Lab 01. Molcas installation, maintenance, tools

1 Using molcas help system.

- Find a list of all keywords for module scf.
- Get help for GV code
- Get help for environment variable MOLCAS_OUTPUT
- Find out available basis sets for Cu
- Find the list of DFT functionals

2 Simple editing of XYZ file.

File *doc/samples/problem_based_tutorials/CH4.xyz* contains 'broken' (prepared for geometry optimization exercise) coordinates. Fix it.

Hint 1. to select a bond click on a first atom, and on a second atom. If bond selected: try + and - . Use F4 for typing the bond length.

Hint 2. Use space or middle mouse button to remove selection. If you made a mistake - use Backspace for Undo.

Hint 3. Check geometry by using F8 (with no selected atoms).

Hint 4. Don't forget to save the file (F2)

3 Making antracene

Start from benzene molecule, and create coordinates for antracene.

Hint 1. Check *Coord* directory for benzene structure

Hint 2. To remove an atom - select it (ot mark by using Shift+mouse), and press Delete.

Hint 3. To add a dummy atom in the middle of a bond - select two atoms, and press End

Hint 4. To apply symmetry: select 1 atom (for inversion) and press F8.

4 (Optional) Making symmetric molecules

Create durene (1,2,4,5-tetramethylbenzene).

Hint 1. Delete one H atom, and select C atom. Use F3 to add CH3 group. Note that F3 works different if you don't atoms selected

5 Fixing the symmetry

Start from benzene molecule, and move an atom slightly out of plane. How to restore the symmetry?

Hint 1. Select three atoms, and apply symmetry (F8)

6 (Optional) making a crystal

$CsCl$ crystal has the following structure:
Cs atoms creates a cube with a size 4.1$\mathring{A}$, Cl atom is located in the middle of the cube.

Create coordinates of a cube in 'vi'. Edit file in GV, and add Cl atom. Now use translation symmetry (select 2 atoms, and press F8).

Mark four atoms, and press '6' in order to select a new cell.

7 My first molcas calculation

Create a simple input for Molcas, containing calls to &GATEWAY, &SEWARD, &SCF, and &GRID_IT. (or use file SCF.energy.CH4.input from samples).

Loot at the orbitals, and modify active space.

Hint 1. To see all orbitals - press F3 in GV

Hint 2. Use hot keys (fi123sd) to select the orbital type, and save orbital file.

8 Simple DFT calculation.

Modify the input, to run DFT calculation.

Compare densities computed with HF and DFT

Hint 1. Use: molcas gv -a -1.0 SCF.grid DFT.grid

9 Set of calculations for potential energy curves

Create an input file, which can be used for the set of calculations with different interatomic distance between atoms, or with different geometries.

Hint 1. Use $XX in inline(!) XYZ file
molcas XX=0.4 input will run calculation with this value.

Hint 2. Use FOREACH command to create a loop.

Hint 3. If there is no simple way to construct coordinates - create a set of them using GV, and loop over the file name.

10 EMIL input

Take an example
doc/samples/problem_based_tutorials/DFT.minimum_optimization.H2O

run it, and visualize geometry steps.

Hint 1. Use F3 in GV to display the plot

Hint 2. Use Home, End, PageUp, PageDown keys to navigate between structures

MOLCAS grid and geometry viewer: GV

MOLCAS Grid/Geometry Viewer/Editor (GV) is an OpenGL based code for visualization of molecular orbitals and densities, density differences and spin-densities, and visualization of molecular structures (with the possibility to manipulate them on the screen), and visualization of some properties.

For installation GV requires headers and libraries for GLUT development. For Linux users we recommend to install libraries from *http* : *//www.mesa3d.org/*. Optionally it is possible to compile GV with panel support. In this case GLUI library should be installed. It is not necessary to build GV. MOLCAS distribution provides prebuild executables for GV, located in ***xbin*** directory. If your platform is different from LINUX, you have to edit ***xbin.cfg*** and specify a suitable executable.

GV can operate with different kinds of files:

- grid files (usually with extension grid) (generated by the program GRID_IT),
- XYZ files,
- molden files, generated by MOLCAS.

If a file name is specified in a command line, GV will determine the type of the file, and switch to the appropriate mode. If no file is specified, GV will search the current directory for files with a known type.

GV can run as a ordinary MOLCAS module (via command molcas gv *filename*), or as a stand alone executable.

