

# Extra Large Scale Electronic Structure calculation program package

## ELSES

### Quick start guide

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ELSES Quick start for ELSES v0.02.04

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## 1 How to compile ELSES

### 1.1 Extraction of all files

Extract all files from the ELSES tar file, then change directory to the elses directory generated.

```
prompt> tar zxvf elses-*.tar.gz
prompt> cd elses
```

### 1.2 Specification of your compiler

A Fortran90 compiler and the LAPACK libraries are required to compile the ELSES code. Edit the file 'Makefile.inc' to specify compiler, linker and locations of the Lapack library. A typical description is as follows;

```
## for GNU G95 Fortran compiler (g95)
FC = g95 -mno-cygwin
FFLAGS = -O2 -g
LDFLAGS =
LIBS = -llapack -lblas
```

Examples of the description can be found in Makefile.inc for different compilers such as

- Intel Fortran compiler 10.1.013 (ifort)
- GNU Fortran compiler 4.3.0 (gfortran)

We have confirmed that Intel Fortran compiler appropriately works by using mkl which is included in the package and is compatible with Lapack and BLAS. In addition, if you use Intel Fortran compiler 11, please read §5.3.

### 1.3 Compiling whole codes

ELSES main program and its related tools are compiled by make command as the following manner in the ELSES directory. If your system has gmake command, we recommend gmake command rather than make command.

```
prompt> make
or
prompt> gmake
```

When the compile procedure is completed, the main simulator (bin/elses) and several tools (such as tool/elses-xml-generate) appear as executable programs. If you fail in the compile procedure, please read §5.1.

## 2 How to use ELSSES

### 2.1 Input file

ELSES requires three types of input file; i) configuration file (e. g. config.xml) in which calculation modes and calculation conditions have to be described, ii) structure file (e. g. H2O.xml) in which a molecular structure has to be described, iii) element file (e. g. O.xml) where several atom parameters have to be specified.

The following sample data are prepared in the sample directory for test calculations.

- sample/H2O/ optimization calculation of H2O
- sample/FeO/ optimization calculation of FeO
- sample/C6H6/ optimization calculation of benzene

### 2.2 Execution of ELSSES

The test calculation by using the H2O sample data is performed by executing elses as the following manner.

```
prompt> bin/elses sample/H2O/config.xml > log.txt
```

You had better save the output to an appropriate log file, because many data is outputted. Detailed data is outputted when verbose mode is used as the following way.

```
prompt> bin/elses -verbose sample/H2O/config.xml > log.txt
```

Furthermore, you can fix the verbose level.

### 2.3 Output file

Calculation results are outputted in

- Output.txt Some kinds of energy and force every MD step.
- position.\*\*\* Coordinate of every atom. Extension of file is determined in the configuration file.

The meaning of items in Output.txt are as follows:

- EBD : energy from the electronic system,  $EBD = 2tr[\rho H_0^{TB}]$
- ECSC: energy from the CSC part
- ECC : energy from the repulsive part
- EKE : energy from kinetic energy of the ionic system
- ETOT=EBD + ECSC + ECC : Total energy
- Force Amp. Average : averaged force over all atoms
- Force Amp. Max : maximum force in all atoms
- The atom that gives the max. force amp. : index of the atom which receive the maximum force

MD step is represented by step\_count, and step\_count=0 corresponds the initial structure. Section 4 treats topics of structure visualization.

```
Output; step_count=      0
Output energy
Band      Energy : EBD  [au]:      -5.354889504408413
ECSC      Energy : ECSC [au]:       0.005897357376885
Core-core Energy : ECC  [au]:       0.133744388618370
Kinetic   Energy : EKE  [au]:       0.000000000000000
EBD+ECSC+ECC Energy : ETOT [au]:     -5.215247758413158

Output Force Amplitude
```

