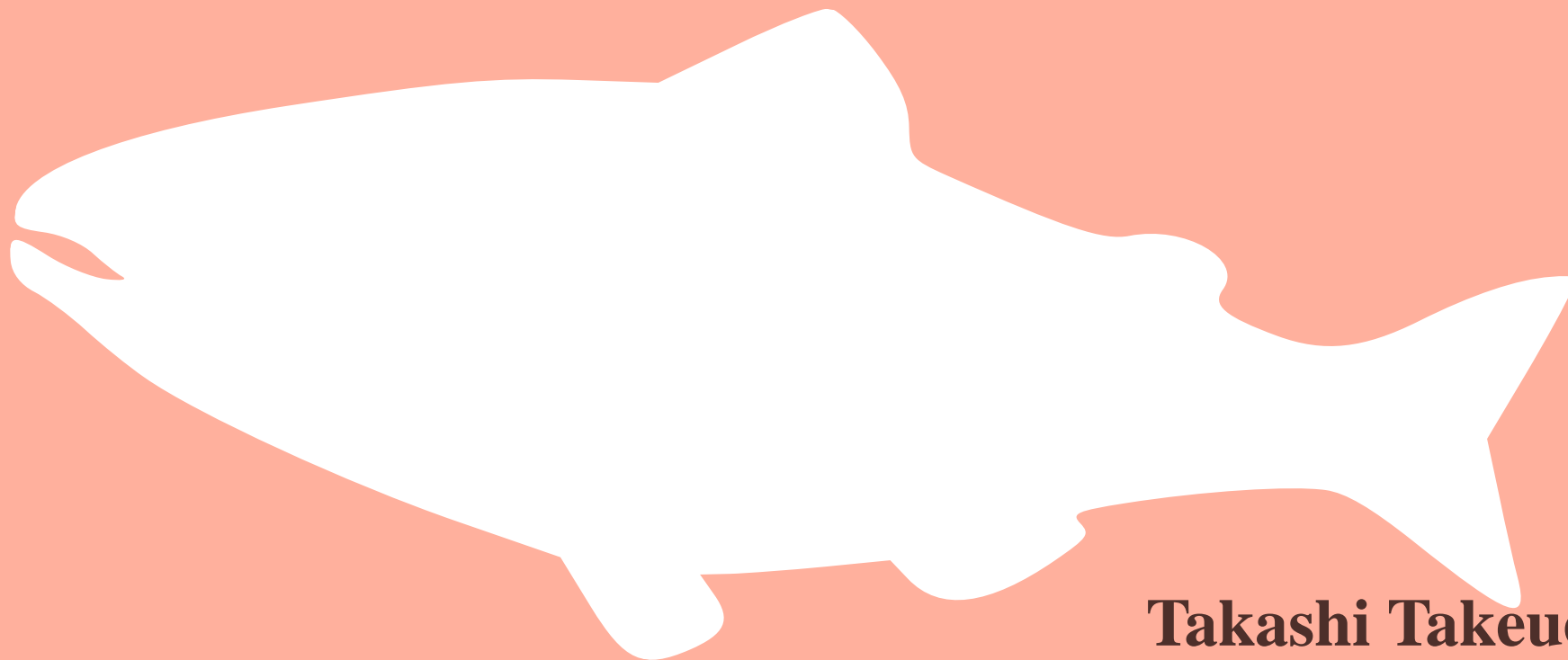


FDTD simulation

Exercise-4-4



Takashi Takeuchi

Center for Computational Sciences, University of Tsukuba

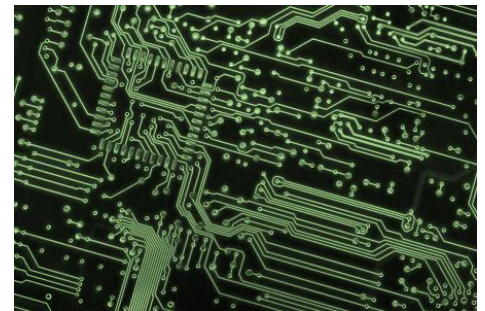
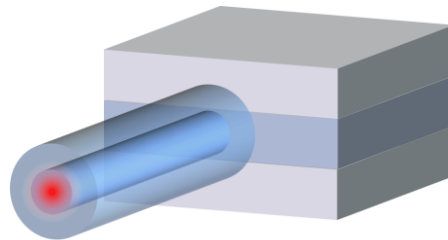
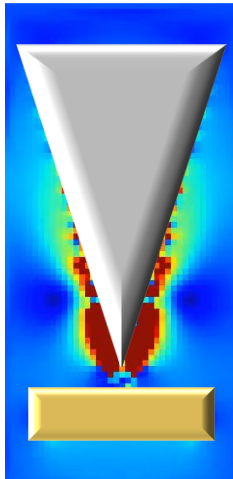
FDTD: Finite-Difference Finite-Time domain

- **What is FDTD ???**

- The FDTD is a real-time and real-space method to solve **classical(macroscopic)** electromagnetic problems.

- **What can we do by FDTD ???**

- can simulate optical and electrical devices such as plasmonics, wave guide, antenna, electric circuit, and so on.



