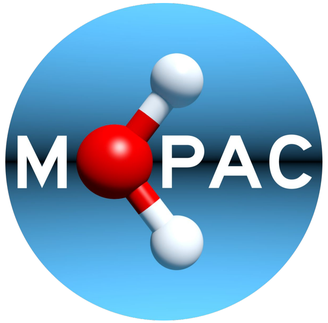
	S22	S66x8	X40	WATER14	L7	S30L	S30Ln	X23
PBE-D3/'CBS'	0.6	0.4	0.5	1.3	2.0	6.6	4.7	1.1
HF-3c	0.6	0.4	1.4	1.1	1.2	6.5	4.0	2.2
HF-3cv	1.7	0.5	2.1	2.3	2.4	7.4	5.3	3.1
DFTB3-D3	1.0	0.8	1.8	0.4	1.7	6.2	3.6	2.4
OM2-D3	0.9	0.8	–	0.9	2.9	6.7	3.7	–
PM6-D3H4X	0.7	0.5	1.2	0.7	2.9	6.7	4.8	–
PM6-D3H+	0.6	0.6	1.5	1.6	2.6	6.2	4.6	–
MSINDO-D3H+	1.5	1.1	1.4	1.5	5.7	9.5	8.8	6.6
PM7	0.8	0.7	1.8	0.5	6.5	16	11	–

MAD / kcal·mol^{-1}

relative error: < 12.5% < < 25% < < 37.5% <

Brandenburg, J. *et al.*, *J. Phys. Chem. Lett*, 5, 24 (2014)

MOPAC



MOPAC manual

MOPAC (Molecular Orbital PACkage) is a semiempirical quantum chemistry program.

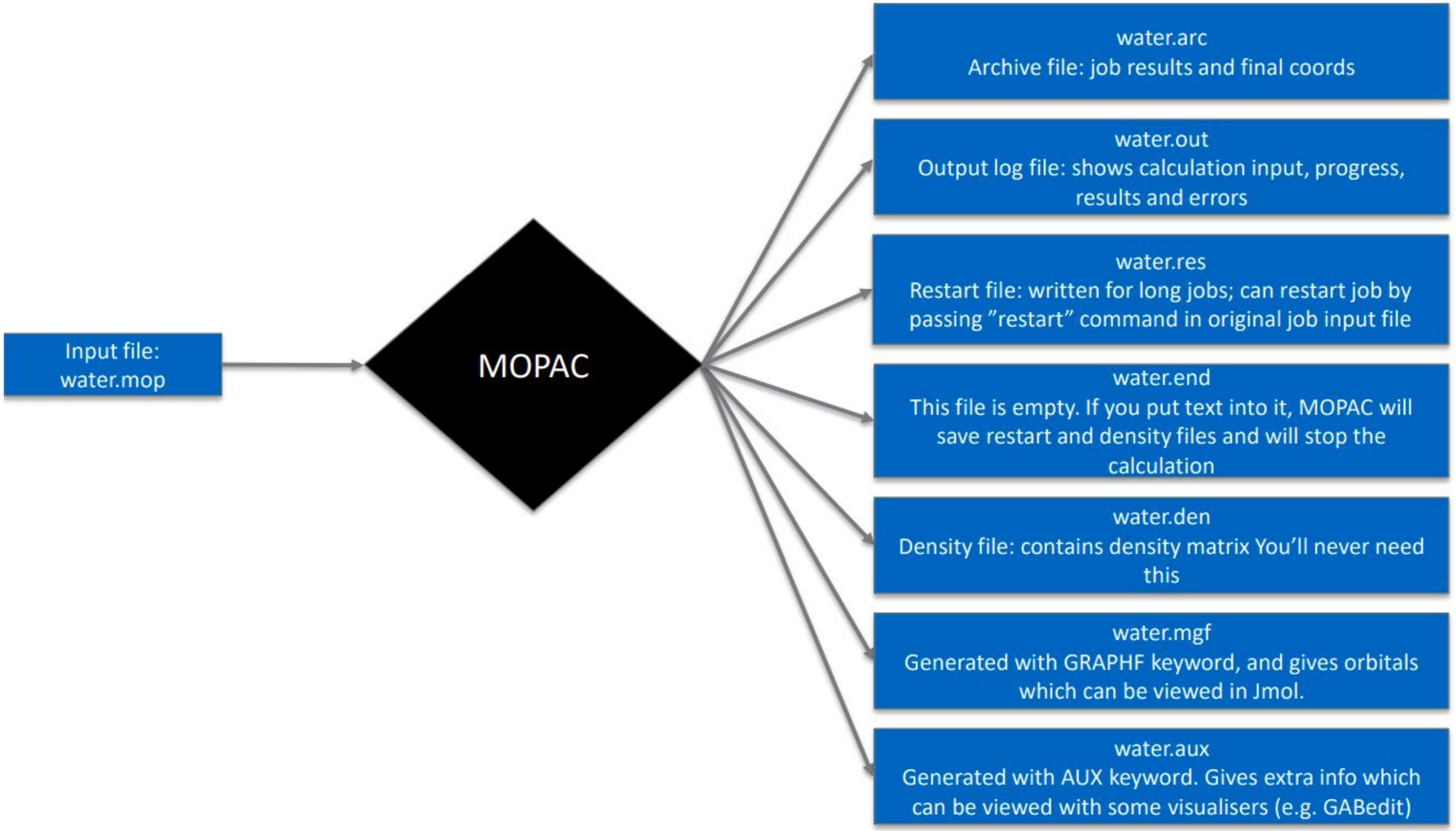
Semiempirical methods contain sets of parameters.

