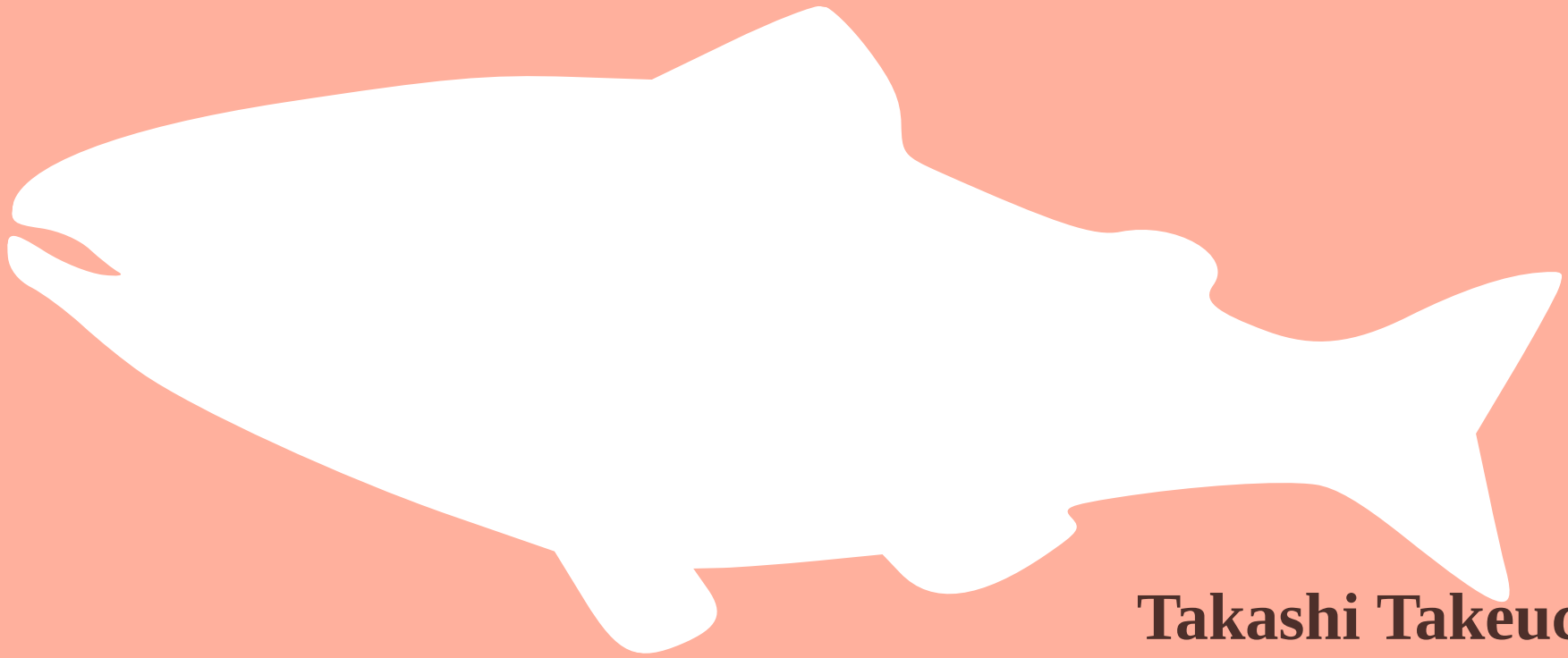
How to Use SALMON -Isolated Systems

Exercise-2



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Demonstration for C_2H_2

- **Linear response calculation**:
  - Ground state calculation → C2H2_gs.inp
  - Real-time TDDFT → C2H2_rt_response.inp

- **Pulse response calculation**:
  - Ground state calculation → C2H2_gs.inp
  - Real-time TDDFT → C2H2_rt_pulse.inp

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- **Pulse response calculation**:
  - Ground state calculation → C2H2_gs.inp
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Input keywords in C2H2_gs.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- &rgrid /
- &scf /
- &functional /
- &atomic_coor /

Basic rules for an input file

```
&category
keyword = xxx
/
```

- The input file consists of categories and keywords with an input value and equal sign(=).
- A character input value requires single quotation marks (‘ ’).
- A real number input value can be written in Fortran style. → e.g. `1.0d-5`
- “ ! ” is used as commented out.
- Space free.
- “&atomic_coor” / “&atomic_red_coor” has to be put at the last part in the input.
- All keywords are described in the SALMON manual.

