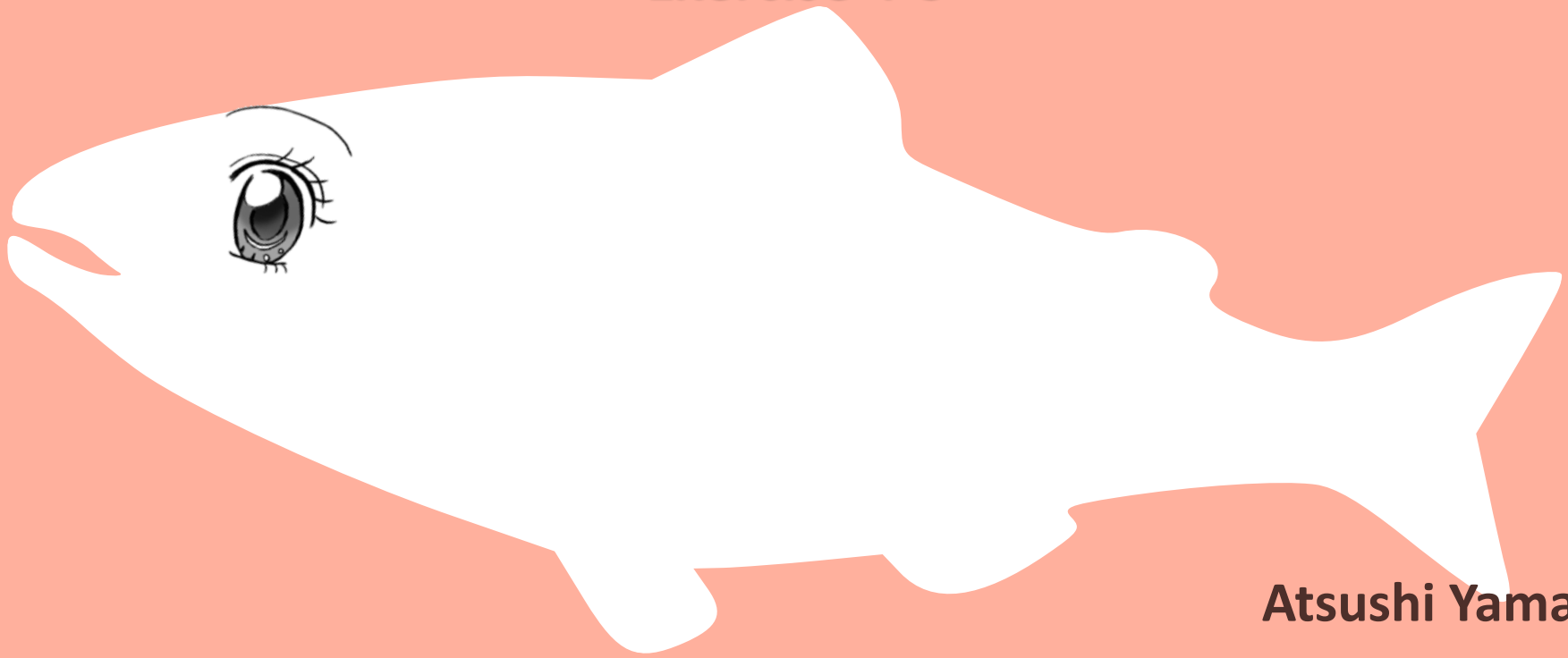
How to Use SALMON: Geometry Optimization and Molecular Dynamics (MD)

Exercise 4-3



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Available Functions

(Trial version now, only for periodic system)

- Geometry Optimization (Conjugated Gradient method)
  (MPI parallelization is not supported (single node only))
- Molecular Dynamics (MD)
  - Type of MD
    - Adiabatic ground-state MD
    - Nonadiabatic Ehrenfest MD (mean-field approximation)

    (surface-hopping, excited state MD are not available)
  - Ensemble
    - NVT (Nose-Hoover thermostat, Velocity scaling)
    - NVE

Note that these functions are currently available only for periodic systems and trial version