Table of Parameters

Parameter	Description	Units	MNDO	AM1	PM3	PM6
U_{ss}, U_{pp}, U_{dd}	*s*, *p*, and *d* atomic orbital one-electron one-center integrals	eV	*	*	*	*
β_s, β_p, and β_d	*s*, *p*, and *d* atomic orbital one-electron two-center resonance integral terms	eV	*	*	*	*
ξ_s, ξ_p, and ξ_d	*s*, *p*, and *d* Slater atomic orbital exponent	$bohr^{-1}$	*	*	*	*
ξ_{sn}, ξ_{pn}, and ξ_{dn}	*s*, *p*, and *d* Slater atomic orbital internal exponent	$bohr^{-1}$	*	*	*	*
α_A	Atom *A* core-core repulsion term	$Å^{-1}$	*	*	*	
α_{AB}	Atoms *A* and *B* core-core repulsion term	$Å^{-1}$				*

A little of technical information

MOPAC: Input file



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MOPAC: Input file

‘Method’ ‘Some parameters’
‘User comments’
‘Empty string’
*Geometry**

```
 PM7 GNORM=0
Geometry optimization

C     1.397   1    0           1    0 1
C     0.6985  1    1.20983749  1    0 1
C    -0.6985  1    1.20983749  1    0 1
C    -1.397   1    0           1    0 1
C    -0.6985  1   -1.20983749  1    0 1
C     0.6985  1   -1.20983749  1    0 1
H     2.481   1    0           1    0 1
H     1.2405  1    2.14860903  1    0 1
H    -1.2405  1    2.14860903  1    0 1
H    -2.481   1    0           1    0 1
H    -1.2405  1   -2.14860903  1    0 1
H     1.2405  1   -2.14860903  1    0 1
```

*Each line starts with the atomic symbol, followed by x,y,z coordinates. Whether these parameters are variables or constants during the geometry optimization is indicated by a trailing 0 (constant) or 1 (variable).

MOPAC: Methods used in the Lab 1

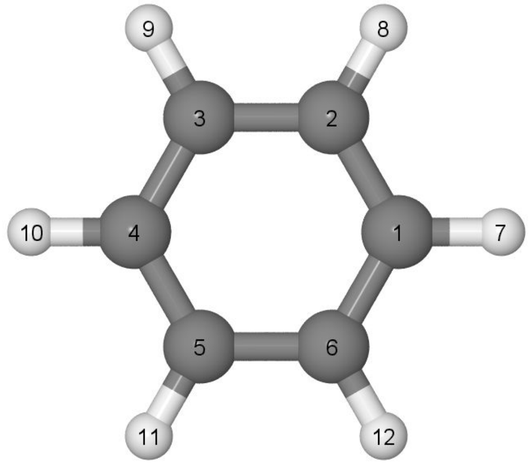
PM7 is the Modified Neglect of Diatomic Overlap, Parametric Method Number 7

- PM7 uses a "D2" type correction for the elements: H, He, B, C, N, O, F, Ne, P, S, Cl, Ar, Br, and Kr. For the other elements, a core-core Gaussian attractive terms is used to mimic dispersion. This means that some form of dispersion is present for all elements. The core-core Gaussian terms are optimized to reproduce reference geometries and heats of formation.