Input keywords in C2H2_gs.inp

- **&units /** 
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- &control /
- &system /
- &pseudo /
- &rgrid /
- &scf /
- &functional /
- &atomic_coor /

unit_system = 'A_eV_fs'
→ Unit system by Å, eV, and fs.
(Default is atomic unit system.)

Input keywords in C2H2_gs.inp

- &units /
- **&calculation /** ⇨
- &control /
- &system /
- &pseudo /
- &rgrid /
- &scf /
- &functional /
- &atomic_coor /

calc_mode = 'GS'
→ Ground state calculation.

Input keywords in C2H2_gs.inp

- &units /
- &calculation /
- **&control /** ⇒
- &system /
- &pseudo /
- &rgrid /
- &scf /
- &functional /
- &atomic_coor /

sysname = 'C2H2'
→ Session name of output files.
→ This is used for a prefix of output files.

Input keywords in C2H2_gs.inp

- &units /
- &calculation /
- &control /
- **&system /** ⟹
- &pseudo /
- &rgrid /
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- &functional /
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iperiodic = 0
→ Number of directions to apply periodic boundary condition.
→ 0 is for isolated systems.

al = 16d0, 16d0, 16d0
→ Side lengths (x,y,z) of system domain.

nstate = 5
→ Number of orbitals.

nelem = 2
→ Number of atomic elements (species).

natom = 4
→ Number of atoms.

nelec = 10
→ Number of valence electrons.

Input keywords in C2H2_gs.inp

- &units /
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- &control /
- &system /
- **&pseudo /** ⟹
- &rgrid /
- &scf /
- &functional /

izatom(1) = 6, izatom(2) = 1
→ Atomic number of each atomic element.

pseudo_file(1) = 'C.cpi', pseudo_file(2) = 'H.cpi'
→ Name of pseudopotential files.

lmax_ps(1) = 1, lmax_ps(2) = 0
→ Maximum angular momentum of pseudopotential projectors.

lloc_ps (1) = 1, lloc_ps(2) = 0
→ Angular momentum of pseudopotential that will be treated as local.

- $V_{ion} = V_{local} + \sum_{lm} \frac{|\psi_{lm}^{PS} v_l\rangle\langle v_l \psi_{lm}^{PS}|}{\langle \psi_{lm}^{PS}|v_l|\psi_{lm}^{PS}\rangle}$

V_{local}: local part of pseudopotential
v_l: non-local part of pseudopotential
ψ_{lm}^{PS}: pseudowavefunction

Input keywords in C2H2_gs.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- **&rgrid /** 
- &scf /
- &functional /
- &atomic_coor /

dl = 0.25d0, 0.25d0, 0.25d0
→ Spacing of real-space grids.

Input keywords in C2H2_gs.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- &rgrid /
- **&scf /** ⇒
- &functional /
- &atomic_coor /

ncg = 4
→ Number of iteration of Conjugate-Gradient method for each scf-cycle.
(Default is 5.)

nscf = 1000
→ Number of maximum scf cycle.

convergence = 'norm_rho_dng'
→ Convergence is checked by
$||\text{rho\_iter}(ix)-\text{rho\_iter}_{-1}(ix)||^2$ / (number of grids).
(Default is rho_dne)
(Difference of electron density / 1 electron)

threshold_norm_rho = 1.d-15
→ Threshold for convergence.
(Default is 1d-17.)

Input keywords in C2H2_gs.inp

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- &control /
- &system /
- &pseudo /
- &rgrid /
- &scf /
- **&functional /** ⇨
- &atomic_coor /

xc = 'PZ'
→ Functional.
→ 'PZ': Perdew-Zunger LDA :Phys. Rev. B 23, 5048 (1981).