Command line parameters for GV

Command	*Purpose*
filename	: name of a grid file, or XYZ file, or molden file. If this parameter is omitted program will try to find a first relevant file in the current directory.
-h	display help information
-n filename	create an empty XYZ file
-d real	set an initial size for the molecule
-f filename	set the basename of output files (.xyz, .tga, .eps, .pov). By default the basename is taken from the filename.
-s integer	Set initial size for the screen.
-g	Run GV with panels (GV should be compiled with GLUI library)

-G	similar to -g, but display panels as a separate window.

The rest of command line parameters have meaning only for displaying grid files:

Command	*Purpose*
-l real	: set initial isolevel value
-i real	: set increment value for changing isovalue
-t real	: set transparency level (between 0.0 and 1.0) for isosurfaces
-b color	: set initial background color ($white|gray|black$)
-o integer	: set the number of initial orbitals (by default: display density)
filename2	: name of a second grid file to display a density difference
-a real	: a weight of second grid. The default is -1 (to calculate density difference).
–out filename	: specify output file name for a grid constructed with -a option.
–version	: print the version number

`GV` also can display a molecular structure from a native seward input. In this case a flag '-c' should be placed before the filename.

For an advance configuration of `GV` one can save the current configuration (see below), and edit the ASCII formatted configuration files. The configuration files are located in the subdirectory *`.molcasgv`* in user home directory. File *`gv.rc`* contains global settings, like colors, transparency, etc. File *`atoms.rc`* contains sizes and colors for each element.

The main control of `GV` can be done by the mouse: the left mouse button is used to rotate the grid or the molecule, right mouse button is used for the on-screen menu. The major operations from menus can also be performed by hot-keys. Note, that behavior of `GV`, e.g. on-screen menus and hot-keys is different for the different types of visualized files.

Some keys like PageUp/PageDown, plus/minus have different meaning in different modes, with a general rule - plus/minus changes a value, PageUp/PageDown changes a property from a list.

Note for Mac users. To press functional keys (F1-F10) you have to use 'fn' button. Insert button (missing on Mac keyboard) can be emulated by 'I' key.

General HotKeys.

Command	*Purpose*
Ctrl-Q	Quit
F10	Exit (exit implies possible back up of edited files).
Escape	unset different editing modes
F1	Display the help screen (with a list of hot-keys)
q/Q	decrease/increase quality of drawing
F2	save INPORB file or XYZ file
F9	Save current settings
Shift+F9	Edit colors for background, labels, orbitals and extra planes.
r/R/g/G/b/B	Interactively change RGB code for the background, labels, and orbitals (selected by Shift-F9 key)
F5	Print screen in tga format. The output files will be named as *filename000.tga*
Shift+F5	Print screen in PostScript format. The output files will be named as *filename000.eps*
P	Print screen in PostScript (level 2) format.
p	Save povray file.
z/Z	Zoom the grid or the molecule
x	Maximize the screen
v/V	Create/restore *.ViewPoint* file (viewing conditions)
Home	Move the molecule to the center of the screen
Up/Down/Left/Right	Move the position of the picture on screen (with shift - make bigger steps)
l	Switch to/from the mode: move the light position with the mouse.
w	Switch between greyscale and colored picture
m	Start/stop animation
W	Switch to Tee time mode

Hot keys in Grid Mode.

Command	*Purpose*
+/-	increase/decrease the isosurface value (the step and initial value can be modified by command line parameters)
PageUp/PageDown	display next/previous orbital. In multiview mode (F3 has been pressed), use magnify glass.
t/T	change transparency level
f/i/1/2(a)/3/s/d	change the type of the current orbital to frozen, inactive, RAS1, RAS2, RAS3, secondary, deleted.
Space/middle mouse	change the type of the current orbital (by loop)
F2	save INPORB file (file will be saved as *filename.GvOrb*)
F3	Switch to/from multiview mode. In multiview mode the orbital type is shown by different backgrounds (rainbow colors). User can modify the type of orbitals, by pressing middle mouse button (or Space).
F4	Enter an isovalue, or an orbital number, or create a filter (for more information check tutorial for GV).
Delete	Hide the orbital from the list
Insert	Restore all hidden orbitals

If GV is used to display a molecule, it is possible to make a selection of an atom, a bond, an angle, or a dihedral angle by clicking (by left mouse button) on the atom. First selected atom will be displayed with a blue colored net, the rest (for bond and angle) with a magenta colored net. Using hot keys it is possible to make modification of the selected part of the structure. In addition to selection (note that only 4 atoms can be selected), it is possible to mark a group of atoms. Marking is made either by mouse (is Shift button is hold), or by keyboard (F7 button). Marked atoms can be modified as a single unit - e.g. rotated, moved. To remove current selection - press middle mouse button or space. If user has both selected and marked atoms - the first press of space button will unselect 'selected', and the second one - unselect 'marked' atoms.