- The best method for general chemistry, and for solids. Optimized to reproduce the Standard Heat of Formation, ΔH_f.

- Perfectly fits for inorganic solids.

Lab 1 practice



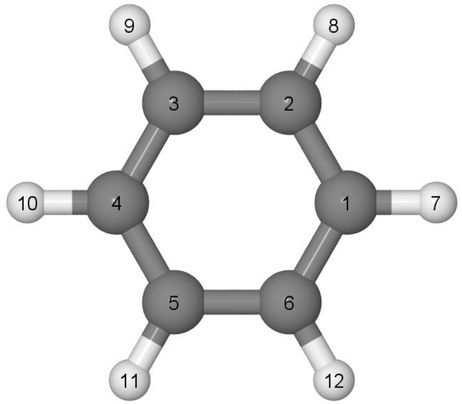
1. Geometry optimization

```
 1  PM7 GNORM=0
 2  Geometry optimization
 3
 4  C     1.397   1    0           1    0 1
 5  C     0.6985  1    1.20983749  1    0 1
 6  C    -0.6985  1    1.20983749  1    0 1
 7  C    -1.397   1    0           1    0 1
 8  C    -0.6985  1   -1.20983749  1    0 1
 9  C     0.6985  1   -1.20983749  1    0 1
10  H     2.481   1    0           1    0 1
11  H     1.2405  1    2.14860903  1    0 1
12  H    -1.2405  1    2.14860903  1    0 1
13  H    -2.481   1    0           1    0 1
14  H    -1.2405  1   -2.14860903  1    0 1
15  H     1.2405  1   -2.14860903  1    0 1
```

molec_PM7_em.mop ***.mop extension***

```
[a.boev@cest-cms-ccmm Lab1_benzene]$ mopac molec_PM7_em.mop
```

GNORM is geometry optimization termination criteria. Allows the geometry optimization to exit as soon as the gradient norm dropped below 0.01 kcal/mol/Ångstrom



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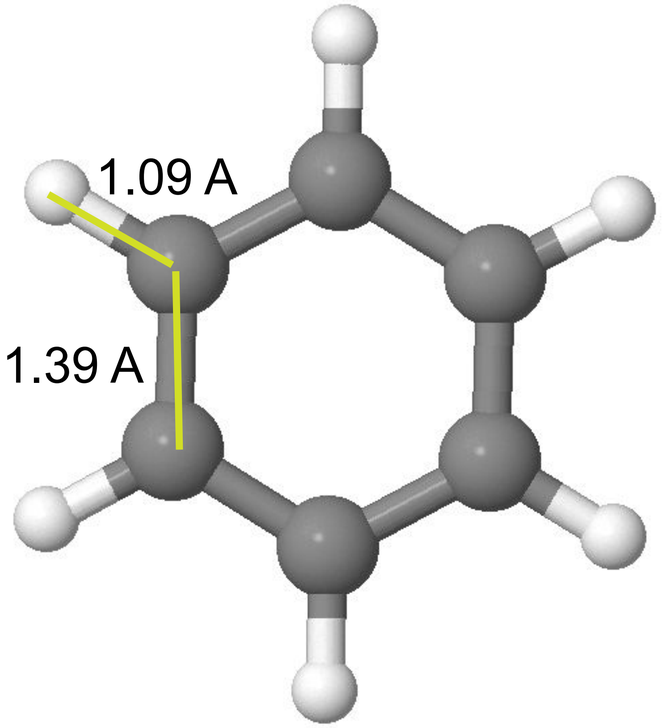
1. Geometry optimization

molec_PM7_em.out

```
FINAL HEAT OF FORMATION =         22.95542 KCAL/MOL =      96.04546 KJ/MOL


COSMO AREA              =        119.70 SQUARE ANGSTROMS
COSMO VOLUME            =        108.36 CUBIC ANGSTROMS

GRADIENT NORM           =          0.00697          =       0.00201 PER ATOM
IONIZATION POTENTIAL    =          9.824057 EV
HOMO LUMO ENERGIES (EV) =         -9.824  0.236
NO. OF FILLED LEVELS    =         15
MOLECULAR WEIGHT        =         78.1134         POINT GROUP:  D6h

MOLECULAR DIMENSIONS (Angstroms)

  Atom       Atom       Distance
  H    12    H     9     4.96376
  H    10    H     7     4.29870
  H     8    C     4     0.00000


SCF CALCULATIONS        =         17

WALL-CLOCK TIME         =      0.070 SECONDS
COMPUTATION TIME        =      0.095 SECONDS
```