Input keywords in C2H2_gs.inp

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- &system /
- &pseudo /
- &rgrid /
- &scf /
- &functional /
- **&atomic_coor /⇨**

	x ↓	y ↓	z ↓	
'C'	0.000000	0.000000	0.599672	1
'H'	0.000000	0.000000	1.662257	2
'C'	0.000000	0.000000	-0.599672	1
'H'	0.000000	0.000000	-1.662257	2

→ Cartesian coordinates of atoms and index number of atomic element.

Output files by C2H2_gs.inp

- variables.log
  → All input variables and values used in the calculation.
- out_gs.log
  → Standard output file.
- C2H2_info.data
  → System information including number of states, electrons, and energy, etc..
- C2H2_gs.bin
  → "Ground state data in binary format (for RT calculation).
- C2H2_eigen.data
  → Orbital energies.
- PS_C_KY_n.dat & PS_H_KY_n.dat
  → Pseudo potential and wave function for radial direction.

out_gs.log

- `less out_gs.log`

Press "q" for quit

iteration count

Iteration count for V_h

```
-------------------------------------------
iter =    54      Total Energy =      -339.58127310     Vh iteration =   1

     1       -18.4138       2       -13.9736       3       -12.4006       4       -7.3403

     5        -7.3403
iter and ||rho_i(ix)-rho_i-1(ix)||**2/(# of grids) =     54 0.67366858E-15

 Ne=  10.00000000000000
```