Demonstration of FDTD

- E and H in the Maxwell's equations are simulated based on the spatial grids.

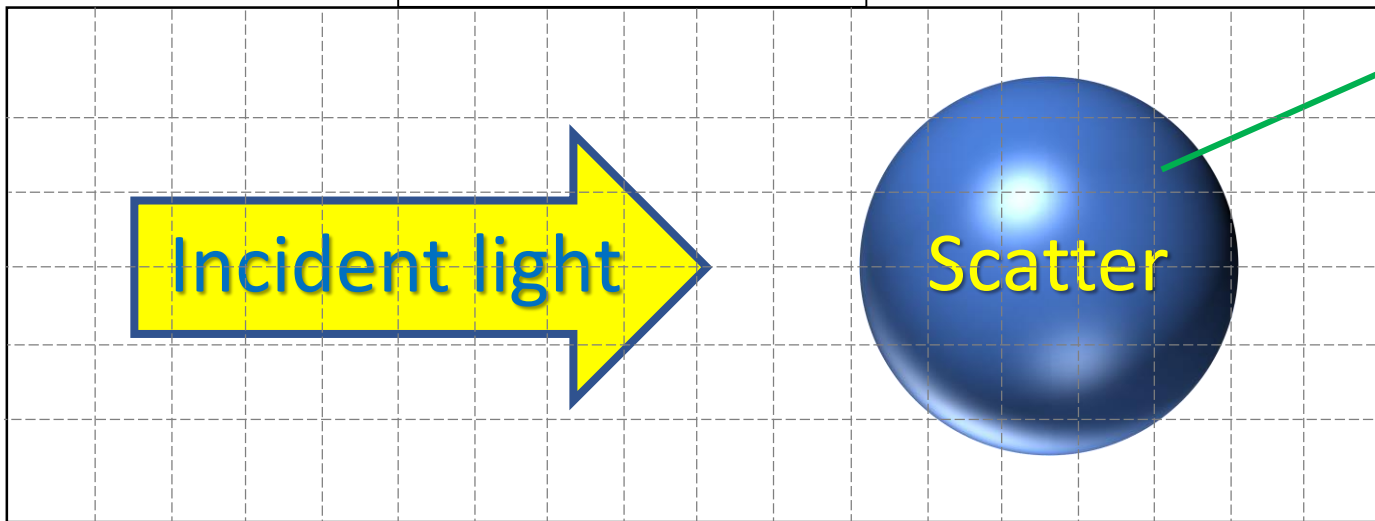
$$\left\{ \begin{array}{l} \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} = \frac{\epsilon}{c} \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{4\pi\sigma}{c} \mathbf{E} - \frac{4\pi}{c} \mathbf{J} \\ \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = \frac{\mu}{c} \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E} \end{array} \right.$$

Shape: arbitrary

Medium:

- ① Constant ϵ , μ , and σ
- ② Drude model
- ③ Perfect Electric Conductor(PEC)