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2. Vibrational frequency calculation

```
 1   AUX(MOS=0,PRECISION=4) PM7 FORCE
 2  Vibrations
 3
 4  C       1.39399329 1      0.00000000 1      0.00000000 1
 5  C       0.69699665 1      1.20723360 1      0.00000000 1
 6  C      -0.69699665 1      1.20723360 1      0.00000000 1
 7  C      -1.39399329 1      0.00000000 1      0.00000000 1
 8  C      -0.69699665 1     -1.20723360 1      0.00000000 1
 9  C       0.69699665 1     -1.20723360 1      0.00000000 1
10  H       2.48186046 1      0.00000000 1      0.00000000 1
11  H       1.24093023 1      2.14935421 1      0.00000000 1
12  H      -1.24093023 1      2.14935421 1      0.00000000 1
13  H      -2.48186046 1      0.00000000 1      0.00000000 1
14  H      -1.24093023 1     -2.14935421 1      0.00000000 1
15  H       1.24093023 1     -2.14935421 1      0.00000000 1
```

molec_PM7_freq.mop

FORCE – shows the force constants for the molecule.

2. Vibrational frequency calculation

HEAT OF FORMATION = 22.956501 KCALS/MOLE

ZERO POINT ENERGY 60.211 KCAL/MOL

NORMAL COORDINATE ANALYSIS (Total motion = 1 Angstrom)

Root No.	1	2	3	4	5	6	7	8
	1 E2u	1 E2u	1 B1g	1 E2g	1 E2g	1 A2u	1 E1g	1 E1g
	346.1	346.1	592.1	600.3	600.3	757.3	900.2	900.2

DESCRIPTION OF VIBRATIONS

VIBRATION	2 1E2u	ATOM PAIR	ENERGY CONTRIBUTION	RADIAL
FREQUENCY	346.12	C 2 -- C 3	+22.7% (110.3%)	0.0%
TRANSITION DIPOLE	0.0000	C 5 -- C 6	+22.7% (110.3%)	0.0%
TRAVEL (Ang.)	0.4069	C 3 -- C 4	+13.5% (85.0%)	0.0%
REDUCED MASS	1.1769	C 1 -- C 6	+13.5% (85.0%)	0.0%
EFFECTIVE MASS	18.7542			
FORCE CONSTANT	0.0831			

VIBRATION	3 1B1g	ATOM PAIR	ENERGY CONTRIBUTION	RADIAL
FREQUENCY	592.06	C 4 -- C 5	+13.1% (49.8%)	0.0%
TRANSITION DIPOLE	0.0000	C 5 -- C 6	+13.1% (49.8%)	0.0%
TRAVEL (Ang.)	0.4437	C 1 -- C 6	+13.1% (49.8%)	0.0%
REDUCED MASS	0.5786	C 3 -- C 4	+13.1% (49.8%)	0.0%
EFFECTIVE MASS	10.0031	C 1 -- C 2	+13.1% (49.8%)	0.0%
FORCE CONSTANT	0.1195	C 2 -- C 3	+13.1% (49.8%)	0.0%

3. Single point calculation

```
 GRAPHF PM7 1SCF ALLVEC AUX(MOS=99999,PRECISION=4)
Single point

C        1.39399329 1       0.00000000 1       0.00000000 1
C        0.69699665 1       1.20723360 1       0.00000000 1
C       -0.69699665 1       1.20723360 1       0.00000000 1
C       -1.39399329 1       0.00000000 1       0.00000000 1
C       -0.69699665 1      -1.20723360 1       0.00000000 1
C        0.69699665 1      -1.20723360 1       0.00000000 1
H        2.48186046 1       0.00000000 1       0.00000000 1
H        1.24093023 1       2.14935421 1       0.00000000 1
H       -1.24093023 1       2.14935421 1       0.00000000 1
H       -2.48186046 1       0.00000000 1       0.00000000 1
H       -1.24093023 1      -2.14935421 1       0.00000000 1
H        1.24093023 1      -2.14935421 1       0.00000000 1
```

molec_PM7_sp.mop

GRAPHF – writes a formatted file, ***<name>.mgf*** with the Information about Molecular Orbitals, which can be visualized with Jmol program.

