Overview of Molcas

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Today we will learn..

- Installation of Molcas
- HowTo get help
- HowTo run Molcas
- HowTo create input
- General structure of the input

A code called Molcas

- source code (Fortran, C) + scripts (Perl, bash)
- can be configured for
  - different platforms: Unix, Linux, Windows, MacOS
  - serial, parallel (SMP or cluster), grid
  - 32- and 64- bit
  - all major compilers: gfortran, Intel, PGI, NAG, SunStudio
- a compiled code includes:
  - set of executables to solve a QCh problem
  - driver scripts to parse input, and run executables
  - tools and interface programs
  - databases (e.g. basis set library)

Configuration

prerequisite software

- Fortran77/90 and C compilers, Perl interpreter
- GNU make, sharutils
- GUI related software/libraries: OpenGL, glut, etc..

Configuration:

- *./configure* (execute setup script)
- *./configure -compiler intel -speed fast*

Installation

- *make*
  - build GA library (can be done externaly)
  - build the code
  - build databases
  - make a first run (to verify: it runs!)
- *molcas getextra* - download GUI
- *config.extra* - build GUI (not recommended)

Reconfiguring

- *make distclean; ./configure [flags]; make*

molcas command

- molcas driver (which version to run?)
- molcas.exe (license and parser)
- molcas commands:
  - molcas input [flags]
  - molcas tool [arguments]
- Multiple installations of Molcas
  - case 1: Current (or parent) directory is MOLCAS
  - case 2: MOLCAS environment is set
  - case 3: latest molcas installation (.Molcas/molcas)

Help!!

- on-line documentation *www.molcas.org*
- molcas help command
  - *molcas help*
  - *molcas help scf*
  - *molcas help scf charge*
  - *molcas help -t b3lyp*
  - *molcas help environment MOLCAS_OUTPUT*
  - *molcas help basis Cu*
- Solving problems
  - Molcas user's billboard
  - Bug report system
  - direct mail: *molcas@teokem.lu.se*

input example

File: Water.DFT.input

```
/* DFT/B3LYP calculation of water */
&GATEWAY
   COORD = water.xyz
   Basis = ANO-S-MB
&SEWARD
&SCF
   KSDFT = B3LYP
```

First molcas run

molcas Water.DFT.input -f
after run:

- Output
  - Water.DFT.log
  - Water.DFT.err
- Extra files
  - Water.DFT.ScfOrb
  - Water.DFT.scf.molden
- Intermediate files
  - /tmp/Water.DFT.5024/Water.DFT.RunFile
  - /tmp/Water.DFT.5024/Water.DFT.OrdInt

Directories

- CurrDir - submit directory
  we can write:

  ```
  coord=water.xyz
  ```

  or,

  ```
  coord=$CurrDir/water.xyz
  ```

  by default: all outputs will be collected here.
- WorkDir - scratch area
  by default - a random name under */tmp*

Changing defaults: by environment variables.

MOLCAS environment variables

- *molcas help environment*
- *molcas setuprc* – interactive script to redefine settings

Examples:

- *MOLCAS_WORKDIR* parent directory for all scratch directories
- *MOLCAS_PRINT* - set up print level
- *MOLCAS_OUTPUT* - to set up output directory for additional output files
- *Project* - set up Project name
- *WorkDir* - set up scratch area ($MOLCAS_WORKDIR/$Project)

Usage:

- molcasrc file (created by setuprc)
- export KEY=VALUE
- molcas KEY=VALUE input

Running molcas

- output goes to screen:
  - *molcas file.input*
- output goes to log and error files (.log and .err) :
  - *molcas file.input* **-f**
- include environment into command:
  - *molcas MOLCAS_PRINT = 3 file.input -f*
  - *CPUS = 2; export CPUS; molcas file.input*

input example

Processing of molcas input:

- preprocessing (clean and massage the input)
- execute molcas modules or commands
- control of the execution (mini programming language)

```
/* set MOLCAS_PRINT */
>>export MOLCAS_PRINT=NORMAL

/* run module GATEWAY */
&GATEWAY
/* input for module GATEWAY */
   COORD = water.xyz
   Basis = ANO-S-MB

/* run module SEWARD */
&SEWARD
```

Enhanced Molcas Input Language (EMIL)

- Comment lines: $*$ at the beginning of line;
  /* */ multiline comments.
- &*MODULE* is a call of module *MODULE*
- input for a module ends by new module,
  or by command, or 'End of input'
- strings $*VAR* replaced by the value of *VAR*
- Short notation: ; and = replaced by a new line
- EMIL commands started from > sign
  > unix echo 'hello'
  >>>>>>>>>>> unix echo 'hello' <<<<<<<<<<<
- @ - macros: @GEOM or @DFT(B3LYP)

