Extra Large Scale Electronic Structure calculation program package

ELSES

Quick start guide

6. Mar. 2017
ELSES Quick start for ELSES v0.07.00dev

Contents

1 How to compile ELSES

See the read-me file of

```
README.md
```

in the package.
Note: The quick start explains the miminum configuration case, the case without the MPI directive and optional external libraries.

2 How to use ELSES

2.1 Input file

The following three types of input files are used;

- configuration XML file (e.g. config.xml) $\cdots$ for calculation conditions
- structure XML file (e.g.C6H6.xml) $\cdots$ for atomic structure
- element XML file (e.g.C.xml) $\cdots$ for TB-model parameters required for each atom species

Among them, the element XML files are optional. If no element file is prepared, the default values built in the code are used.

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

- `sample/sample_geno/C6H6_opt/` structure optimization of benzene
- `sample/sample_geno/C6H6_dyn/` finite-temperature dynamics of benzene

Each directory contains a directory (named `result`) for resultant files.

2.2 Execution of ELSES

The test calculation by using the benzene data (`sample/sample_geno/C6H6_opt/`) is performed by executing elses as the following manner.

```
prompt> cd sample/sample_geno/C6H6_opt/
prompt> ../../../bin/elses config.xml > log.txt
```

You had better save the output to an appropriate log file, because many data is outputted. Another log file, named `log-node00000.txt` is also generated. The verbose mode can be used when you specied

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

so as to obtain detailed information. [1]

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 : electronic structure energy (EBD= $2\mathrm{Tr}[\rho H_0^{TB}]$)
- ECSC: charge-selfconsistent (CSC) part energy (zero among non-CSC calculations)
- ECC : 'rest-part' (repulsive) energy (mainly ion-ion repulsion)
- EKE : kinetic energy of the ionic system (nonzero only among finite-temperature dynamics)
- 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

[1] The verbose level can be specified as '-verbose=10'. The default level is one.

MD step is represented by step_count, and step_count=0 corresponds the initial structure. Section 5 treats topics of structure visualization.

An example of `Output.txt` is described as follows; (Here, several lines is truncated, owing to the limitation of paper width).

```
@@ Main output : ELSES version 0.03.15
INFO: config_name = C6H6_geno_opt_20121218
INFO-MPI-OMP: P_MPI, P_OMP=         1        12
Date: 2012 12 18; Time: 19 52 46
-----------------------------------------------------------------
Output; step_count=         0
 Output energy
 Band         Energy : EBD  [au]:            -21.074627243244468
 ECSC         Energy : ECSC [au]:              0.000000000000000
 Core-core    Energy : ECC  [au]:              0.647213749370900
 Kinetic      Energy : EKE  [au]:              0.000000000000000
 EBD+ECSC+ECC Energy : ETOT [au]:            -20.427413493873569
 Energy summary (explan.):  step_count        EBD+ECSC+ECC      EBD+ECSC+ECC+EKE  EBD
 Energy summary (au     ):            0      -20.42741349      -20.42741349      -21.07462724
 Energy summary (eV/atom):            0      -46.32188375      -46.32188375      -47.78952722
 SD energy difference per atom [eV]=         0        0.00019272172572821044
 Output Force Amplitude
 Force Amp. Average [au] [eV/A]=              0.000035411685775             0.001820957125198
 Force Amp. Max     [au] [eV/A]=              0.000061352314869             0.003154888914855
 The atom that gives the max. force amp. =          6
 Force_summary(ave[eV/A],max[eV/A],atom for max)=         0        0.0018209571251982 8338
-----------------------------------------------------------------
Output; step_count=         1
 Output energy
 Band         Energy : EBD  [au]:            -21.074258569701925
 ECSC         Energy : ECSC [au]:              0.000000000000000
 Core-core    Energy : ECC  [au]:              0.646764619148410
 Kinetic      Energy : EKE  [au]:              0.000000000000000
 EBD+ECSC+ECC Energy : ETOT [au]:            -20.427493950553515
 Energy summary (explan.):  step_count        EBD+ECSC+ECC      EBD+ECSC+ECC+EKE  EBD
 Energy summary (au     ):            1      -20.42749395      -20.42749395      -21.07425857
 Energy summary (eV/atom):            1      -46.32206620      -46.32206620      -47.78869121
 SD energy difference per atom [eV]=         1        0.00015499142578130867
 Output Force Amplitude
 Force Amp. Average [au] [eV/A]=              0.000028478925492             0.001464457315618
 Force Amp. Max     [au] [eV/A]=              0.000045665333030             0.002348225218168
 The atom that gives the max. force amp. =          3
 Force_summary(ave[eV/A],max[eV/A],atom for max)=         1        0.0014644573156175 4074
-----------------------------------------------------------------
```

2.4 Output of computational time

Total simulation time is outputted at the end of the standard output as the following style.

```
.....Total Simulation time (sec )    =                      0.05100
.....Total Simulation time (hour)    =                      0.00001
.....Total Simulation time (day )    =                      0.00000
```

In the above case, the total simulation time is about 0.05 seconds.

If the last line of the node log (log-node00000.txt) is

```
..... ELSES ended successfully (without MPI)
```

the message means that the calculation is over without error.

The simulation time for each MD step can be found by searching the word 'MDloop' in the node log (log-node00000.txt).

```
prompt> grep MDloop log-node000000.txt
elaps-time(befor  MDloop)=             0       0.006400       0.000000       0.000000
elaps-time(lap    MDloop)=             1       0.003500       0.000000       0.000000
elaps-time(lap    MDloop)=             2       0.001400       0.000000       0.000000
elaps-time(lap    MDloop)=             3       0.001300       0.000000       0.000000
```

This example shows that it takes about 0.0064 second to perform the calculation before MD and simulation time of each MD step are about 0.0035 seconds.

