

Hands-on course of autcc ver.11

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1 software

- python
- sqlite3
- sqlite3 python interface

are necessary.

2 Assumption

Assumptions of the environment.

- The local PC handles DB.
- The local PC can't handle the computational server directly.
- The computational server uses the job scheduler, that the local PC can't submit jobs directly.

Remember that the facts of the output of the program,

- The errors of the program is different of the errors of the job scheduler.
- The errors of the program is different of the result of the program, e.g., whether the SCF is achieved or not.

3 directory structure

- inputdata
- calcddata

```
$ ls inputdata
Fdd2
$ ls inputdata/Fdd2
xsf_2_i0040 xsf_2_i0042 xsf_2_i0044 xsf_2_i0046 xsf_2_i0048
xsf_2_i0041 xsf_2_i0043 xsf_2_i0045 xsf_2_i0047 xsf_2_i0049
$ ls -a inputdata/Fdd2/xsf_2_i0040
.  ..  3.xsf  input_scf.txt  output_scf.txt
```

4 add .ID

hash.py can add hex digest.

```
$ pwd
/home2/kino/tmp/autcc/inputdata/Fdd2
$ ls
xsf_2_i0040  xsf_2_i0042  xsf_2_i0044  xsf_2_i0046  xsf_2_i0048
xsf_2_i0041  xsf_2_i0043  xsf_2_i0045  xsf_2_i0047  xsf_2_i0049
$ for n in xsf_2_i004*; do (cd $n; ../../../hash.py $PWD > .ID);done
$ ls -a xsf_2_i0040
.  ..  .ID  3.xsf  input_scf.txt  output_scf.txt
$ cat xsf_2_i0040/.ID
1b16160e003f0b8ed8541db046880ac11267baf1
\end{verbatim}
```

```
\section{create DB}
\begin{verbatim}
$ ./db11.py
./db11.py <options>
<options>
-createdb
-init
-send
-updatestatus
-recv
-purge

-status
-history
-help
$ ./db11.py -createdb
mode= createdb
createdb done
```

rundata.sqlite3 is made.

5 register directries in DB

```
$ ./db11.py -init
mode= createdb
createdb done
$ sqlite3 rundata.sqlite3
SQLite version 3.8.2 2013-12-06 14:53:30
Enter ".help" for instructions
Enter SQL statements terminated with a ";"
sqlite> select * from materialdata;
9d47efe361cb99a7b869a3d2fc6dd470d2fe3dc9|inputdata/Fdd2/xsf_2_i0041|metal1|new|0|idle|2015-05-28 23:
4435a45b0ef7ca11cce11ce420c2a8a87aae7a83|inputdata/Fdd2/xsf_2_i0049|metal1|new|0|idle|2015-05-28 23:
1b16160e003f0b8ed8541db046880ac11267baf1|inputdata/Fdd2/xsf_2_i0040|metal1|new|0|idle|2015-05-28 23:
5b600d251de1acf57a02e5db5ab2bee282ff8aac|inputdata/Fdd2/xsf_2_i0044|metal1|new|0|idle|2015-05-28 23:
71198b9bf3de59a7e47325988f2282321b05470b|inputdata/Fdd2/xsf_2_i0043|metal1|new|0|idle|2015-05-28 23:
7287588e927eefadf94f7daf67bb663c29357005|inputdata/Fdd2/xsf_2_i0047|metal1|new|0|idle|2015-05-28 23:
bda2dcf7090fcf8fe1b63a49174881c9aa7ad546|inputdata/Fdd2/xsf_2_i0046|metal1|new|0|idle|2015-05-28 23:
1178f9860baff27f5f6ec857ca0b8f53072f81d2|inputdata/Fdd2/xsf_2_i0042|metal1|new|0|idle|2015-05-28 23:
947390dc28b02f2f4b66a37266615ac2fa0e6953|inputdata/Fdd2/xsf_2_i0045|metal1|new|0|idle|2015-05-28 23:
751aa565288af342b02e4cec013f0a3e02f2751d|inputdata/Fdd2/xsf_2_i0048|metal1|new|0|idle|2015-05-28 23:
```

The directories that have a .ID file is added to the DB.

6 make inputdata

```
$ ./db11.py -send
mode= send
make 10 directories
calcddata/9d47efe361cb99a7b869a3d2fc6dd470d2fe3dc9.0/input_scf.txt is changed.
calcddata/4435a45b0ef7ca11cce11ce420c2a8a87aae7a83.0/input_scf.txt is changed.
calcddata/1b16160e003f0b8ed8541db046880ac11267baf1.0/input_scf.txt is changed.
calcddata/5b600d251de1acf57a02e5db5ab2bee282ff8aac.0/input_scf.txt is changed.
calcddata/71198b9bf3de59a7e47325988f2282321b05470b.0/input_scf.txt is changed.
calcddata/7287588e927eefadf94f7daf67bb663c29357005.0/input_scf.txt is changed.
calcddata/bda2dcf7090fcf8fe1b63a49174881c9aa7ad546.0/input_scf.txt is changed.
calcddata/1178f9860baff27f5f6ec857ca0b8f53072f81d2.0/input_scf.txt is changed.
calcddata/947390dc28b02f2f4b66a37266615ac2fa0e6953.0/input_scf.txt is changed.
calcddata/751aa565288af342b02e4cec013f0a3e02f2751d.0/input_scf.txt is changed.
send done
```