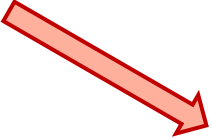
Computational domain



Input keywords in ftdt.inp

- `&units` → 'A_eV_fs' is used now.
('au' and 'A_eV_fs' are available.)
- `&calculation`
- `&control`
- `&system`
- `&emfield` → A y-polarized pulse(E_y component) is employed.
- `&maxwell`


Input keywords in ftdt.inp

- &units
- **&calculation** 
- **&control** 
- &system
- &emfield
- &maxwell

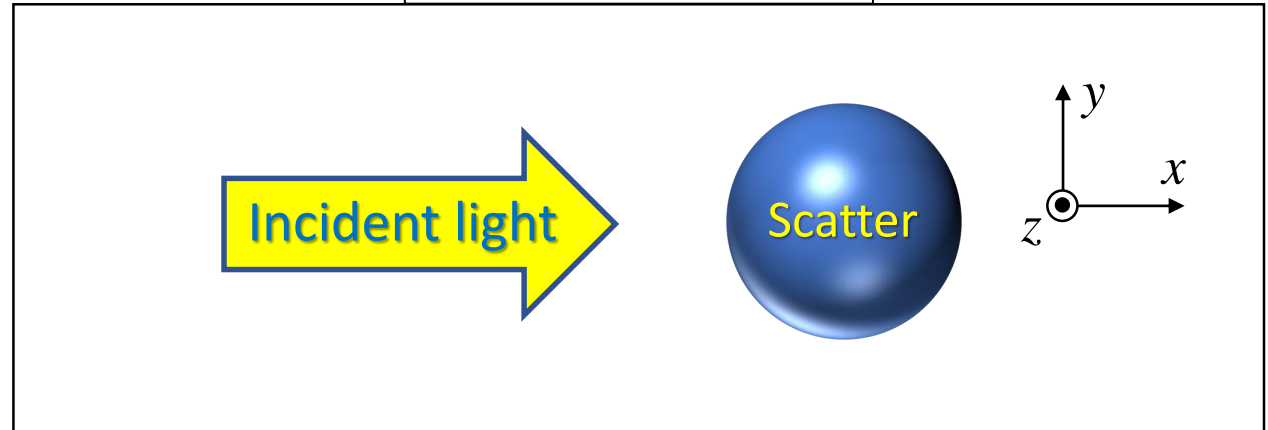
theory = 'Maxwell'
→ Type of theory in the simulation.
→ **Default is 'TDDFT'**.

directory = './result/'
→ Directory name for out put.
→ **Default is './'**.

Input keywords in ftdt.inp

- `&units`
- `&calculation`
- `&control`
- `&system`
- `&emfield`
- `&maxwell` 

Computational domain



`al_em = 16.25d0, 16.25d0, 16.25d0`

→ Computational domain length.

`dl_em = 0.25d0, 0.25d0, 0.25d0`

→ Spacing of real-space grids.


`nt_em = 300`

→ Number of total time steps for real-time propagation.