Menu of Exercise

Menu of the exercise

Calculations of single water molecule
(with periodic boundary condition at gamma-point) :

1. Geometry Optimization

- Input Files ---- in exercise4-3_md/1_H2O_opt/
  (H2O_opt.inp, O_rps.dat, H_rps.dat, k1x1x1.dat)

2. Ehrenfest MD simulation

- Input Files ---- in exercise4-3_md/2_H2O_md/
  (H2O_md.inp, O_rps.dat, H_rps.dat, k1x1x1.dat)

1. Geometry Optimization (Job Submission)

This example performs geometrical optimization of single water molecule
(periodic boundary condition with gamma-point ; just test system)

Prepare files →

```
%> ls
H2O_opt.inp  H_rps.dat  k1x1x1.dat  O_rps.dat
```

Check following input files in the same directory

- `H2O_opt.inp` (input file)
- `H_rps.dat`, `O_rps.dat` (PS potential data)
- k1x1x1.dat (read-in k-point data (Γ-point))

Submit job →

```
%> (job submit command)
```

Calculation of Geometrical Optimization (Input File)

Important input keywords for optimization in Example input file

```
&calculation
  calc_mode = 'GS'
  use_geometry_opt = 'y'
/
```

Optimization option in combination with GS mode

```
&opt
  convrg_opt_fmax  = 1d-3
/
```

Convergence threshold of optimization (Maximum Force) [a.u.]

```
&atomic_coor
'H'   3.5   2.5   2.5   1 y
'H'   2.5   3.5   2.5   1 y
'O'   2.5   2.5   2.5   2 y
/
```

Put "y" for the atoms to be optimized.
(but in the current version, all atoms must have 'y')

Note:

- Algorism to find the structure with force=0 is used (not energy minimization algorism)
- If you choose a functional of inaccurate force calculation, the optimization will not converge.
- option to read the pre-calculated ground state orbitals (gs_wfn_k/) as initial guess is available using read_gs_wfn_k='y'
- The threshold of ground state SCF in the optimization iteration is from &scf block. If this is tight, the optimization calculation takes long time. Additional threshold of ground state SCF is available specifying in &opt block.

Calculation of Geometrical Optimization (Output File, Check of Result, Restart)

Important Output Files

- `out.log` --- standard log (Here, just example name: the file name given in the job script file)
- `H2O_trj.xyz` --- atomic coordinates at each optimization step [Å]

Checks of Output Files

Maximum Force

```
%> grep Fmax out.log
```

```
%> grep Fmax out.log
   Convergence threshold of Fmax   =  1.0000000E-03
 step=(perp=  0, line=  0)  Fmax= 0.2361E+00  Fave= 0.2135E+00  E= -0.16761049E+02  dE-perp=  0.0000E+00
 step=(perp=  1, line=  1)  Fmax= 0.2228E-01  Fave= 0.2206E-01  E= -0.16797253E+02  dE-perp= -0.3620E-01
 step=(perp=  2, line=  1)  Fmax= 0.4918E-02  Fave= 0.4593E-02  E= -0.16822598E+02  dE-perp= -0.2535E-01
 step=(perp=  3, line=  1)  Fmax= 0.8861E-03  Fave= 0.8109E-03  E= -0.16822264E+02  dE-perp=  0.3347E-03
```

converged maximum force

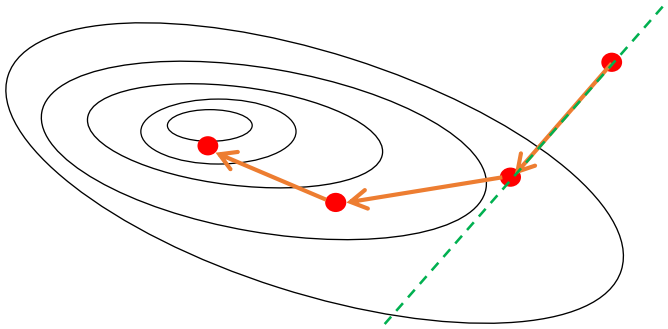
Total energy at each main optimization step