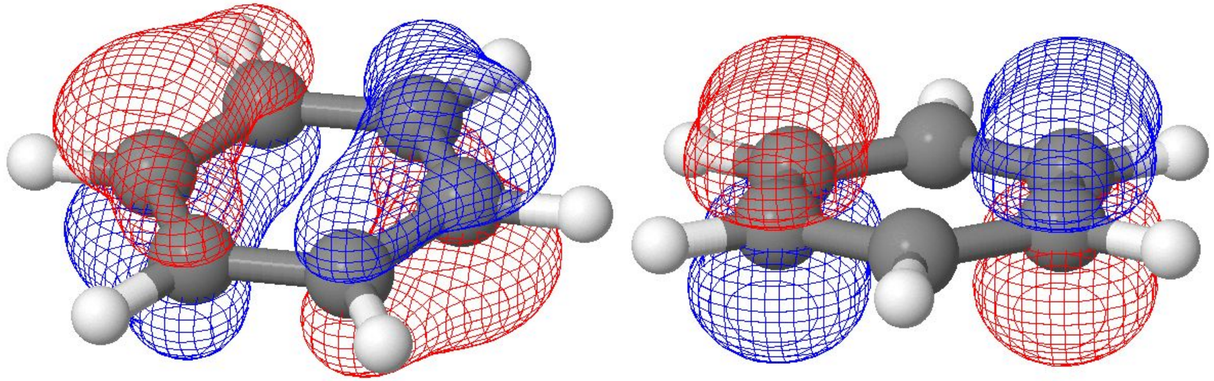
1SCF – is a single SCF calculation of a geometry.

ALLVEC – allows printing of all the MO into the output file.

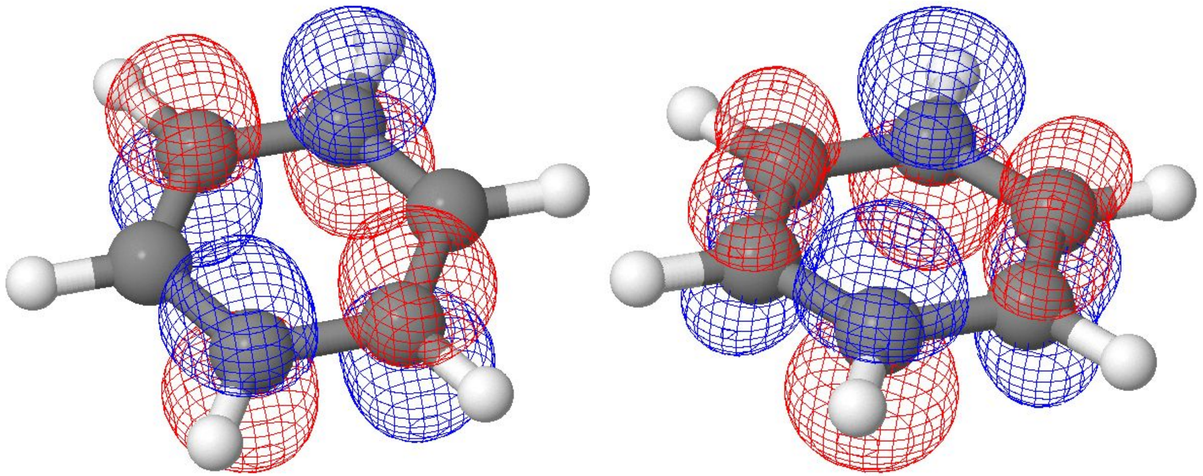
3. Single point calculation

Jmol → molec_PM7_sp.mgf → RButton → Surfaces → Molecular Orbitals

HOMO: -9.82 eV (Doubly generated)



LUMO: 0.24 eV (Doubly generated)



4. Localized Molecular orbitals

```
 1   GRAPHF AUX(MOS=99999,PRECISION=4) PM7 1SCF LOCALIZE ALLVEC
 2  Localized MO
 3
 4  C        1.39399329 1       0.00000000 1       0.00000000 1
 5  C        0.69699665 1       1.20723360 1       0.00000000 1
 6  C       -0.69699665 1       1.20723360 1       0.00000000 1
 7  C       -1.39399329 1       0.00000000 1       0.00000000 1
 8  C       -0.69699665 1      -1.20723360 1       0.00000000 1
 9  C        0.69699665 1      -1.20723360 1       0.00000000 1
10  H        2.48186046 1       0.00000000 1       0.00000000 1
11  H        1.24093023 1       2.14935421 1       0.00000000 1
12  H       -1.24093023 1       2.14935421 1       0.00000000 1
13  H       -2.48186046 1       0.00000000 1       0.00000000 1
14  H       -1.24093023 1      -2.14935421 1       0.00000000 1
15  H        1.24093023 1      -2.14935421 1       0.00000000 1
```