In addition, the computational time for some routines can be found by using grep command for the the node log (log-node00000.txt) as the following manner.

```
prompt> grep -i time log-node00000.txt
```

For an example, when the diagonalization solver is specified in the geno work flow, the following message appears

```
  TIME for LAPACK (DSYGV) =             0.0017000000
```

This message represents that it takes 0.0017 seconds for the diagonalization routine of LAPACK(DSYGV)

2.5 Execution of the sample test tool

The sample test tool, a shell script,

```
/sample/shell_scripts/elses_sample_test.sh
```

executes several sample data and checks the numerical result. The tool is prepared, so as to confirm that the build procedure is finished without problem. The tool is executed, as follows;

```
$ cd sample
$ ./shell_scripts/elses_sample_test.sh
```

If the test does not detect a problem, an example of the output is

```
-------------------------------------------------------------------------------
ELSES sample test
-------------------------------------------------------------------------------
TEST for C6H6_opt (GENO)
2013/08/09 PM 06:56:12
.....Total Simulation time (sec )    =                       0.10900
-----------------------------------
TEST for C6H6_dyn (GENO)
2013/08/09 PM 06:56:12
.....Total Simulation time (sec )    =                       0.19280
-----------------------------------
TEST for VCNT_100atom (non-geno)
    (with generation of initial XML file and final eigen values)
2013/08/09 PM 06:56:13
.....Total Simulation time (sec )    =                       3.92220
.....Checking the resultant eigen levels
-----------------------------------
TEST for Au_NW_0143atom (non-geno;NRL)
    (with generation of the element file)
2013/08/09 PM 06:56:17
.....Total Simulation time (sec )    =                       7.52500
ELSES sample test .... ended successfully, if no numerical data appears above
-------------------------------------------------------------------------------
ELSES band calculation test : carbon diamond with Cerda spd orbitals
```

```
 test> ../../../../bin/elses -band -verbose ./config.xml > logfile.txt
 test> ../../../../bin/band > log-band.txt
 test> diff EigenEnergy.txt result/EigenEnergy.txt
---> Test ended successfully, if no numerical data appears above
```

Additional numerical value appears in the above output, when the test detects a problem. The above output is just one example and the tool may be updated. One can find the output file for the latest test tool as

```
sample/shell_scripts/result/result_elses_sample_test.txt
```

2.6 Aborting a run before the completion

One can abort an MD (iterative) simulation before its completion by a 'stop signal'. The stop signal is to put the file

```
00_stop_signal.txt
```

on the working directory. The first line of the file should be a number except 0 (zero). No information is needed at the other lines. At each MD step, ELSES tries to detect the stop signal or search the file. When detects, the simulation will ends after saving the output files. Note: If the first line of the file is 0 (zero), the file is ignored.

3 Input files

3.1 Cconfiguration XML file

The calculation conditions are specified by the configuration XML file (typical filename : `config.xml`).

Popular calculation modes are those for structure optimization and for finite-temperature dynamics. A example of the configuration file for the former and latter mode is

```
sample/sample_geno/C6H6_opt/config.xml
```

or

```
sample/sample_geno/C6H6_dyn/config.xml
```

respectively. The content of `sample/sample_geno/C6H6_opt/config.xml` is shown below:

```
<?xml version="1.0" encoding="UTF-8"?>
<config name="C6H6_geno_opt_20121218">

<system>
  <cluster structure="C6H6.xml" />
  <boundary x="nonperiodic" y="nonperiodic" z="nonperiodic" />
  <element  name="C" model="geno"  filename="C.xml"> </element>
  <element  name="H" model="geno"  filename="H.xml"> </element>
</system>

<calc mode="optimization">
  <solver scheme="eigen"> </solver>
  <genoOption>
   <CSC_method> ELSTNER </CSC_method>
   <CSC_max_loop_count> 0 </CSC_max_loop_count>
   <CSC_charge_convergence>  1d-5 </CSC_charge_convergence>
   <CSC_charge_mixing_ratio> 0.1 </CSC_charge_mixing_ratio>
  </genoOption>
  <optimization>
   <sd_ratio> 0.2 </sd_ratio>
   <max_num_iter> 2000 </max_num_iter>
   <convergence_criteria mode="energy_per_atom" unit="eV"> 1.0d-5 </convergence_criteria>
  </optimization>
</calc>

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

</config>
```

Among them, the configuration name in

```
<config name="C6H6_geno_opt_20121218">
```

does not affect the calculation result and is arbitrary.

3.1.1 Call of the structure file

The structure file is specified by the cluster tag in the system tag.

```
<cluster structure="C6H6.xml" />
<boundary x="nonperiodic" y="nonperiodic" z="nonperiodic" />
```

The `boundary` tag specifies the periodic or non-periodic boundary condition for the x, y, z directions. The above example is one for the non-periodic boundary conditions. The periodic boundary condition is imposed, when the word 'nonperiodic' is replaced by 'periodic'.

Details of the structure file are explained below.

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 ELSES 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="C" model="geno"  filename="C.xml"> </element>
```

3.1.3 Temperature and heat-bath mass

Finite-temperature dynamics is realized by the thermostat method [2] and requires the temperature and the heat-bath mass. An example can be found in the file of `sample/C6H6_dyn/config.xml`.

The temperature of the system is specified by the temperature tag in the system tag. The unit of the temperature can be 'kelvin' or 'a.u.' (default).

```
<temperature unit="kelvin"> 500 </temperature>
```

The heat-bath mass is specified by the heat-bath mass per atom.