Convergence

```
%> tail out.log
```

```
 ================================================

  Optimization Converged
     Iteration step=    3
     Force(maximum)=  0.8860836326E-03 [a.u.]
     Force(average)=  0.8108601090E-03 [a.u.]
     Total Energy  = -0.1682226358E+02 [a.u.]
  ================================================
```



Restart

Copy the atomic coordinate at the last step printed in H2O_trj.xyz and paste into &atomic_coor in the next input file, and run

2. Ehrenfest Molecular Dynamics (Job Submission)

This example performs Ehrenfest molecular dynamics simulation of single water molecule using the optimized structure in the previous step
(but in this tutorial, the optimized coordinates are already given in the input file by a shortcut.)

The room temperature is given as initial condition.
The electric field is not applied now, but of course external field is available!

Prepare files →

```
%> ls
H2O_md.inp  H_rps.dat  k1x1x1.dat  O_rps.dat
```

Check following input files in the same directory

- `H2O_md.inp` (input file)
- `H_rps.dat`, `O_rps.dat` (PS potential data)
- k1x1x1.dat (read-in k-point data (Γ-point))

Submit job →

```
%> (job submit command)
```

Calculation of Ehrenfest MD (Input File)

Important input keywords for Ehrenfest MD in Example input file

```
&calculation
  calc_mode = 'GS_RT'
  use_ehrenfest_md = 'y'
/
```

Ehrenfest MD option in combination with RT mode

```
&md
  ensemble = "NVE"
  set_ini_velocity='y'
  temperature0_ion = 300.0d0
  step_update_ps=      50
  step_update_ps2=     200
/
```

Ensemble: NVE is corresponding to energy conservation condition, without temperature controller

Set initial velocity (give temperature at t=0)

Setting temperature [K].
temperature at t=0 as initial velocity in this case

Time step interval to update pseudopotential:
step_update_ps → interval of fully updating
step_update_ps2 → interval of update without re-allocation
(Note: calculation gets slower if the interval is small)

```
&atomic_coor
'H'    3.6867868204    2.3313961921    2.4999999893  1
'H'    2.3313961246    3.6867870709    2.4999999912  1
'O'    2.5139878343    2.5139878474    2.5000000182  2
/
```

Atomic coordinate. Usually in MD calculation, optimized structure is used.

Calculation of Ehrenfest MD (Output File, Check of Results, Restart)

Important Output Files

- `H2O_trj.xyz` --- Atomic coordinates [Å], velocity [a.u.] and force [a.u.] at each time step
- `H2O_rt.data`
- `H2O_rt_energy.data`

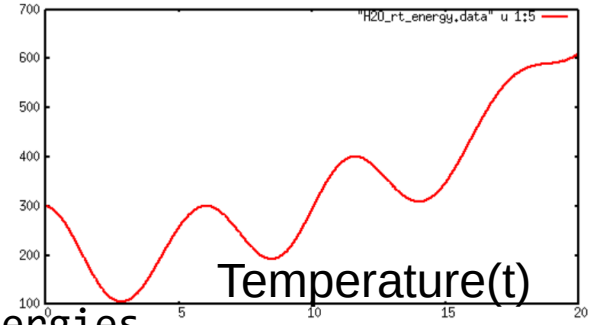
Checks of Output Files

- Animation:
  animation can be made by using visualization software such as VMD reading H2O_trj.xyz
  (but not in the tutorial menu)
- `Plot of temperature.`

(Smaller grid spacing is necessary to get appropriate results.)

```
%> gnuplot
```

```
gnuplot> p “H2O_rt_energy.data” u 1:5 w l
```