GV can understand an extended syntax of XYZ file, and draw additional elements: axises, polygons, etc. Such extra data can be produced by other codes, in particular by ZYX interpreter.

Hot keys in Coordinate mode.

Command	*Purpose*

F2	Save coordinates (file will be saved as *filename000.xyz*)
Shift-F2	Save coordinates (overwrite the file)
left mouse	select an atom by clicking on it.
left mouse + shift	mark an atom
drag left mouse + shift pressed, followed by left click	mark atoms in the area
F3	display menu with fragments.
M	if Mopac is installed - optimize geometry (you might need to modify *sbin/runmopac* script and fix the location of Mopac installation)

Hot keys in if no atoms are selected

Command	*Purpose*
+/-	change a size of atoms and bonds
Insert	add an atom, or last inserted fragment
End	add dummy atoms (reference points) on the direction of axis.
a	Mark hydrogen atoms in the molecule
F8	analyze the symmetry of the molecule and display symmetry elements.
Delete	delete dummy atoms
Home	Move the molecule to the center of screen
*	Reverse the selection
#	if several atoms are marked, sort them, and place into the beginning of xyz file.

Hot keys in Selection mode (1 atom is selected)

Command	*Purpose*
Space/middle mouse	remove selection.
F3	display a menu with fragments, to be inserted close to selected atom
Insert	add an atom (or last selected fragment) near selected atom

Delete	delete selected atom
Home	place the origin to the position of selected atom
PageUp/PageDown	Change selected atom to one from the list (H,C,N,O,F,S,Cl)
F4 or =	invoke an edit box, where you can type an element name for selected atom.
F7	Mark atoms connected to the selected atom.
a	Mark all atoms which are the same elements as selected
F8	apply Inversion symmetry around selected atom
-/+	desaturate the color of the atom

Hot keys in Selection mode for bond (2 atoms are selected)

Command	*Purpose*
Space/middle mouse	remove selection.
Insert	create a bond between selected atoms
Delete	delete the bond between selected atoms
PageUp/PageDown	change the type of the bond between atoms
+/-	change the distance between atoms. Note that first selected atom (blue) will move.
F4 or =	invoke an edit box, where you can type an interatomic distance
F7	Mark all connected atoms around the first atom in a selected bond into a group.
F8	apply translational symmetry for a vector specified by selected atoms.
F6	Watch the value of selected bond
#	Change the order of selected atoms

Hot keys in Selection mode for angle (3 atoms are selected)

Command	*Purpose*
Space/middle mouse	remove selection.

+/-	change the angle between selected atoms. Note that first selected atom (blue) will move.
PageUp/PageDown	change the angle according to 'standard' angle values (by loop)
F4 or =	invoke an edit box, where you can type an angle value (or, you may type the value directly)
F8	apply mirror symmetry around an plain specified by selected atoms.
F6	Watch the value of selected angle
3	draw a triangle between selected atoms
4	draw a plane going through selected atoms

Hot keys in Selection mode for dihedral angle (4 atoms are selected)

Command	*Purpose*
Space/middle mouse	remove selection.
+/-	change the dihedral angle between selected atoms. Note that first selected atom (blue) will move.
F4 or =	invoke an edit box, where you can type a dihedral angle value (or, you may type the value directly)
F6	Watch the value of selected angle
F7	Mark atoms located at other side from the plain defined by selected atoms 2-3-4, in comparison to atom 1
F7+Shift	Use selected atoms as a cell, and mark atoms outside this cell
6	draw a cell, using selected atoms as axis definition

Hot keys in Molden mode for a orbital file (e.g. scf.molden)

Command	*Purpose*
PageUp/PageDown	Display charges

Hot keys in Molden mode for a frequency file

Command	*Purpose*

PageUp/PageDown	load next/previous vibration mode
F3	draw graphical information in a separate window.
+/-	change the speed of vibrations

Hot keys in Molden mode for a geometry file

Command	*Purpose*
PageUp/PageDown	load next/previous geometry
F3	draw graphical information in a separate window.
Home	show initial structure
End	show the resulting structure