Force Amp. Average [au] [eV/A]=	0.001726821055051	0.088797441728644
Force Amp. Max [au] [eV/A]=	0.002523260806207	0.129752358387033
The atom that gives the max. force amp. =	2	
-----		
Output; step_count=	1	
Output energy		
Band Energy : EBD [au]:	-5.353486452101532	
ECSC Energy : ECSC [au]:	0.005849513281715	
Core-core Energy : ECC [au]:	0.131352808940064	
Kinetic Energy : EKE [au]:	0.000000000000000	
EBD+ECSC+ECC Energy : ETOT [au]:	-5.216284129879754	
Output Force Amplitude		
Force Amp. Average [au] [eV/A]=	0.001492961265475	0.076771788591698
Force Amp. Max [au] [eV/A]=	0.002132810129885	0.109674411643693
The atom that gives the max. force amp. =	2	

## 3 How to control ELSSES

### 3.1 Adjustment of the configuration file

The file /sample/H2O/config.xml is the configuration file of the sample data of H<sub>2</sub>O molecule. The configuration file has the following contents. The numerical values of various kinds of calculation conditions in ELSSES can be controlled by editing this file.

```
<?xml version="1.0" encoding="UTF-8"?>
<config name="H2O">

<system>
  <cluster structure="H2O.xml" />
  <boundary x="nonperiodic" y="nonperiodic" z="nonperiodic" />
  <temperature unit="kelvin"> 273.15 </temperature>
  <element name="H" model="geno" filename="H.xml"/>
  <element name="O" model="geno" filename="O.xml" />
</system>

<calc mode="optimization">
<genoOption>
  <CSC_method> ELSTNER </CSC_method>
  <CSC_max_loop_count> 10000 </CSC_max_loop_count>
  <CSC_charge_convergence> 1d-6 </CSC_charge_convergence>
  <CSC_charge_mixing_ratio> 0.1 </CSC_charge_mixing_ratio>
</genoOption>
  <optimization>
    <sd_ratio> 0.2 </sd_ratio> <max_num_iter> 200 </max_num_iter>
  </optimization>
  <dynamics scheme="velocity verlet">
    <delta unit="fsec"> 1.00 </delta>
    <total unit="fsec"> 500.00 </total>
  </dynamics>
</calc>

<output>
  <restart filename="restart.xml" interval="1" />
  <position filename="position.xyz" interval="1" />
</output>

</config>
```

#### 3.1.1 Call of the structure file

The structure file is specified by the cluster tag in the system tag. Explanation of structure file is given later.

```
<cluster structure="H2O.xml" />
```

#### 3.1.2 Call of element files

The element file is specified by the element tag in the system tag. Description of file name is necessary to execute ELSSES even when you carry out calculations by default atom parameters without element files. It is note that the calculation is performed by using default parameters when the element file specified in the configuration file is not found.

```
<element name="H" model="geno" filename="H.xml"/>
```

#### 3.1.3 For changing temperature

The temperature of the system is specified by the temperature tag in the system tag.

The unit of value will be treated as Kelvin if a keyword "kelvin" is specified in the unit attribute, meanwhile, it will be treated as atomic unit if "a.u." is specified

```
<temperature unit="kelvin"> 273.15 </temperature>
```

### 3.1.4 For changing the calculation mode

ELSES can carry out the structure optimization calculation and the molecular dynamics calculation. The calculation mode is specified by the mode attribute in the calc tag. The structure optimization calculation is performed out when a keyword "optimization" is specified, and the molecular dynamics calculation is carried out when a keyword "dynamics" is specified.

```
<calc mode="optimization">  
</calc>
```

```
<calc mode="dynamics">  
</calc>
```

### 3.1.5 For changing the total optimization step

In the case of the optimization mode, total optimization step is specified by the max\_num\_iter. The function of convergence judgement have not been implement yet.

```
<optimization>  
  <sd_ratio> 0.2 </sd_ratio>  
  <max_num_iter> 200 </max_num_iter>  
</optimization>
```