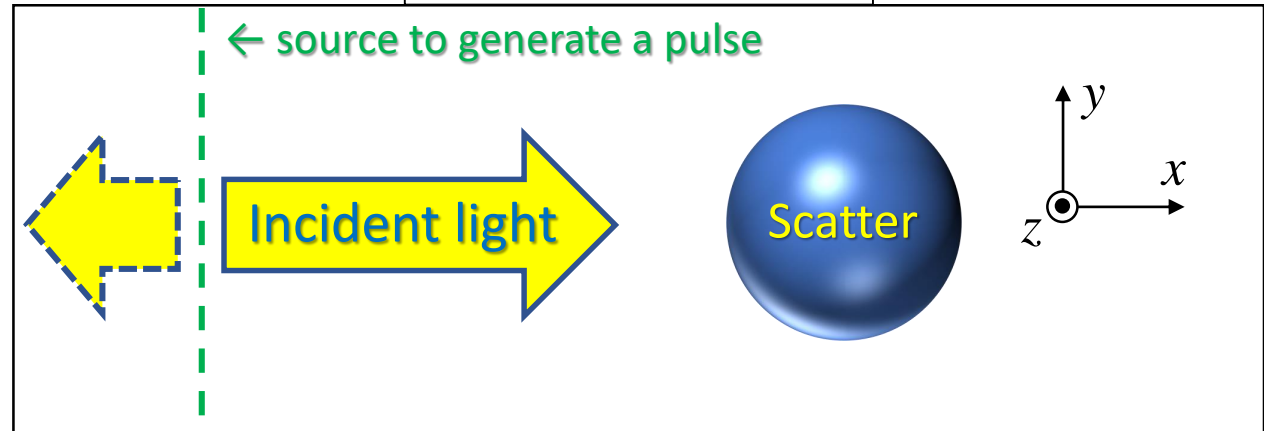
! `dt_em = **`

→ Time step (not necessary here).

Input keywords in ftdtd.inp


- `&units`
- `&calculation`
- `&control`
- `&system`
- `&emfield`
- `&maxwell` 

Computational domain

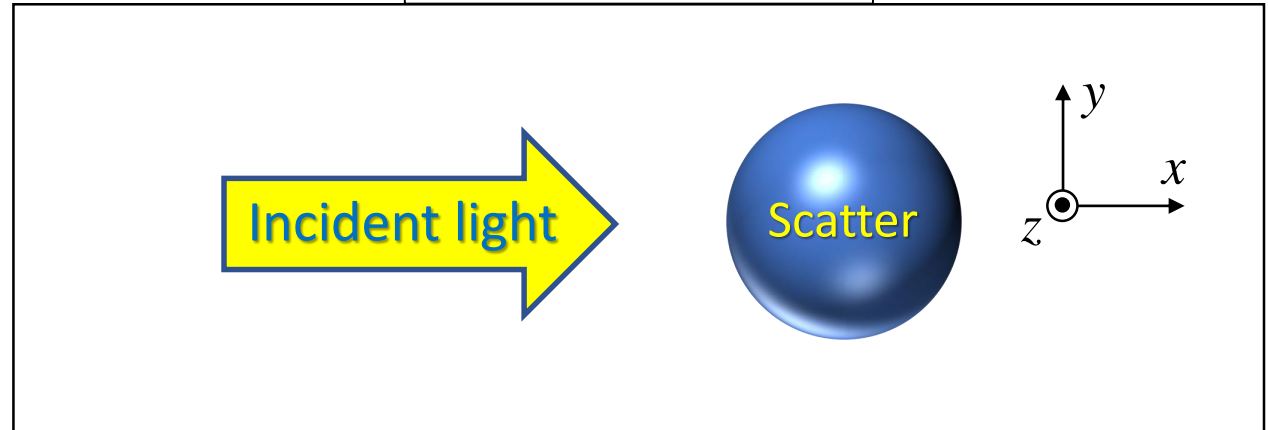


`wave_input = 'source'`
→ Type how to generate pulse.
→ In v.1.2.0, this is 'source' only.
`source_loc1 = -5.0d0, 0.0d0, 0.0d0`
→ Location of source 1.
`ek_dir1 = 1.0d0, 0.0d0, 0.0d0`
→ Direction that the pulse propagates.
(x-direction, y-direction, z-direction)

Input keywords in ftdtd.inp

- `&units`
- `&calculation`
- `&control`
- `&system`
- `&emfield`
- `&maxwell` 

Computational domain



- **imedia_num = 1**
→ Number of media.
- **shape_file = 'shape.cube'**
→ Name of shape-file
- **epsilon(1) = 2.0d0**
→ Relative permittivity.
- **rmu** and **sigma** are permeability and conductivity.
- **type_media = 'pec' or 'drude'**.
- If 'drude', set **omega_p_d** and **gamma_d**.

SALMON utilities



SALMON

Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience

▸ Sitemap

▸ Japanese

HOME > Utilities

- Home
- About SALMON
- Download
- Install and Run
- Input Variables
- Exercises
- Documents
- References
- User Community
- Events

Utilities

Structure Generation

- [salmon_inp](#) - by M. Uemoto at University of Tsukuba. This package is an input file generator which translates CIF (Crystallographic Information File) data to SALMON input file.