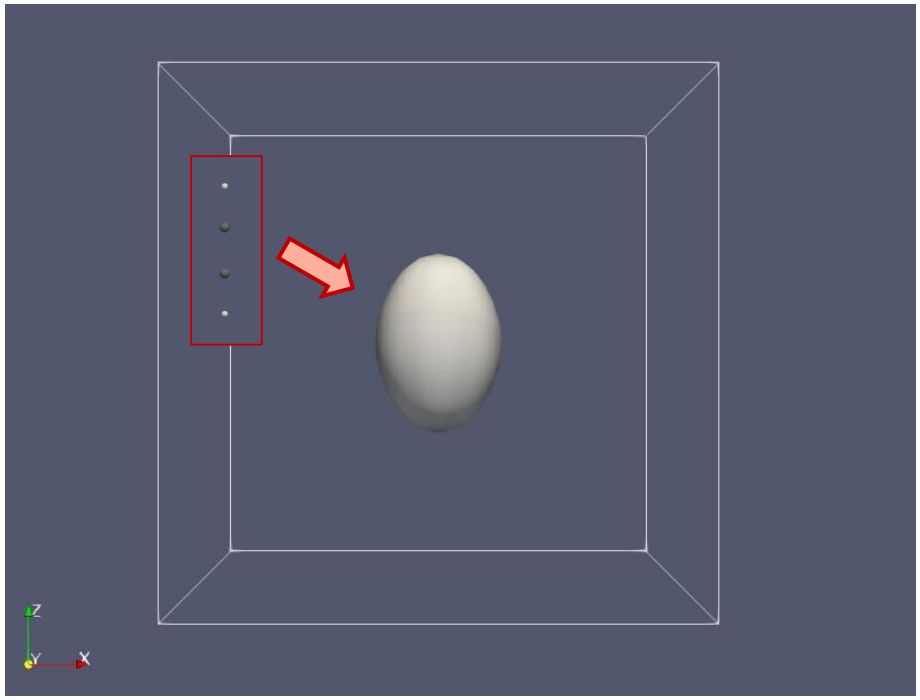
Orbital energies

Number of electros

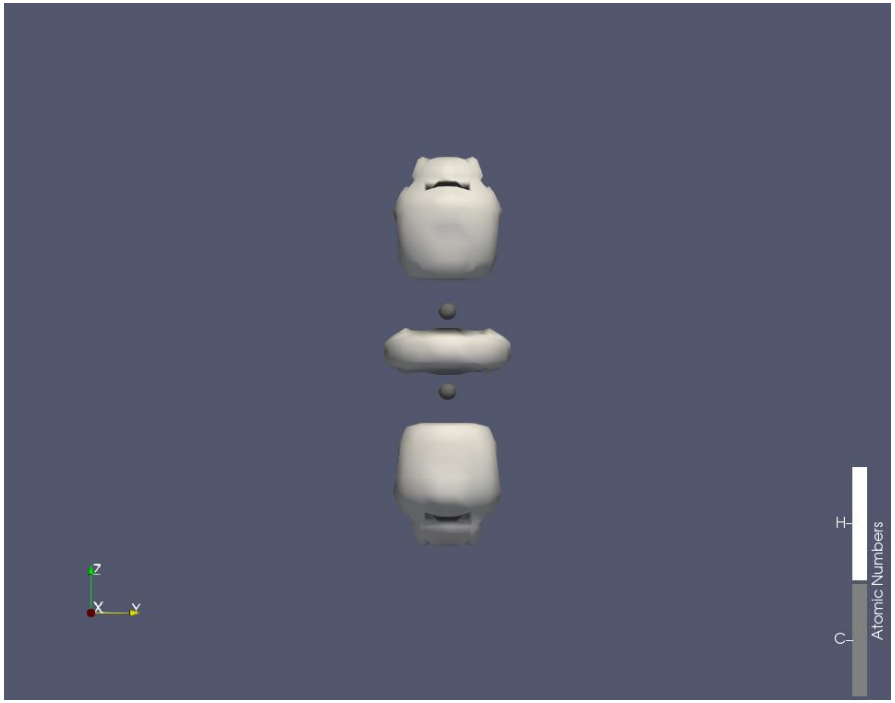
Convergence check

Visualization by ParaView

Electron density



Electron localization function



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- **Pulse response calculation**:
  - Ground state calculation → C2H2_gs.inp
  - Real-time TDDFT → C2H2_rt_pulse.inp

Input keywords in C2H2_rt_response.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- &functional /
- &tgrid /
- &emfield /
- &atomic_coor /

Input keywords in C2H2_rt_response.inp

- &units /
- **&calculation /** ⇨
- &control /
- &system /
- &pseudo /
- &functional /
- &tgrid /
- &emfield /
- &atomic_coor /

calc_mode = 'RT'
→ Real-time TDDFT calculation.

Input keywords in C2H2_rt_response.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- &functional /
- **&tgrid /** 
- &emfield /
- &atomic_coor /

dt = 1.25d-3
→ Time step size.

nt = 5000
→ Number of total time steps.

Input keywords in C2H2_rt_response.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- &tgrid /
- &functional /
- **&emfield /** 
- &atomic_coor /

ae_shape1 = 'impulse'
→ Impulsive fields.

epdir_re1 = 0.d0,0.d0,1.d0
→ Real part of polarization vector of the pulse field.

Output files by C2H2_rt_response.inp

- out_rt.log (`less out_rt.log`)
  → Standard output file.