### 3.1.6 For changing MD time slice

The delta time, short time slices between MD steps is specified by the delta tag in the dynamics tag. The total elapsed time is also specified by the total tag in the dynamics tag.

```
<dynamics scheme="velocity verlet">  
  <delta unit="fsec"> 1.00 </delta>  
  <total unit="fsec"> 256.00 </total>  
</dynamics>
```

The unit of value will be treated as femto-second if a keyword "fsec" is specified in the unit attribute, meanwhile, it will be treated as atomic unit if "a.u." is specified

### 3.1.7 Setting of the charge self-consistent calculation

The charge self-consistent (CSC) calculation is performed when a keyword "ELSTNER" is specified in the CSC\_method tag.

```
<genoOption>  
  <CSC_method> ELSTNER </CSC_method>  
  <CSC_max_loop_count> 10000 </CSC_max_loop_count>  
  <CSC_charge_convergence> 1d-6 </CSC_charge_convergence>  
  <CSC_charge_mixing_ratio> 0.1 </CSC_charge_mixing_ratio>  
</genoOption>
```

The execution without the CSC calculation is carried out when you set CSC\_max\_loop\_count tag to 0.

```
<genoOption>  
  <CSC_method> ELSTNER </CSC_method>  
  <CSC_max_loop_count> 0 </CSC_max_loop_count>  
  <CSC_charge_convergence> 1d-6 </CSC_charge_convergence>  
  <CSC_charge_mixing_ratio> 0.1 </CSC_charge_mixing_ratio>  
</genoOption>
```

### 3.1.8 For changing an output file for MD visualization

The whole coordinates and forces of each atom at each MD step are saved in a file for the following visualizations of the molecular dynamics. The file name is specified by the filename attribute of the position tag in the output tag. The interval, frequency for saving this data is specified by the interval attribute of the same tag.

The whole coordinates, velocity, and acceleration of each atom at the last MD step are saved in a file for the future use to continue the calculation. The file name is specified by the filename attribute of the restart tag in the output tag. The interval, frequency for saving this data is specified by the interval attribute of the same tag.

```
<output>
  <restart filename="restart.xml" interval="1" />
  <position filename="position.xyz" interval="1" />
</output>
```

Furthermore, ELSESES can make output file in some types of format by changing file extension in the file name attribute of position tag as the following manner.

```
(1) xyz format for vmd, molden and vesta(*)
<position filename="position.xyz" interval="1" />
  output file : position.xyz

(2) axsf format for xcrysden
<position filename="position.axsf" interval="1" />
  output file : position.axsf

(3) xsf format for xcrysden and vesta(**)
<position filename="position.xsf" interval="1" />
  output file : MD_step.xsf
(e. g. position0000000000.xsf, position0000000010.xsf, ...)

(4) pdb format for vmd, rasmol, molden and vesta
<position filename="position.pdb" interval="1" />
  output file : MD_step.pdb
(e. g. position0000000000.pdb, position0000000010.pdb, ...)
Note: script file for a batch transaction of rasmol, also, is outputted.
  output file : rasmol-batch.txt、rasmol- setting.txt

(*) Only the first snapshot is read in.
(**) Substituting atomic number for atom symbol is necessary.
    (e. g. 「H」 「1」)
```

## 3.2 Adjustment of the element file (GENO type Hamiltonian)

You can adjust atom parameters by editing the element file. If the element file is not found, ELSESES use the default parameter as is described in ELSESES manual. It is note that all tags have to be set when you use the element file. The sample file /sample/H2O/O.xml is described below.

```
<?xml version="1.0" encoding="UTF-8"?>
<element type="Huckel" name="O">
  <mass> 16.0d0 </mass>
  <initial_charge> 0 </initial_charge>
  <principal_quantum_number> 2 2 2 2 </principal_quantum_number>
  <initial_occupation> 2.d0 1.333d0 1.333d0 1.333d0 </initial_occupation>
  <initial_diagonal_elements> -28.20d0 -12.4d0 -12.4d0 -12.4d0 </initial_diagonal_elements>
  <zeta> 2.575d0 2.275d0 2.275d0 2.275d0 </zeta>
  <chemical_hardness> 12.4d0 </chemical_hardness>
  <repulsive_rescaling> 1.0 1.0 1.0 1.0 </rescaling_zeta>
</element>
```