```
<heatbath_mass mode="on">
  <mass_per_atom unit="a.u."> 25.0d0 </mass_per_atom>
</heatbath_mass>
```

If one write 'mode="off"', the tag is ignored.

Note: The priority treatment in multiple definitions of the heat-bath mass $\cdots$ The value of the heat-bath mass can appear, not only the configuration XML file, but also the structure XML file (for example, in a case of continued simulation). The priority treatment in multiple definitions of the heat-bath mass is as follows; (case I) If the value appears in the configuration XML file, the value is chosen. In such a case, the value of the structure XML file is ignored, if exists. (case II) If the value does not appear in the configuration XML file and appears in the structure XML file, the value of the structure XML file is chosen. (case III) If no value appears among the two XML files, the default value ((heatbath per atom)=25 au) is chosen. [3]

3.1.4 For changing interaction range of Hamiltonian

The interaction range of the Hamiltonian is specified by the cluster tag in the system tag as the following manner.

```
<cluster structure="structure.xml" cutoff_radius="10.0d0" />
```

The unit of value will be treated as atomic unit. Furthermore, this cutoff radius is applied to the range of the overlap matrix. It is noted that this setting is applied to systems constructed by GENO type and NRL type Hamiltonian.

3.1.5 For changing the calculation mode

ELSES can carry out mainly 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>
```

[2] S. Nosé, Mol. Phys. **52**, 255 (1984); J. Chem. Phys. **81**, 511 (1984).

[3] The present default value is a recommended one. A proper value should be set. See textbooks of classical (or quantum) molecular dynamics simulation.

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

Other calculation modes are explained in §3.6.

3.1.6 Optimization mode

Calculations condition of the optimization mode are specified in the optimization tag as the following manner.

```
<optimization>
  <sd_ratio> 0.2 </sd_ratio>
  <max_num_iter> 200 </max_num_iter>
  <convergence_criteria mode="energy_per_atom" unit="eV"> 1.0d-5 </convergence_criteria>
</optimization>
```

Iteration ratio of the steepest descent method is specified in sd_ratio tag. The value of the max_num_iter tag represents the maximum number of the optimization step. The convergence criteria of the optimization calculation is optionally specified in the convergence_criteria tag. This criteria is defined by the difference of the total energy from the previous optimization step divided by the total atom number δE (eV). When specification of this tag is omitted, the optimization calculation of the maximum number of the optimization step specified in the max_num_ite tag is carried out.

The energy difference δE at each optimization step is outputted in the output file named Output.txt at default setting as the following way.

```
 SD energy difference per atom [eV]=         0        0.00019272172572821233
```

The first value represents the step count.

3.1.7 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

3.1.8 Setting of the calculation solver

The A type of the generalized Krylov-subspace solver is applied to the calculation of the quantum part for a nonorthogonal basis, namely for the GENO type Hamiltonian and the NRL type Hamiltonian, when the solver tag is set into the calc tag as the following manner.

```
<solver scheme="gKrylov_A">
</solver>
```

Furthermore, it is necessary to set the interaction range of the Hamiltonian(see §3.1.4), in order to perform calculations by using this solver.

The diagonalization solver is applied when the solver tag is omitted or the solver tag is set into the calc tag as the following manner.

```
<solver scheme="eigen">
</solver>
```

3.1.9 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.

The matrix element of the Hamiltonian depends on the charge distribution, so that the loop of the CSC calculation does not finish until the charge distribution converges. Therefore, the large number of the CSC loop makes the calculation time longer.

```
<genoOption>
 <CSC_method> ELSTNER </CSC_method>
 <CSC_max_loop_count> 1000 </CSC_max_loop_count>
 <CSC_charge_convergence>  1d-6 </CSC_charge_convergence>
 <CSC_charge_mixing_ratio> 0.6 </CSC_charge_mixing_ratio>
</genoOption>
```

The tag CSC_charge_convergence specifies a criterion of the charge convergence. The convergence criterion becomes strict, when a smaller value is fixed. The tag CSC_charge_mixing_ratio specifies the charge mixing ratio in the CSC loop. The number of the CSC loop also depends on this value. This value should be larger than 0 and smaller than 1, and the conventional value is from 0.4 to 0.6. It is noted that the charge mixing ratio is automatically adjusted to take account of the behaviour of the charge fluctuation in the CSC loop, while the specified value is treated as the initial value.

The number of the CSC loop can be confirmed by the following manner;

```
prompt> grep CSC (standard output file) | grep converge
```

As a result, the loop number is shown as the following format;

```
INFO:CSC loop is converged:loop num., dq=         9 0.898594E-06
INFO:CSC loop is converged:loop num., dq=         4 0.725716E-06
INFO:CSC loop is converged:loop num., dq=         4 0.247496E-06
INFO:CSC loop is converged:loop num., dq=         4 0.230907E-06
```

This result shows that the number of the CSC loop is nine for the first MD step,and four for the next MD step. The quantity which evaluates the charge convergence is shown below the loop number. This value should be smaller than the value specified in the tag CSC_charge_convergence.

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> 0.6 </CSC_charge_mixing_ratio>
</genoOption>
```

3.1.10 Adjustment of the Wolfsberg-Helmholtz constant K

We can change κ and δ to adjust the Wolfsberg-Helmholtz K in the HML_kappa tag and HML_small_delta tag as the following manner. It is noted that the unit of the δ is Å^{-1}.

```
<genoOption>
 <HML_kappa> 1.00 </HML_kappa>
 <HML_small_delta> 0.35 </HML_small_delta>
</genoOption>
```

The constant K formalism independent of the inter-atomic distance is applied when the HML_constant_K tag is set and the value of K is specified by the HML_K tag as the following manner.