Press q for quit

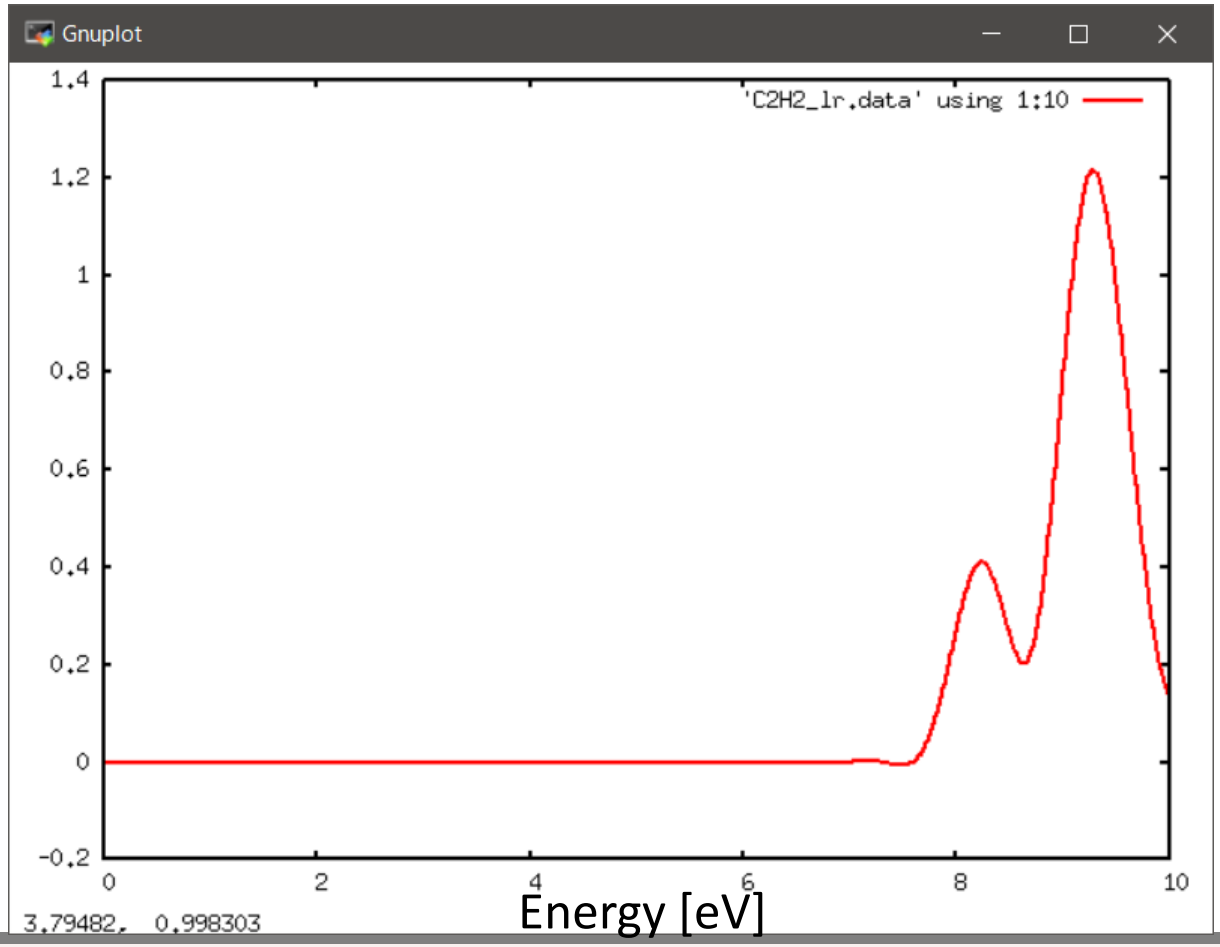
```
 timestep   time[fs]    Dipole moment(xyz)[A]      electrons         Total energy[eV]    iterVh

 ----------------------------------------------------

        1    0.00125000  0.16755557E-10 -0.23698286E-09  0.27416845E-02    10.00000000     -339.56762344   97
```

- C2H2_p.data
  → Dipole moment at each time step.
- C2H2_lr.data
  → The dipole moment in frequency domain and Oscillator strength.

Oscillator strength by C2H2_rt_response.inp

- `gnuplot`
- `plot 'C2H2_lr.data' u 1:10 w l lw 2`

To finish gnuplot → exit



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  - Ground state calculation → C2H2_gs.inp
  - **Real-time TDDFT → C2H2_rt_pulse.inp**

Real-time calculation by C2H2_rt_pulse.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- &functional /
- &tgrid /
- &emfield /
- &atomic_coor /

Input keywords in C2H2_rt_pulse.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- &functional /
- **&tgrid /** 
- &emfield /
- &atomic_coor /

dt = 1.25d-3
→ Time step size.

nt = 4800
→ Number of total time steps.

Input keywords in C2H2_rt_pulse.inp

- &units /
- &calculation /
- &control /
- &system /
- &pseudo /
- &functional /
- &tgrid /
- **&emfield /** 
- &atomic_coor /

ae_shape1 = 'Ecos2'
→ Envelope of pulse field: $\cos^2$ type.

epdir_re1 = 0.d0,0.d0,1.d0
→ Real part of polarization vector of the pulse field.

rlaser_int_wcm2_1 = 1.d8
→ Pulse intensity at peak(W/cm2).

omega1 = 9.28d0
→ (Mean) pulse frequency (or photon energy).

pulse_tw1 = 6.d0
→ Duration of the pulse.