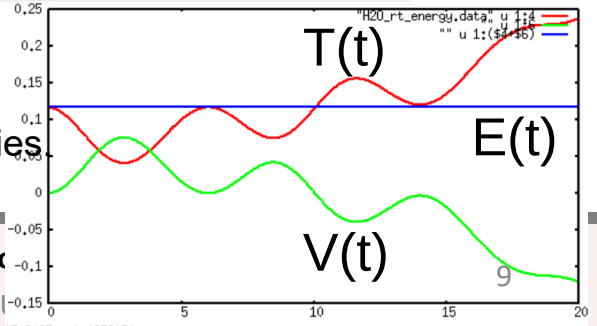


- `Plot of kinetic, potential(electrons), and total energies.`

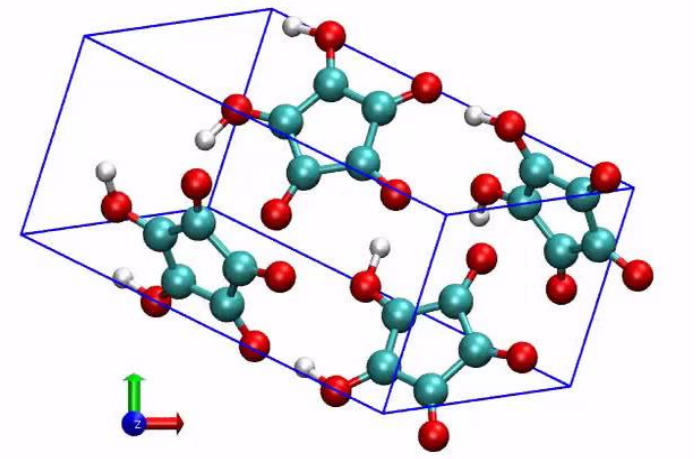
```
gnuplot> p “H2O_rt_energy.data” u 1:4 w l, “” u 1:6 w l, “” u 1:($4+$6) w l
```

Restart

(1) use “write_rt_wfn_k=‘y’” in the first run,
(2) copy or link the printed directory “rt_wfn_k” from the first to next directories,
(3) use “read_rt_wfn_k=‘y’” in the next run



Example of adiabatic GS-MD

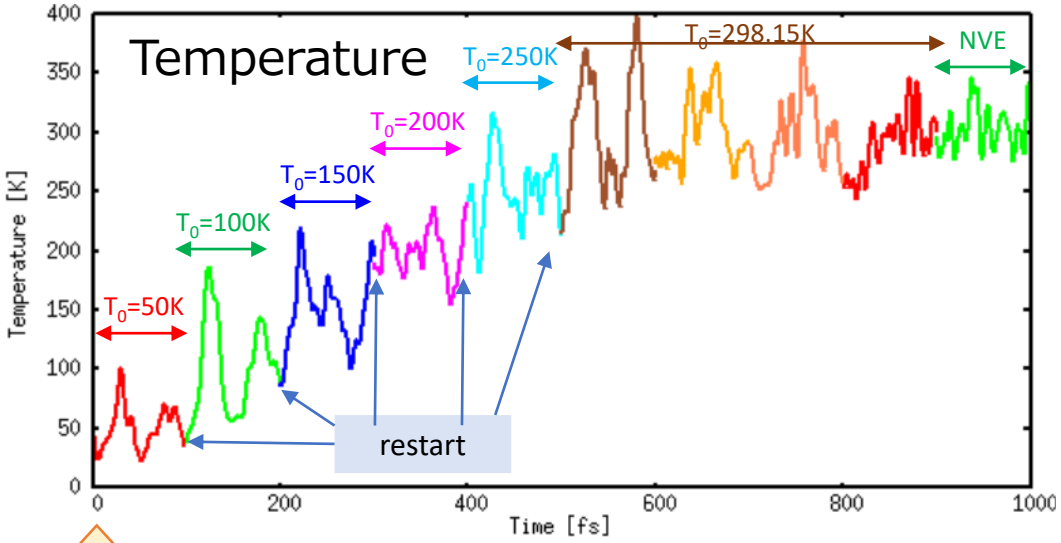


Input keywords (example)

```
&calculation
   calc_mode='GS'
   use_adiabatic_md='y'
/
```

```
&md
   ensemble='NVT'
   thermostat='nose-hoover'
   thermostat_tau=100
   temperature0_ion = 298.15
   set_ini_velocity='r'
   file_ini_velocity="ini_vel.dat"
   stop_system_momt ='y'
/
```

Equilibration process by adiabatic ground-state MD (Δt=0.5fs)



Start from optimized structure