```
<genoOption>
 <HML_constant_K> T </HML_constant_K>
 <HML_K> 1.75 </HML_K>
</genoOption>
```

3.1.11 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, ELSES 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" />
¢^^e2^^84^^a2output file °^^c3^^9fposition.xyz

(2) axsf format for xcrysden and vmd(***)
<position filename="position.axsf" interval="1" />
¢^^e2^^84^^a2output file °^^c3^^9fposition.axsf

(3) xsf format for xcrysden, vesta(**) and vmd(***)
<position filename="position.xsf" interval="1" />
¢^^e2^^84^^a2output 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" />
¢^^e2^^84^^a2output file : MD_step.pdb
(e. g. position0000000000.pdb, position0000000010.pdb, ...)
Note: script file for a batch transaction of rasmol, also, is outputted.
¢^^e2^^84^^a2output 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 °^^e2^^97^^8a¢^^e2^^84^^a2 °÷ 1 °^^e2^^97^^8a)
(***) The visualization of forces is not supported.
```

The information on the unit cell is additionally outputted in the position file into the xyz format when the “cell_info" attribute is specified in the position tag as follow,

```
<position filename="position.xyz" cell_info="on" interval="1" />
```

This function does not put in motion when the attribute is fixed as "off". The cell length Lx, Ly, Lz () are outputted every snapshots in the xyz file as the following format.

```
12       10.00000000000000000000       10.00000000000000000000       10.00000000000000000000
```

3.1.12 Controlling the elapsed simulation time

The simulation is terminated before the total MD (optimization) step set in the configuration file by specifying the “limit" tag in the calc tag. For example, the simulation is terminated after 10 minutes run when the limit tag is specified as bellow,

```
 <limit>
   <time unit="min"> 10 </time>
 </limit>
```

The “unit" attribute accepts the following description.

```
°÷ second °^^e2^^97^^8a °÷ seconds °^^e2^^97^^8a °÷ sec °^^e2^^97^^8a °÷ s °^^e2^^97^^8a: second
°÷ minute °^^e2^^97^^8a °÷ minutes °^^e2^^97^^8a °÷ min °^^e2^^97^^8a °÷ m °^^e2^^97^^8a: minute
°÷ hour °^^e2^^97^^8a °÷ hours °^^e2^^97^^8a °÷ h °^^e2^^97^^8a: hour
°÷ day °^^e2^^97^^8a °÷ days °^^e2^^97^^8a °÷ d °^^e2^^97^^8a: day
```

It is noted that the MD (optimization) calculation is terminated when the elapsed time is over the limit time specified by this tag, and then file outputs carry out. This means that the total elapsed time is longer than the limit time. Therefore, you have to set the limit time shorter than the hard limit.

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, ELSES use the default parameter as is described in ELSES 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 </repulsive_rescaling>
</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. The double-ζ is applied to s- and p-orbitals as well as the case of d-orbital, although single-ζ is used for s- and p-orbitals by omitting the zeta2, c1, and c2 tag.

3.2.1 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 ELSES 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>
```

3.2.2 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 ζ 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>
```

3.2.3 For changing the repulsive rescaling factor

The parameter ζ^{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 ζ^{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. It is noted that only ζ_2 is rescaled by the factor in a case of d-orbitals.

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

3.2.4 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>
```

3.3 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 ELSES 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 bin/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>
```

3.4 Adjustment of the structure file

The structure file of H_2O 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.">  0.250000000000000E+02</massperatom>
  <position unit="a.u.">  0.000000000000000E+00   </position>
  <velocity unit="a.u.">  0.000000000000000E+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 Setting of unit cell

The size of the unit cell is fixed by the unit cell tag. In this tag, you can set arbitrary length unit by using myLength option as the following example. In this case, the value specified in the myLength tag is treated as the unit length. The unit of myLength has to be specified by the atomic unit or the angstrom. If the description of the unit is omitted, the length unit is treated as the atomic unit.

```
<unitcell>
  <myLength unit="a.u.">  0.410342853147435E+02   </myLength>
  <vector unit="myLength">  1.0d0  0.000000000000000E+00  0.000000000000000E+00   </vector>
  <vector unit="myLength">  0.000000000000000E+00  1.0d0 0.000000000000000E+00    </vector>
  <vector unit="myLength">  0.000000000000000E+00  0.000000000000000E+00  1.0d0   </vector>
</unitcell>
```

3.4.2 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>
```

3.4.3 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.

3.4.4 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 bin/elses-xml-generate.

3.5.1 Preparation of the XYZ-formatted file

A XYZ-formatted file of a molecule which will be calculated by ELSES 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. Although any comments can be written on the second line in this xyz-formatted file, the error may occur if the line is in blank.

```
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, bin/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.

3.6 Various calculation modes

Various calculation modes introduced in §3.1.5 are implemented in ELSES, in addition to the optimization mode and the dynamics mode. This subsection is devoted to the explanation of the various calculation mode.

3.6.1 File conversion mode

Only conversion of the structure file format from the XML format to other formats is carried out in the file conversion mode. After reading the input file, the position file whose format is specified in the position tag in the configuration file and the restart file of the XML format are generated without any electronic structure calculations, when the file conversion mode is specified as "file_conversion" or "conversion" in the mode attribute of the calc tag in the configuration file by the following way.

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

This mode is also useful to inspect syntax of input files as a configuration file and a structure file, because this mode use the subroutine which reads input files.

3.6.2 Cell change only mode

This mode changes only cell length (AX, AY, AZ) to perform the calculations with varying volume. In the calculation by this mode, atom positions in the structure XML file are read as normalized positions. At this time, absolute values of the cell length are determined from the supplement file explained below. The physical meaning of this calculation for a non-periodic system corresponds to change of scale length. This mode in the current ELSES supports to only orthogonal cell vectors.