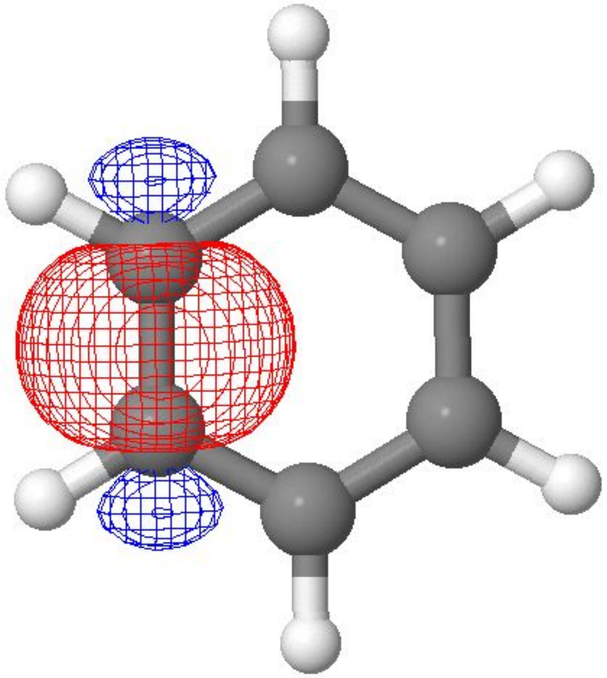
molec_PM7_lmo.mop

FORCE – gives the force constants for the molecule.

LOCALIZE – prints the occupied eigenvectors as transformed into a localized in the output file.

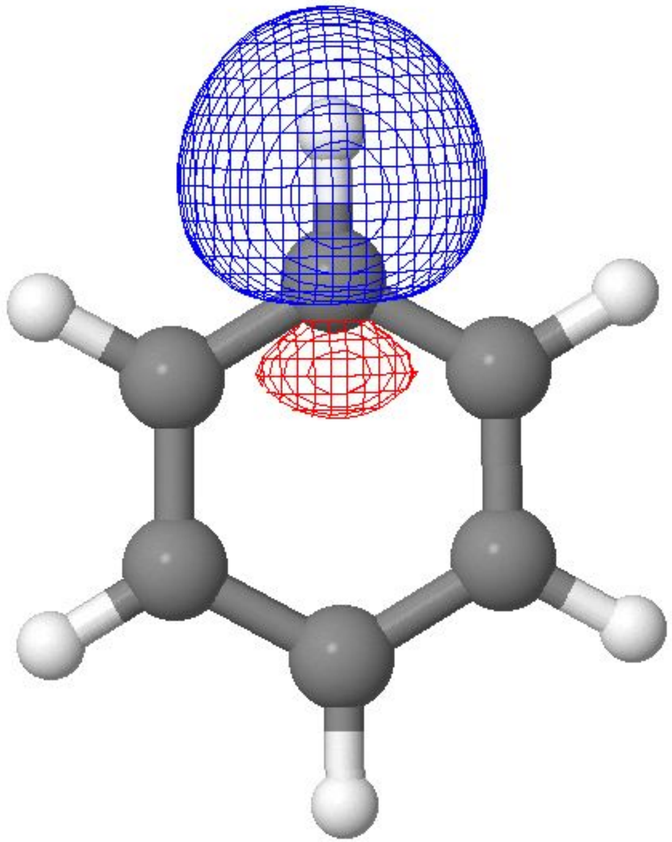
4. Localized Molecular orbitals

C-C σ-bond (-19.94 eV)



molec_PM7_lmo.out

C-H σ-bond (-17.56 eV)