You have to add parameters such as zeta2, c1 and c2 when the calculated system includes d-orbitals. The sample element file for atoms with d-orbitals is prepared in /sample/FeO/Fe.xml.

### 3.3 Adjustment of the element file (NRL type Hamiltonian)

When you perform calculations by using Naval Research Laboratory type Hamiltonian, you have to download parameter files from NRL site (<http://cst-www.nrl.navy.mil/bind>) and transform those into xml format. It is note that the current ELSESES can treat only the system which consists of a single species of atoms.

You can transform the parameter file (e. g. au\_par\_99.txt) to a xml file by using tool/elses-xml-generate-nrl-param as the following manner;

```
prompt> elses-xml-generate-nrl-param au_par_99.txt au_par_99.xml Au
```

The argument has to be provided in order of the download file, the xml file, and the atom.

Furtherer, you describe the element tag under system tag in configuration file as the following manner;

```
<element name="Au" model="NRL" filename="au_par_99.xml"> </element>
```

#### 3.3.1 For changing the atom species

The atomic mass is specified by the mass tag. The initial atomic charge is specified by the initial\_charge tag as the deviation from neutrality. These are treated as the atomic unit.

```
<mass> 16.0d0 </mass>
<initial_charge> 0 </initial_charge>
```

Species of the atomic orbital are specified by the principal\_quantum\_number tag. The current ELSESES can deal with one s-orbital, three p-orbitals, and five d-orbitals. In this tag, the principal quantum number has to be described in order of s-, p-, and d-orbitals. The occupation number of orbitals is specified by the initial\_occupation tag as the principal\_quantum\_number tag.

```
<principal_quantum_number> 2 2 2 2 </principal_quantum_number>
<initial_occupation> 2.d0 1.333d0 1.333d0 1.333d0 </initial_occupation>
```

#### 3.3.2 For changing the STO parameter

The orbital energy is specified by the initial\_diagonal\_element tag as the electron volt unit. In this tag, the orbital energy has to be described in order of s-, p-, and d-orbitals. The STO parameter  $\zeta$  which represents the extent of the Slater orbital is specified by the zeta tag as the atomic unit. The order of the description is the same as the initial\_diagonal\_elements tag.

```
<initial_diagonal_elements> -28.20d0 -12.4d0 -12.4d0 -12.4d0 </initial_diagonal_elements>
<zeta> 2.575d0 2.275d0 2.275d0 2.275d0 </zeta>
```

#### 3.3.3 For changing the repulsive rescaling factor

The parameter  $\zeta^{rep}$  which represents the extent of the STO orbital in the repulsive part is defined as  $\zeta^{rep} = (repulsive\_rescaling) * \zeta$ , so that you can adjust  $\zeta^{rep}$  by varying the repulsive rescaling factor. The repulsive rescaling factor is specified by the repulsive\_rescaling tag. In this tag, you fix the repulsive rescaling factor in order of s-, p-, and d-orbitals.

```
<repulsive_rescaling> 1.0 1.0 1.0 1.0 </repulsive_rescaling>
```

#### 3.3.4 For changing the chemical hardness

The chemical hardness is specified by the chemical\_hardness tag as the electron volt unit.

```
<chemical_hardness> 12.4d0 </chemical_hardness>
```