The cell change only mode is performed by specifying the mode atributte of the calc tag in the configuration XML file as the following manner.

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

In addition, setting the cell_change tag by the following manner needs to read the supplement file.

```
<cell_change scheme="from_file" filename="input_cell_change.txt">
   <max_num_iter> 10 </max_num_iter>
</cell_change>
```

Here, the value of the max_num_iter attribute represents the iteration number of varying cell length. The format of supplement file (an example, input_cell_change.txt) is below.

```
51.136009312574d0  88.5526014925063d0 94.486343888717 8d0
 0   0.8   0.8    0.8
 1   0.85  0.85   0.85
 2   0.9   0.9    0.9
 3   0.95  0.95   0.95
 4   1.0   1.0    1.0
 5   1.1   1.1    1.1
 6   1.2   1.2    1.2
 7   1.3   1.3    1.3
 8   1.4   1.4    1.4
 9   1.5   1.5    1.5
10   1.6   1.6    1.6
```

The values at the first line represent reference values of cell lengths. These values have to be specified by the atomic unit. Four values at other lines represent the step count, the scale value of AX, the scale value of AY, and the scale value of AZ, respectively. It is noted that the step count begins at zero, and the scale value means that the normalized cell length is scaled by these. In the case of step count=0, values of AX, AY and AZ are fixed by multiplying the reference value by 0.8, namely, AX = 51.136009312574×0.8 a.u. If the step count called by this mode is not described in the supplement file, the scaled values at the previous step count are used. On one hand, if max_num_iter is smaller than the maximum step count described in the supplement file, step counts after the max_num_iter are ignored. On the other hand, if the max_num_iter is larger than the maximum step count, the value at the final step count is used after the final step count. For an example, in the above case (max_num_iter=10), lines for step count=0, 1, 2, $\cdots$, 9 are read and a line for step count=10 is ignored in the supplement file. If the value of the max_num_iter tag is specified larger than the maximum step count described in the supplement file, for an example, mux_num_iter=100 in the above case, the cell length fixed at step count=10 is used in calculations after step count=11, so that these calculations are no physical meaning.

The result of the cell change only mode can be confirmed by the following way, as an example;

```
> grep Energy Output.txt | grep summary | grep eV
 Energy summary (eV/atom):             0      -66.97559540
 Energy summary (eV/atom):             1      -70.63700976
 Energy summary (eV/atom):             2      -72.74055923
 Energy summary (eV/atom):             3      -73.80520398
 Energy summary (eV/atom):             4      -74.19291064
 Energy summary (eV/atom):             5      -73.74131018
 Energy summary (eV/atom):             6      -72.47607900
 Energy summary (eV/atom):             7      -70.96731433
 Energy summary (eV/atom):             8      -69.56988810
 Energy summary (eV/atom):             9      -68.50967860
```

In this case, the configuration at step count=4, namely all scale values are one, is most stable in these calculations with varying cell lengths.

4 Output file -Option-

ELSES optionally output the density of states and an intermediate file for visualizing wave functions.

4.1 Output of DOS and eigen levels

The density of states is outputted when a file "input_energy_mesh.txt" exists in the current directory. Calculation conditions for the DOS, such as the energy range, should be described in this file as the following format.

```
an example of input_energy_mesh.txt °^^c2^^a0comments is also written after #) °^^c3^^9f
1        # Mode ( 0 for nothing, 1 for TDOS)
6000     # Number of the energy mesh points
-40      # Lowest energy mesh point in eV
110      # Highest energy mesh point in eV
0.1      # Level broadening parameters in eV
```

When Mode=1 is chosen, the following files include the DOS and eigen levels are outputted.

- output_dos.txt : total DOS
- output_eigen_levels.txt : Eigen energy

The DOS is outputted in output_dos.txt as the following format.

```
tdos=      0      -50.0000000000         0.0000000000         0.0000000000         0.0000000000
```

An index of an energy point, the DOS(1/eV), the NOS, the energy NOS (eV) are in line. The eigen levels are listed in output_eigen_levels.txt as the following format.

```
         1      -30.3114648255         1.0000000000
```

Three successive values represent an index of an energy level k, an eigen energy ε_k(eV), an occupation number $f_k (0 \leq f_k \leq 1)$, respectively. It is noted that this function is available for the diagonalization solver for the GENO type Hamiltonian, up to now.

4.2 Output of an intermediate file for visualizing wave functions

The intermediate file for visualizing wave functions is outputted when the wavefunction tag is added into the output tag in the configuration file as the following format. The utility elses-generate-cubefile (see §6.3) reads this intermediate file to generate the Gaussian Cube file.

```
<output>
 <wavefunction filename="output_wavefunction.txt" />
</output>
```

This file is outputted at the final MD step. While there is no restriction of the file name, you had better set the file name to "output_wavefunction.txt", because elses-generate-cubefile reads the input file of that name. It is noted that this function is available tor the diagonalization solver for the GENO type Hamiltonian, up to now.