FDTD

- [FDTD_make_shape](#) - by T. Takeuchi at University of Tsukuba. This package is a shape file maker for FDTD program in SALMON.
- [FDTD_make_figani](#) - by T. Takeuchi at University of Tsukuba. This package is a figure and animation maker for FDTD program in SALMON.

→usage: ./make_shape.py

Post-Processing


Data Visualization

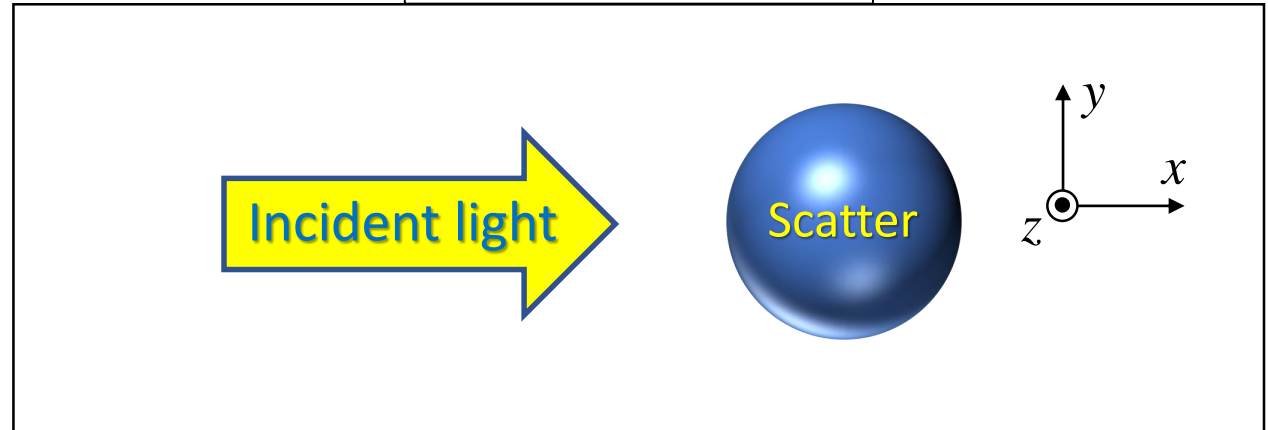
<https://salmon-tddft.jp/utilities.html>

Utilities

FDTD simulation by ftd.inp

Computational domain

- `&units`
- `&calculation`
- `&control`
- `&system`
- `&emfield`
- `&maxwell` 



`iobs_num_em = 1`

→ Number of observation points.

`iobs_samp_em = 5`

→ Sampling time step.

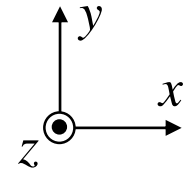
`obs_loc_em(1,:) = 0.0d0, 0.0d0, 0.0d0`

→ Coordinate of the observation point.

Check of calculation by ftdt.inp

Computational domain

PML(Absorbing boundary condition)



- out_ftdtd.log
→ Standard output file.

```
*****
```

```
From CFL condition, dt_em is determined by 4.766437173888290E-005  
in the unit system, A_eV_fs.
```

```
*****
```

```
*****
```

```
PML has been set for x-direction: -8.00000E+00 to -6.00000E+00.  
PML has been set for x-direction: 6.00000E+00 to 8.00000E+00.  
PML has been set for y-direction: -8.00000E+00 to -6.00000E+00.  
PML has been set for y-direction: 6.00000E+00 to 8.00000E+00.  
PML has been set for z-direction: -8.00000E+00 to -6.00000E+00.  
PML has been set for z-direction: 6.00000E+00 to 8.00000E+00.
```

```
*****
```