### 3.4 Adjustment of the structure file

The structure file of H<sub>2</sub>O molecule specified in the previous configuration file has the following contents. By editing this file manually, it could change the initial position, velocity and restriction on motion of each atom.

```
<?xml version="1.0" encoding="UTF-8"?>
<structure name="H2O" mdstep="0">

  <unitcell>
    <vector unit="angstrom"> 10.0 0.0 0.0 </vector>
    <vector unit="angstrom"> 0.0 10.0 0.0 </vector>
    <vector unit="angstrom"> 0.0 0.0 10.0 </vector>
  </unitcell>

  <heatbath>
    <massperatom unit="a.u."> 0.2500000000000000E+02</massperatom>
    <position unit="a.u."> 0.0000000000000000E+00 </position>
    <velocity unit="a.u."> 0.0000000000000000E+00 </velocity>
  </heatbath>

  <atom element="O" class="" motion="free">
    <position unit="angstrom"> 0.000000000 0.000000000 0.000000000 </position>
  </atom>
  <atom element="H" class="" motion="free">
    <position unit="angstrom"> 0.584410971 0.761619206 0.000000000 </position>
  </atom>
  <atom element="H" class="" motion="free">
    <position unit="angstrom"> 0.584410971 -0.761619206 0.000000000 </position>
  </atom>
```

However, this file can be automatically generated by the attached utility program explained in the following section. Therefore, only a few fundamental items are explained later.

#### 3.4.1 For freezing movements of specified atoms

If a keyword 'fixed' is specified to the motion attribute of the atom tag, the movement of the atom will be frozen during the whole process of the MD calculation.

```
<atom element="H" motion="fixed"> ... </atom>
```

#### 3.4.2 For changing initial positions of each atom

The 3-dimensional coordinates of each atom is specified in the position tag inside the atom tag. The unit of value will be treated as angstrom if a keyword 'angstrom' is specified in the unit attribute, meanwhile, it will be treated as atomic unit if 'a.u.' is specified. In addition, if a keyword 'internal' is specified in the unit attribute, it will become the internal coordinates to the principal lattice vectors specified by the unitcell tag.

#### 3.4.3 For changing initial velocities of each atom

The 3-dimensional velocity of each atom is specified in the velocity tag inside the atom tag. The unit of value will be treated as atomic unit if "a.u." is specified.

### 3.5 How to generate the structure file

The XML-formatted structure data file can be generated semi-automatically from XYZ-formatted file by using attached utility program tool/elses-xml-generate.



### 3.5.1 Preparation of the XYZ-formatted file

A XYZ-formatted file of a molecule which will be calculated by ELSESES is required in order to generate the structure file. The XYZ format is the simplest format where the element name and coordinates of each atom of a molecule or cluster is saved in the following manner. The unit of the coordinates in this file is angstrom.

```
3
H2O
O  0.000000000  0.000000000  0.000000000
H  0.584410971  0.761619206  0.000000000
H  0.584410971 -0.761619206  0.000000000
```

### 3.5.2 Preparation of the generation specification file

The file which has the following contents is also required. This file specifies how to generate a XML-formatted file from XYZ-formatted files.

```
<?xml version="1.0" encoding="UTF-8"?>
<generate name="H2O">
  <unitcell>
    <vector unit="angstrom"> 10.0  0.0  0.0 </vector>
    <vector unit="angstrom"> 0.0  10.0  0.0 </vector>
    <vector unit="angstrom"> 0.0  0.0  10.0 </vector>
  </unitcell>

  <cluster structure="H2O.xyz">
  </cluster>
</generate>
```

The file actually specifies only the shape of the rectangular system by the three ‘vector’ tags inside the ‘unitcell’ tag. Temporally, only orthogonal cells are supported.

### 3.5.3 Generation of the structure file

Execute the attached utility program, tool/elses-xml-generate as following manner.

```
prompt# elses-xml-generate generate.xml H2O.xml
```

Here, the first argument of this command is the generation specification file for input, and the second argument is the XML-formatted structure file for output.