EMIL/UNIX commands

```
>> UNIX ls
>> Export A=7
>> Eval B=$A+1
>> UNIX echo $B
>> Exit [returncode]
>> COPY File1 File2
>> LINK File1 File2
>> RM File
```

Note! $>$ *Export*! $=$ *export*, $>$ *COPY*! $=$ *cp*, $>$ *LINK*! $=$ *ln*
Note! all commands are executed at WorkDir

EMIL commands for preprocessing

```
>> include filename
>> verbatim
  /* No preprocessing here!
     */
 A=B; $C
>> end verbatim
```

IF control statements

```
>>>> If ( Iter = 1 ) <<<<
   ...
>>>> EndIf    <<<<

>>>> If ( $VAR = 7 ) <<<<
   ...
>>>> EndIf    <<<<

>>>> If ( -FILE file ) <<<<
   ...
>>>> EndIf    <<<<

>>>> If ( $VAR = 7 ) GOTO JUMP
   ...
>>>>LABEL JUMP
```

LOOP statements

```
>>>> Do While <<<<
....
&SLAPAF ( or &LOOP) /* module with special RC */
>>>> EndDo    <<<<

>>>> ForEach VAR IN ( 1, 2, 3 ) <<<<
....
>>>> EndDo    <<<<

>>>> ForEach VAR IN ( 1 .. 100 ) <<<<
....
>>>> EndDo    <<<<
```

input example

```
/* this is an example of geometry
   optimization of
   water molecule using DFT */
  &GATEWAY
     COORD=water.xyz
     Basis=ANO-S-MB
>>>>Do While
  &SEWARD
  &SCF ; KSDFT=B3LYP
  &SLAPAF
>>>> EndDo
```

input example

```
>>export DIST=1.0
>>foreach DFT in (BLYP,B3LYP,LDA)
>>foreach L in ( 1,2,3 )
   >>eval DIST=$DIST+0.1
     &GATEWAY
       Coord
        2
        inlined coordinates for H2
        H 0 0 0
        H $DIST 0 0
        BASIS= ANO-S-MB
     &SEWARD; &SCF; KSDFT=$DFT
>>enddo
>>enddo
```

Gateway module

- Coordinates
  - 'Native' molcas input
  - XYZ input (as a separate file or inline)

```
2  <- Number of atoms
comment line <- ( a.u., transformation)
O  0.0 0.0 0.0 <-  element(†)
C  1.2 0.0 0.0     cartesian coordinates
```

    (†) Element name can contain a basis set label.
- Basis set
  - RI/CD basis set
- Symmetry
- External field (PCM,Xfield)

'Native' molcas input

- default symmetry: C_1
- default units: atomic
- only symmetry unique atoms
- atoms with unique labels

```
&GATEWAY
Title =  water, ano-s(dzp) basis set
Symmetry =  x y
Basis set
H.ano-s...2s1p.
H1 -0.783975899  0.000000000 -0.184686472 Angstrom
End of basis
Basis set
O.ano-s...3s2p1d.
O  0.0   0.0 .369372944 Angstrom
End of basis
```

XYZ input

- default symmetry is highest available (D_{2h} subgroup)
- default units: Ångstrom
- 'plain' xyz formatted file (inline or an external file)
- Global or local basis set labels

```
&GATEWAY
  COORD
   3
   water molecule (in Angstrom)
   H -0.783975899  0.000000000 -0.184686472
   H  0.783975899  0.000000000 -0.184686472
   O  0.000000000  0.000000000 .36937294400
  Basis = ANO-S-VDZP
```

advanced XYZ input

```
 Basis
 ANO-S-VDZP, H.ANO-S-VDZP, O.ANO-S...3s2p1d.
 Group = C1
*  Group = x y
```

- for C_1 group: Group=C1, or NoSym
- To 'freeze' the molecule: NoMove
- to hack: $*WorkDir*/*findsym.std*

Grid/Geometry Viewer/Editor (gv)

- visualization and edit of coordinates:
  molcas gv file.xyz
  molcas gv -n new.xyz
- visualization of densities and orbitals
  molcas gv file.grid
  molcas gv -a -1.0 file1.grid file2.grid –out res.grid
- selection of active space
  molcas gv file.grid –> Save file.GvOrb
- visualization of molden files
  molcas gv file.geo.molden
  molcas gv file.freq.molden
  molcas gv file.scf.molden

Hints for GV usage

- Read the manual and tutorial!
- F1 - for a quick help
- Grouping (marking) and selection:
  - left mouse click - select an atom (up to 4)
  - left mouse + Shift - mark an atom (for group operations)
  - middle mouse click (or Space) - unselect/ungroup
- Operations:
  - +/− change a value
  - PageUp/PageDown change a property
  - F2 - save
  - F3 - view
  - F4 - edit
  - F5 - print