4.3 Output of electron number

The valence electron number of each atom is outputted in a file for a certain interval, when the output_atom_charge tag is added into the output tag in the configuration file as the following format. The interval, frequency for saving this data, and the file name are specified by the interval attribute and the filename attribute of the same tag, respectively.

```
<output>
<atom_charge filename="output_atom_charge.txt" interval="2" />
</output>
```

After the number of atoms and the number of MD steps, the data on the electron number are described in the outputted file. In the case which the system includes s orbitals and p orbitals, the data are represented in order of the atom index, the symbol of an element, the initial valence electron number (n_ini), the difference between the valence electron number and n_ini, the s orbital electron number, the p orbital electron number, the electron number of each p orbital, and the number of atoms which are in the interaction range of the Hamiltonian, as the following format.

```
ex. the result of sample/C6H6
         12
 mdstep=           0
   1     C   4.00000   0.0146392611   1.16593   2.84871   0.92298 °°0.92573   1.00000         12
   2     C   4.00000   0.0146410769   1.16593   2.84871   0.92504 °°0.92367   1.00000         12
   3     C   4.00000   0.0146380523   1.16593   2.84871   0.92504 °°0.92367   1.00000         12
   4     C   4.00000   0.0146392611   1.16593   2.84871   0.92298 °°0.92573   1.00000         12
   5     C   4.00000   0.0146410769   1.16593   2.84871   0.92504 °°0.92367   1.00000         12
   6     C   4.00000   0.0146380523   1.16593   2.84871   0.92504 °°0.92367   1.00000         12
   7     H   1.00000  -0.0146392814   0.98536   0.00000   0.00000 °°0.00000   0.00000         12
   8     H   1.00000  -0.0146408406   0.98536   0.00000   0.00000 °°0.00000   0.00000         12
   9     H   1.00000  -0.0146382684   0.98536   0.00000   0.00000 °°0.00000   0.00000         12
  10     H   1.00000  -0.0146392814   0.98536   0.00000   0.00000 °°0.00000   0.00000         12
  11     H   1.00000  -0.0146408406   0.98536   0.00000   0.00000 °°0.00000   0.00000         12
  12     H   1.00000  -0.0146382684   0.98536   0.00000   0.00000 °°0.00000   0.00000         12
```

Furthermore, the maximum value and the minimum value of n-n_ini are shown in the standard output, as the following format. The numbers represent the number of MD steps, the index of the atom which consists of the maximum (minimum) n-n_ini, the difference between the electron number (n) and the initial electron number (n-n_ini).

```
INFO:Max of elec_num ( n - n_ini )=         0         5   0.01464
INFO:Min of elec_num ( n - n_ini )=         0         8  -0.01464
```

5 Visualization of MD calculations

In this section, we briefly explain how to visualize the result of MD calculation using free software. ELSES 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 §3.1.11 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)

5.1 Batch transaction by rasmol

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

5.1.1 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.

5.1.2 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

5.1.3 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.

5.1.4 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.

6 Utility tool

ELSES package includes some utility tools. This section is devoted to brief explanation of these tools. It is noted that the tool "mkSupercell.pl" requires the perl and libXML module for the perl. Please refer to appropriate documentations for installing these.

6.1 mkSupercell

The utility mkSupercell (/bin/Perl/mksupercell.pl) generates a structure file of a certain supercell for ELSES from an unit cell file and a supercell file. The unit cell file includes the definition of the unit cell, and the supercell file includes the definition of the translational vector.

The format of the unit cell file (unitcell.xml) is shown below. The size of the unit cell, atom species, and positions of these atoms are specified in the unitcell tag as the following manner.

```
<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>

<atom element="O" class="" motion="free">
<position unit="angstrom">  0.000000000   0.0000000000  0.00000000 </position>
</atom>

<atom element="H" class="" motion="free">
<position unit="angstrom">  0.584410971   0.761619206  0.00000000 </position>
</atom>

<atom element="H" class="" motion="free">
<position unit="angstrom">  0.584410971  -0.761619206  0.00000000 </position>
</atom>

</unitcell>
```

The format of the supercell file (supercell.xml) is shown below. The information of the heat bath is specified in the heatbath tag, and the translation vector is specified in the unitcell tag. These tags are included in the structure tag.

```
<structure>

 <heatbath>
  <massperatom unit="a.u.">  0.250000000000000E+02</massperatom>
  <position unit="a.u.">  0.000000000000000E+00   </position>
  <velocity unit="a.u.">  0.000000000000000E+00   </velocity>
 </heatbath>

 <unitcell>
   <vector unit="angstrom">  50.0   0.0   0.0 </vector>
   <vector unit="angstrom">   0.0  50.0   0.0 </vector>
   <vector unit="angstrom">   0.0   0.0  50.0 </vector>
 </unitcell>

 </structure>
```

The structure file of the supercell (supercell_new.xml) is generated by executing the mkSupercell utility from two files of unitcell.xml and supercell.xml as the following manner.

```
prompt> mksuperecell.pl unitcell.xml supercell.xml
```

6.2 band

The utility band(`/bin/band`) calculates a band structure from following input files.

- ForBandCalc.txt: Structure data
- OverlapAndHamiltonian.txt: Matrix elements of the Hamiltonian and the overlap
- SymLine.txt: Symmetric line data

ForBandCalc.txt can be generated by the utility mkSupercell.pl (see §6.1).