## 4 Visualization of MD calculations

In this section, we briefly explain how to visualize the result of MD calculation using free software. ELSEES can make an output file in a variety of formats for some visualization software. Each software can read some particular formats, so that you have to fix the appropriate format of output file as §3.1.7. In the following section, the batch transaction of rasmol is explained. Note that the same manner can be applied to Jmol.

- rasmol (<http://openrasmol.org/>)
- Jmol (<http://jmol.sourceforge.net/>)
- molden (<http://www.cmbi.ru.nl/molden/molden.html>)
- xcrysden (<http://www.xcrysden.org/>)
- VMD (<http://www.ks.uiuc.edu/Research/vmd/>)
- VESTA ([http://www.geocities.jp/kmo\\_mma/crystal/jp/vesta.html](http://www.geocities.jp/kmo_mma/crystal/jp/vesta.html))

### 4.1 Batch transaction by rasmol

The visualization software rasmol can carry out batch transaction. We briefly explain the actual manner.

#### 4.1.1 Adjustment of the interval of output

Before the simulation, please adjust a value of interval parameter in the input file config.xml.

```
<position filename="H2O-position.pdb" interval="4" />
```

In the above case, positions of atoms will be recorded by four MD steps. Tentatively, the filename parameter is ignored. After the simulation, a lot of files for visualization are generated.

#### 4.1.2 Output file

After the MD simulation, pdb files of each MD step and the script file for rasmol are outputted.

- rasmol-batch.txt
- rasmol-setting.txt

#### 4.1.3 Batch transaction of rasmol

Please launch the rasmol program. Type the following command in the command-line window of rasmol.

```
RasMol > set write on  
RasMol > script rasmol-batch.txt
```

The snapshots are visualized in the visualization window sequentially. At the same time, these images are recorded in gif-formatted image files. See manuals of rasmol for details.

## 4.2 Batch files

Setting for each snapshot is described in rasmol-batch.txt as the following.

```
zap  
set specular on  
background white  
load pdb snap0000000001.pdb  
echo load snap0000000001.pdb  
script rasmol-setting.txt  
write gif snap0000000001.gif
```

Image files in the other format are generated if you change "gif" to the other format in the last line.

The setting of image visualization is described in rasmol-setting.txt as the following.

```
select all
color green
spacefill 150
wireframe 100
#pause
```

If you want to stop the motion by one snapshot, please remove “#” in the last line. In this case, the next snapshot appears every time you press the return key.

## 5 Trouble shooting

### 5.1 Compile error

If you fail in the compile procedure, please carry out the following command successively and let us know the results.

```
prompt> make clean
prompt> make xml
prompt> make elses
prompt> make tool
prompt> make tool-LDOS
```

### 5.2 Execution error: XML parsing Error

“XML parsing Error” in the execution indicates that an input xml file does not obey the xml grammar (e. g. a tag is not closed). Although there is also detailed information about the error so that you may find the origin of the error, you had better use the xml checker (e. g. xmllint).

xmllint works by typing the following command.

```
prompt> xmllint -noout filename
```

### 5.3 Execution error: alloc. error

“alloc. error” in the execution indicates that allocation of array fails due to the lack of memory.

### 5.4 Bug of Intel Fortran compiler 11

The compile procedure will not be completed if you use Intel Fortran compiler version between 11.0 and 11.1.046, according to bugs of the compiler. We include the patch which is provided by an user of ELSESES in the package to solve the problem. Please read the document `elses-ice-20090606.ReadMe` and apply the patch `elses-ice-20090606.patch`.

Furthermore, even if you use Intel Fortran compiler version 11.1.056, it is possible that the compile procedure fails and the following message is displayed.

```
elses-md-main.f90(26): internal error: Please visit
'http://www.intel.com/software/products/support' for assistance.
call get_elapse_wall_clock_time(elapse_time)
[ Aborting due to internal error. ]
```

This is caused by bugs of the compiler, too. Although we need to wait for the improvement of the compiler by Intel, you will possibly complete the compile procedure by repeating the make.