5. Triplet geometry optimization

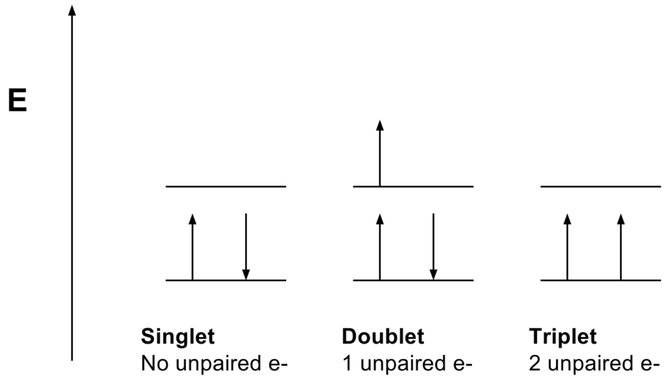
```
 PM7 UHF TRIPLET GNORM=0
To get correctly oriented molecule we slightly expanded C2-C3 and C5-C6 bonds

C       1.39399358 1      0.00000000 1      0.00000000 1
C       0.71699679 1      1.20723386 1      0.00000000 1
C      -0.71699679 1      1.20723386 1      0.00000000 1
C      -1.39399358 1     -0.00000000 1      0.00000000 1
C      -0.71699679 1     -1.20723386 1      0.00000000 1
C       0.71699679 1     -1.20723386 1      0.00000000 1
H       2.48186088 1      0.00000000 1      0.00000000 1
H       1.24093044 1      2.14935457 1      0.00000000 1
H      -1.24093044 1      2.14935457 1      0.00000000 1
H      -2.48186088 1      0.00000000 1      0.00000000 1
H      -1.24093044 1     -2.14935457 1      0.00000000 1
H       1.24093044 1     -2.14935457 1      0.00000000 1
```

UHF – the unrestricted Hartree-Fock Hamiltonian is to be used.

TRIPLET – triplet state is defined.

GNORM – geometry optimization stop criterion. Allows the geometry optimization to exit as soon as the gradient norm dropped below 0.01 kcal/mol/Ångstrom.

molec_T_PM7_em.mop



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5. Triplet geometry optimization

```
FINAL HEAT OF FORMATION =         76.82977 KCAL/MOL =     321.45576 KJ/MOL


COSMO AREA              =       119.88 SQUARE ANGSTROMS
COSMO VOLUME            =       108.45 CUBIC ANGSTROMS

GRADIENT NORM           =         0.00607           =       0.00175 PER ATOM
IONIZATION POTENTIAL    =         7.393328 EV
ALPHA SOMO LUMO (EV)    =        -7.393  0.656
BETA  SOMO LUMO (EV)    =       -10.311 -2.048
NO. OF ALPHA ELECTRONS  =        16
NO. OF BETA  ELECTRONS  =        14
MOLECULAR WEIGHT        =        78.1134          POINT GROUP:  D2h
```

C2–C3 and C5–C6 bonds are elongated to 1.482 A and other bonds are compressed to 1.386 A.

6.Triplet Vibrational frequency calculation

```
 1   AUX(MOS=0,PRECISION=4) PM7 UHF TRIPLET FORCE
 2  Vibrations
 3
 4  C        1.42788504 1       0.00000000 1       0.00000000 1
 5  C        0.74084873 1       1.20340293 1       0.00000000 1
 6  C       -0.74084873 1       1.20340293 1       0.00000000 1
 7  C       -1.42788504 1       0.00000000 1       0.00000000 1
 8  C       -0.74084873 1      -1.20340293 1       0.00000000 1
 9  C        0.74084873 1      -1.20340293 1       0.00000000 1
10  H        2.51842877 1       0.00000000 1       0.00000000 1
11  H        1.24433052 1       2.15780940 1       0.00000000 1
12  H       -1.24433052 1       2.15780940 1       0.00000000 1
13  H       -2.51842877 1       0.00000000 1       0.00000000 1
14  H       -1.24433052 1      -2.15780940 1       0.00000000 1
15  H        1.24433052 1      -2.15780940 1       0.00000000 1
```

molec_T_PM7_freq.mop

UHF – the unrestricted Hartree-Fock Hamiltonian is to be used.

TRIPLET – triplet state is defined.

FORCE – gives the force constants for the molecule.