The file SymLine.txt should include the number of symmetric lines and number of data points as the following format (some comments are also described after #).

```
 # number of symmetric lines
   6
# number of points between b_start and b_end, b_start(x,y,z), b_end(x,y,z)
# all fist and last points of symmetric lines should be given in a unit of 2*pi/aLat
# where aLat=|a_1| (a_i are the translation vectors of Bravais lattice (a.u.)
 40   0.5    0.5    0.5    0.0    0.0    0.0       #L-G
 40   0.0    0.0    0.0    0.0    1.0    0.0       #G-X
 20   0.0    1.0    0.0    0.5    1.0    0.0       #X-W
 30   0.5    1.0    0.0    0.5    0.5    0.5       #W-L
 20   0.5    0.5    0.5    0.0    0.75   0.75      #L-K
 40   0.0    0.75   0.75   0.0    0.0    0.0       #K-G
```

First, you have to prepare two files (ForBandCalc.txt and supercell_new.xml) by using the utility mkSupercell.pl (see §6.1). After that, please execute ELSES with the config file where the supercell_new.xml file is specified in the cluster tag. The file OverlapAndHamiltonian.txt is outputted by executing ELSES with band option as the following manner.

```
prompt> elses -band config.xml
```

After preparing these files in the current directory, the band calculation is performed by using the utility band as the following manner.

```
prompt> /bin/band/src/band
```

As a result, the band structure is outputted in the file “EigenEnergy.txt" as the following format.

```
# kx ky kz K E1 E2 E3 ...

horizontal axis K
vertical axis E1, E2, E3,... in eV-unit
```

Sample files for the diamond structure are placed in the following directory.

```
/bin/band/sample/
```

6.3 elses-generate-cubefile

The utility ‘elses-generate-cubefile’ (/bin/elses-generate-cubefile) generates Gaussian Cube files for visualizing wave functions. This utility reads the intermediate file explained in §4.2. This utility is executed as the following way.

```
prompt> elses-generate-cubefile N1 N2
```

When two arguments (N1 and N2) are inputted, wave functions from N1-th to N2-th are outputted. The outputted file is named “eigen_state_000003", for an example. When one argument is inputted at this time, only N1-th eigen state is outputted.

```
prompt> elses-generate-cubefile N1
```

If there is no argument, all eigen states are outputted.

```
prompt> elses-generate-cubefile
```

In addition, the mesh grid of the Gaussian Cube file can be changed by the input file “input_mesh_grid.txt". The number of mesh points for x, y and z directions is described on the first line in this input file.

```
60 70 80   # Mesh points in the x,y,z directions
```

If the input file does not exist, the number of the mesh point is set to 80 for all directions.

6.4 elses-dos

The utility “elses-dos" calculates the DOS from energy levels in the input file “levels.txt". The utility also needs the another file (input_energy_mesh.txt) where calculation conditions are described. The format of this file is same as the file explained in §4.1.

It is necessary to input total number of levels N when this utility is executed, so that you had better confirm it.

```
prompt> elses-dos
Input # of levels
```

An outputted file is named “output_tdos.txt". Up to now, elses-dos can read only the Gaussian output format. This utility searches the word “Orbital energy" first, and then reads energy levels described below the word. Therefore, please edit the input file (levels.txt) appropriately.

6.5 msd

The utility “msd" (/bin/msd) calculates the mean-squared displacement (MSD) averaged over all atoms from two input files of the position file (position.xyz) and the configuration file (input_msd.txt). This utility is executed by the following command, when the input files exist.

```
prompt>msd
```

The configuration file has to be described as below.

```
240     # natom: total number of atoms
10000   # total_md_step: total number of MD steps
500     # tmax: number of MD steps used for MSD
10      # it0: sampling interval
500     # t0max: number of initial positions to be stored
10.0    # dt: time interval of MD step [fs]
```

These values have to correspond to the information on the position file, e. g. in the case of a MD simulation of 1000 steps with the interval of 1fs and the atom position is outputted at every 10fs, namely the number of times it is outputted is 1000, total_md_step and dt are set to be 1000 and 10, respectively. In addition, the inequality it0$\times$t0max $>$ tmax has to be satisfied.

6.6 xyz2xml.pl

The utility “xyz2xml.pl" (/bin/Perl/xyz2xml.pl) extracts a certain snapshot from the position file “position.xyz" outputted through a simulation and makes the structure file named “restart_new.xml". This utility requires two input files of the position file (position.xyz) and the restart file (restart.xml). The N-th snapshot is extracted and the structure file of the snapshot is made by the following manner.

```
prompt> xyz2xml.pl position.xyz restart.xml N
```

It is noted that the final snapshot is extracted when the argument N is omitted.

6.7 xyz2xyz.pl

The utility “xyz2xyz.pl" (/bin/Perl/xyz2xyz.pl) converts the position file (position.xyz) into the new position file (position_new.xyz) where atom positions are reduced into the unit cell specified in the structure file. This utility is executed by specifying two files of the structure file (structure.xml) and the position file (position.xyz) as the following manner.

```
prompt> xyz2xyz.pl structure.xml position.xyz
```

6.8 xml-check

The utility “xml-check" helps us find spelling mistakes in tag names in a configuration file (config.xml) and a structure file (structure.xml) by the following manner.

```
prompt> xml-check filename
```

Two example results are shown below.

- case A (sample/C6H6/config.xml) °Ã§

```
XML tag checker
scanned file name=config.xml
---------------Tag check starts--------------------
tag starts:config tag starts:system tag starts:cluster
...
tag ends:position
tag ends:outputm
tag ends:config
---------------Tag check ends--------------------
scanned file name=config.xml
RESULT: OK !
```

- case B(a spelling mistake is made in optimization tag in sample/C6H6/config.xml)

```
XML tag checker
scanned file name=config.xml
---------------Tag check starts--------------------
tag starts:config tag starts:system tag starts:cluster
...
unknown tag=optimisation
...
tag ends:outputm
tag ends:config
---------------Tag check ends--------------------
scanned file name=config.xml
RESULT:ERROR:unknown tag is found!
```

All tags included in this quick start are registered in the utility. However, the xml-check may show “unknown tag" for some tags which are experimentally implemented. You had better carry out also other method to check the syntax, before using the xml-check, by following methods;

- drag the xml file onto a certain web browser
- using the UNIX command xmllint (see §8.2)

It is noted that the xml-check is not omnipotent, so that some kinds of error are not found by the tool. Furthermore, a calculation is possibly executed even in the case we prepare a incorrect input files. Therefore, we recommend checking syntax error by the above method. Some kinds of xml error are shown below, and ELSES can not detect the error (b)-(d).