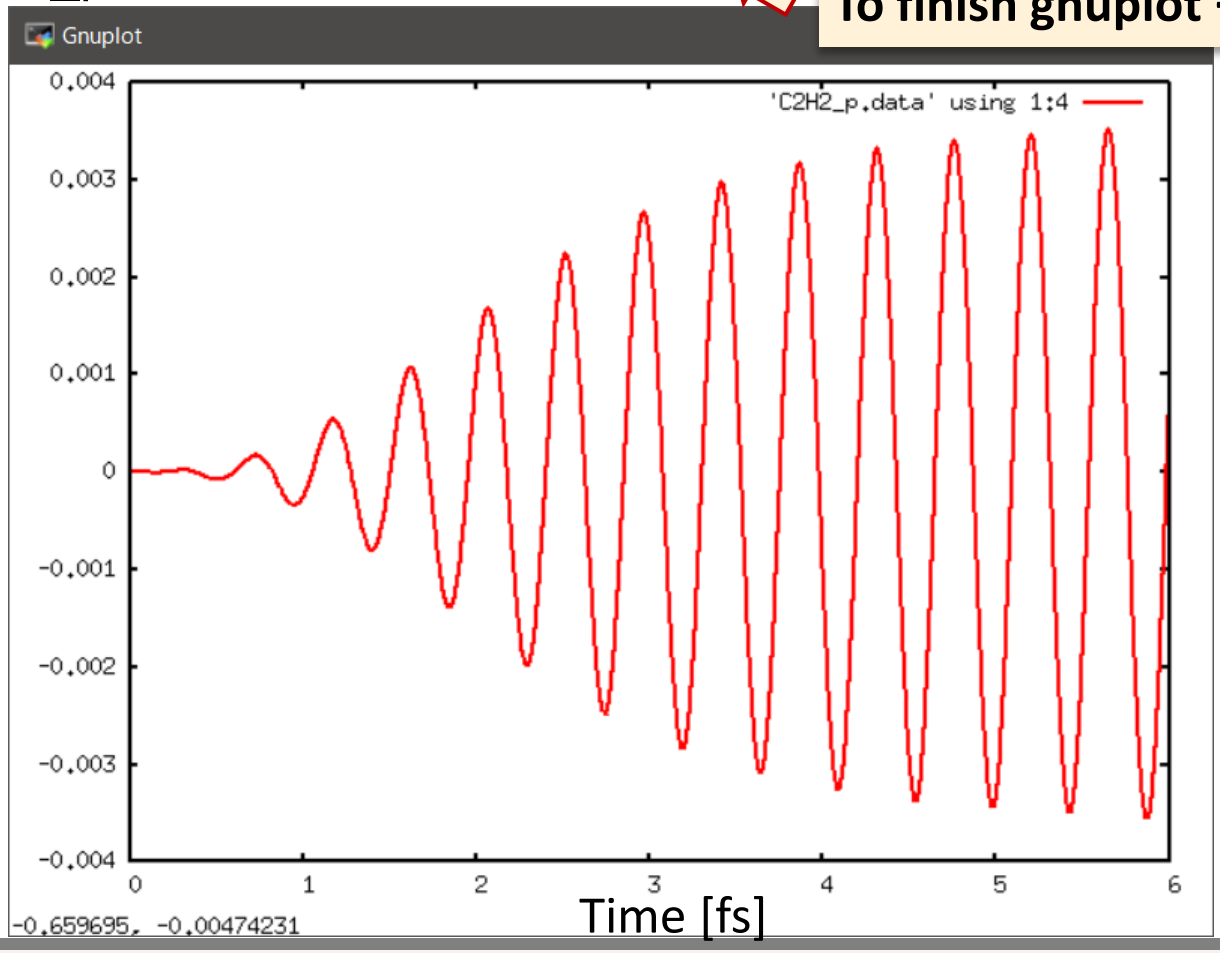
phi_cep1 = 0.75d0
→ Carrier envelope phase of the pulse.

Dipole moment by C2H2_rt_pulse.inp

C2H2_ps.data
→ The dipole moment in frequency domain and the power spectrum.

- `gnuplot`
- `plot 'C2H2_p.data' u 1:4 w l lw 2`

To finish gnuplot → exit



Visualization by ParaView