6.Triplet Vibrational frequency calculation

HEAT OF FORMATION = 76.829766 KCALS/MOLE

ZERO POINT ENERGY 56.229 KCAL/MOL

NORMAL COORDINATE ANALYSIS (Total motion = 1 Angstrom)

Root No.	1	2	3	4	5	6	7	8
	1 Au	1 B2g	1 B3u	1 B3g	1 Ag	2 B3u	1 B1g	2 B2g
	103.7	232.4	297.5	501.4	575.9	670.0	741.0	779.2

7. Triplet Single point calculation

```
 1   GRAPHF PM7 UHF TRIPLET 1SCF ALLVEC AUX(MOS=99999,PRECISION=4)
 2  Single point
 3
 4  C        1.42788504 1       0.00000000 1       0.00000000 1
 5  C        0.74084873 1       1.20340293 1       0.00000000 1
 6  C       -0.74084873 1       1.20340293 1       0.00000000 1
 7  C       -1.42788504 1       0.00000000 1       0.00000000 1
 8  C       -0.74084873 1      -1.20340293 1       0.00000000 1
 9  C        0.74084873 1      -1.20340293 1       0.00000000 1
10  H        2.51842877 1       0.00000000 1       0.00000000 1
11  H        1.24433052 1       2.15780940 1       0.00000000 1
12  H       -1.24433052 1       2.15780940 1       0.00000000 1
13  H       -2.51842877 1       0.00000000 1       0.00000000 1
14  H       -1.24433052 1      -2.15780940 1       0.00000000 1
15  H        1.24433052 1      -2.15780940 1       0.00000000 1
```

molec_T_PM7_sp.mop

GRAPHF – writes a formatted file, ***<name>.mgf*** with the Information about Molecular Orbitals needed by Jmol program.

1SCF – is a single SCF calculation of a geometry.

ALLVEC – allows printing of all the MO into output file.

UHF – the unrestricted Hartree-Fock Hamiltonian is to be used.

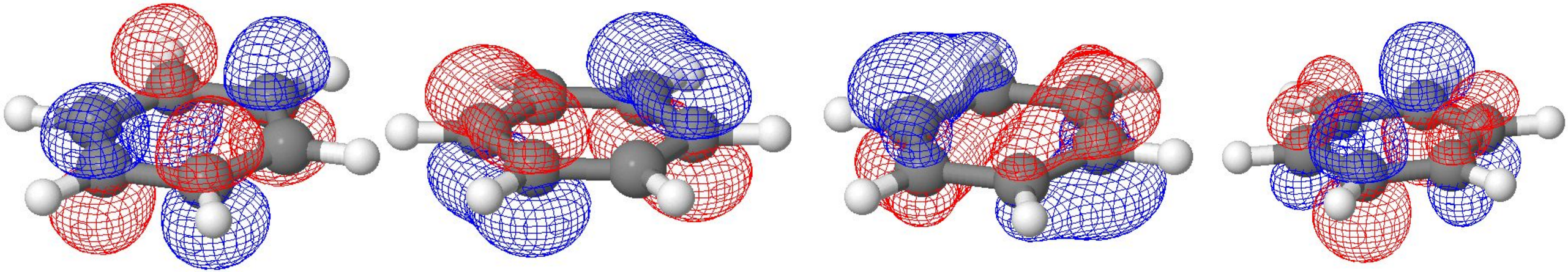
TRIPLET – triplet state is defined.

7. Triplet Single point calculation

Jmol → molec_T_PM7_sp.mgf → RButton → Surfaces → Molecular Orbitals

α ß

SOMO: -7.39 eV LUMO: -2.05 eV SOMO: -10.31 eV LUMO: 0.65 eV



SOMO is singly occupied MO

Parameters for advances calculations: Full list of parameters

Eigenvalues – units of eV; **Frequencies** – units of cm^{-1}.

GRADIENT NORM — kcal/mol/Angstrom multiply by 43.37 to get eV/Ångstrom, 0.01 kcal/mol/Ångstrom = 0.4 meV/A.

Heat of Formation (ΔH_f) – the change in enthalpy, in kcal mol^{-1} or kj mol^{-1}, when one mole of a system is formed from its elements, with everything being in its standard state.

ITER – shows information on SCF.

COSMO area (COnductor-like Screening MOdel) – model for solvation.

FINAL HEAT OF FORMATION – relative to elements in **standard states**.

IONIZATION POTENTIAL – Vertical IP = – HOMO according to the **Koopman's theorem**.

DIPOLE POINT-CHG. vs HYBRID – different methods to calculate dipole charge. For more details, look in the **manual**.

CHARGE – Used to calculate properties of ions and specifies system charge.

Thx

Skoltech