(a) syntax error
°°correct °Ã§ <calc></calc>
°°incorrect °Ã§ <calc></kalc> (The end of the tag is inconsistent with the top of it.)
°°correct °Ã§ <calc><solver></solver></calc>
°°incorrect °Ã§ <calc><solver></calc> (The tab is not closed)
→ The syntax check described above can detect this type of error, and ELSES also possibly detect it.

(b) spelling mistake of a tag name
°°correct °Ã§<calc></calc>
°°incorrect °Ã§<kalc></kalc> (a spelling mistake of tag name calc)
→ The xml-check can detect this type of error.

(c) incorrect tag class
°°correct °Ã§<calc><solver></solver></calc>
incorrect °Ã§<calc></calc><solver></solver> (The solver tag has to be in the calc tag)
→ The xml-check detects part of this error.

(d) incorrect attribute
°°correct °Ã§ <A unit="a.u."></A>
°°incorrect: <A vnit="a.u."></A> (a spelling mistake of the attribute name)
→ No way to detect this error so far.

7 Important updates

This section lists important updates at each version, in particular, specification changes without the backward compatibility.

7.1 v0.03.10

Executive files (mainly of tool) as are listed below move in the directory bin (/bin).

```
tool/elses-xml-generatenrl-param
tool/elses-xml-generate
tool/Perl/mksupercell.pl
tool/band/src/band
tool/plot eigenstates/src/elses-generate-cubefile
tool/DOS/elses-dos
tool/Perl/xyz2xml.pl
tool/Perl/xyz2xyz.pl
```

7.2 v0.03.12

Information displayed on the standard output by the way (elses > log.txt) in the previous version of ELSES is outputted into the log file named log-node00000.txt. This file name is fixed in the current package. This kind of change will be successively carried out without announcement, and finally, only specific information such as error messages will be outputted into the log file.

7.3 v0.03.13

Default solver of the quantum part for the non-orthogonal basis model (GENO, NRL) and the orthogonal basis model (others) is set to eigen, while it is eigen for the non-orthogonal model and is krylov for the orthogonal model in the previous version of ELSES. In addition to this change, the solver tag is added into the config file for the orthogonal model in sample files as the following.

```
<solver scheme="krylov">  </solver>
```

7.4 v0.03.15

The sample directory (`/sample/`) is reorganized. The sample data without GENO systems are moved into a subdirectory (`/sample/sample_non_geno/`).

7.5 v0.03.16

The sample directory (`/sample/`) is reorganized, as follows;

```
/sample/sample_geno/
/sample/sample_geno_mpi/
/sample/sample_non_geno/
/sample/shell_script/
```

The subdirectories contain samples with GENO system, samples of GENO system for MPI calculation, samples of non-GENO system, related shell scripts.

7.6 v0.07.00

We modified slightly how to build ELSES. See Sec.1.

8 Trouble shooting

8.1 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
```

8.2 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
```

8.3 Execution error: alloc. error

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

8.4 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 ELSES 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 you had better upgrade your compiler to a more recent version, you will possibly complete the compile procedure by repeating the make.

8.5 Setting error in double-ζ parameters

The parameters, zeta1, zeta2, c1 and c2, which determine the functional form of double-ζ function are not independent variables, and these have to satisfy the normalization condition of the basis function. The error message as the following is displayed and the calculation is going to halt, when the normalization condition is not satisfied.

```
c1,c2=  7.23130306240707E-01  6.00000000000000E-01
z1,z2=  2.12500000000000E+00  2.50000000000000E+01
sqrt(z1.z2)     =  9.60113094396169E-01
Suggested c1,c2 =  7.53172006986839E-01  6.24926379508812E-01
ERROR:Please correct the element XML file for the double-zeta parameters
renormalizeDoubleZeta in SetAtomParameters: erroneous normalization of double zeta
```

The suggested values of c1 and c2 satisfy the normalization condition with keeping the ratio c1/c2 as is set before, so that the calculation by using these values is executable.

The details how to set up the double-ζ parameters proposed in the manuscript (Cerdä and Soria, Physical Review **B 61**, 7965 (2000)) are explained below, for an example. The Wolfsberg-Helmholtz constant K is fixed to constant in their modelling and the double-ζ function is adopted. Although parameters of ζ_1, ζ_2, c1, and c2 are listed in Table

I, some parameters of strongly localized basis are not shown in the manuscript. They explain that the value of ζ is omitted in the case of ζ >20, because the larger value of ζ does not affect results. While we confirmed this fact, all parameters of the double-ζ function have to be specified as these satisfy the normalization condition for executing ELSES.

For an example, the manner how to set up the double-ζ parameter in the case of the 2s orbital on the C atom is explained below. In the manuscript, although values of ζ_1 and c1 are listed as ζ_1=2.125 and c1=0.790, values of ζ_2 and c2 are not shown. This does not indicate that ζ_2 and c2 are fixed to zero, since c1 will have to be one if c2 is zero due to the normalization condition. It should be mentioned that the calculation by single-ζ function is carried out when the double-ζ parameter c2 is fixed to zero in an element file. Therefore, we make up some parameters such as ζ2 and c2 ourselves, in order to perform the calculation by using the parameter set listed in the manuscript. We had better execute a trial by setting up as ζ_2=25 and c2=0.72, for example, to find appropriate values of parameters. In the calculation, ELSES suggests appropriate values of c1 and c2 as described above, so that we can perform the calculation by using the suggested double-ζ parameter.