The inputfiles are changed according to senario/metal1_? files.

```
$ ls calcddata/
1178f9860baff27f5f6ec857ca0b8f53072f81d2.0  7287588e927eefadf94f7daf67bb663c29357005.0
1b16160e003f0b8ed8541db046880ac11267baf1.0  751aa565288af342b02e4cec013f0a3e02f2751d.0
4435a45b0ef7ca11cce11ce420c2a8a87aae7a83.0  947390dc28b02f2f4b66a37266615ac2fa0e6953.0
5b600d251de1acf57a02e5db5ab2bee282ff8aac.0  9d47efe361cb99a7b869a3d2fc6dd470d2fe3dc9.0
71198b9bf3de59a7e47325988f2282321b05470b.0  bda2dcf7090fcf8fe1b63a49174881c9aa7ad546.0
$ ls -a calcddata/1178f9860baff27f5f6ec857ca0b8f53072f81d2.0
.  ..  .EXECSTATUS  .ID  3.xsf  input_scf.txt  output_scf.txt
```

.EXECSTATUS is made.

```
$ cat calcddata/1178f9860baff27f5f6ec857ca0b8f53072f81d2.0/.EXECSTATUS
idle
```

7 calculate them in the computational server.

Send files into a computaional server. If the job can successfully calculated, change the .EXECSTATUS to "finished". Receive the result from the server.

For example,

```
$ cat calcddata/1178f9860baff27f5f6ec857ca0b8f53072f81d2.0/.EXECSTATUS
finished
```

8 change the execution status

```
$ ./db11.py -updatestatus
mode= updatestatus
updatestatus done
```

The DB read the content of .EXECSTATUS.

9 receive the result and register to the DB.

```
$ ./db11.py -recv
mode= recv
process 10 directories
OK inputdata/Fdd2/xsf_2_i0041 9d47efe361cb99a7b869a3d2fc6dd470d2fe3dc9 0
NG inputdata/Fdd2/xsf_2_i0049 4435a45b0ef7ca11cce11ce420c2a8a87aae7a83 0
OK inputdata/Fdd2/xsf_2_i0040 1b16160e003f0b8ed8541db046880ac11267baf1 0
NG inputdata/Fdd2/xsf_2_i0044 5b600d251de1acf57a02e5db5ab2bee282ff8aac 0
OK inputdata/Fdd2/xsf_2_i0043 71198b9bf3de59a7e47325988f2282321b05470b 0
OK inputdata/Fdd2/xsf_2_i0047 7287588e927eefadf94f7daf67bb663c29357005 0
OK inputdata/Fdd2/xsf_2_i0046 bda2dcf7090fcf8fe1b63a49174881c9aa7ad546 0
OK inputdata/Fdd2/xsf_2_i0042 1178f9860baff27f5f6ec857ca0b8f53072f81d2 0
OK inputdata/Fdd2/xsf_2_i0045 947390dc28b02f2f4b66a37266615ac2fa0e6953 0
NG inputdata/Fdd2/xsf_2_i0048 751aa565288af342b02e4cec013f0a3e02f2751d 0
recv done
$ ls inputdata/Fdd2/
xsf_2_i0040      xsf_2_i0041.o  xsf_2_i0043      xsf_2_i0045      xsf_2_i0046.o  xsf_2_i0048
xsf_2_i0040.o  xsf_2_i0042      xsf_2_i0043.o  xsf_2_i0045.o  xsf_2_i0047      xsf_2_i0049
xsf_2_i0041      xsf_2_i0042.o  xsf_2_i0044      xsf_2_i0046      xsf_2_i0047.o
```

inputdirectory.o is made if the output file shows that the SCF is converged.

10 make the input files again for the failure cases

```
$ ./db11.py -send
mode= send
make 3 directories
calcddata/4435a45b0ef7ca11cce11ce420c2a8a87aae7a83.1/input_scf.txt is changed.
calcddata/5b600d251de1acf57a02e5db5ab2bee282ff8aac.1/input_scf.txt is changed.
calcddata/751aa565288af342b02e4cec013f0a3e02f2751d.1/input_scf.txt is changed.
send done
$ ls calcddata/
1178f9860baff27f5f6ec857ca0b8f53072f81d2.0  7287588e927eefadf94f7daf67bb663c29357005.0
1b16160e003f0b8ed8541db046880ac11267baf1.0  751aa565288af342b02e4cec013f0a3e02f2751d.0
4435a45b0ef7ca11cce11ce420c2a8a87aae7a83.0  751aa565288af342b02e4cec013f0a3e02f2751d.1
4435a45b0ef7ca11cce11ce420c2a8a87aae7a83.1  947390dc28b02f2f4b66a37266615ac2fa0e6953.0
5b600d251de1acf57a02e5db5ab2bee282ff8aac.0  9d47efe361cb99a7b869a3d2fc6dd470d2fe3dc9.0
5b600d251de1acf57a02e5db5ab2bee282ff8aac.1  bda2dcf7090fcf8fe1b63a49174881c9aa7ad546.0
71198b9bf3de59a7e47325988f2282321b05470b.0
```

ID.1 is made. The input files are made using senario/metal1_1 parameter. ...

A definitions

In db11.py

```
DBNAME_define      = "materialdata"
SENARIODIR_define  = "senario"
INPUTDIR_define    = "inputdata"
TEMPORARYDIR_define= "calcddata"
MATERIALKIND_define= "metal1"
DBFILE_define      = "rundata.sqlite3"
```

In QmasOutInfo.py

```
qmas_inputfile="input_scf.txt"  
qmas_outputfile="output_scf.txt"
```

QmasOutInfo.py also determines whether the SCF is achieved from the output file.