SALMON utilities



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→usage: ./make_figani.py

Post-Processing

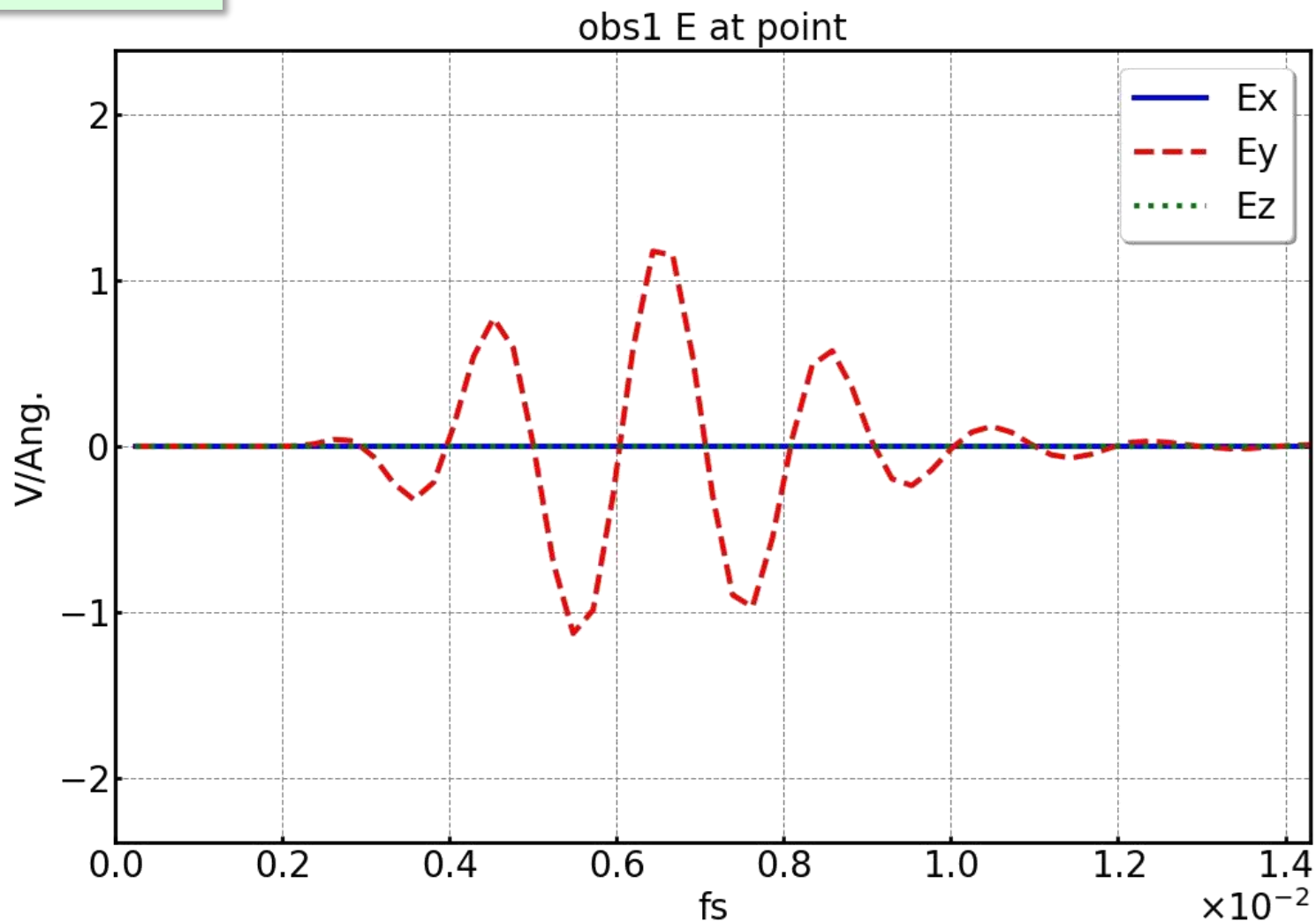
Data Visualization

<https://salmon-tddft.jp/utilities.html>

Utilities

Result: Temporal profile of E by ftdtd.inp

```
./make_figani.py
```



Result: Temporal profile of H by ftdt.inp

```
./make_figani.py
```

