FDTD simulation

Exercise-4-4

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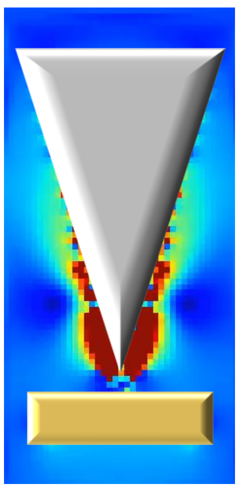
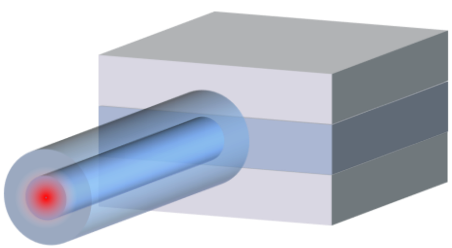
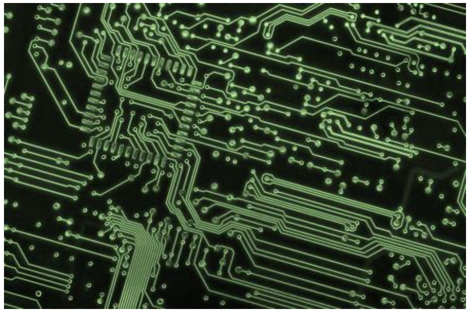
FDTD: Finite-Difference Finite-Time domain

- **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 circit, and so on.

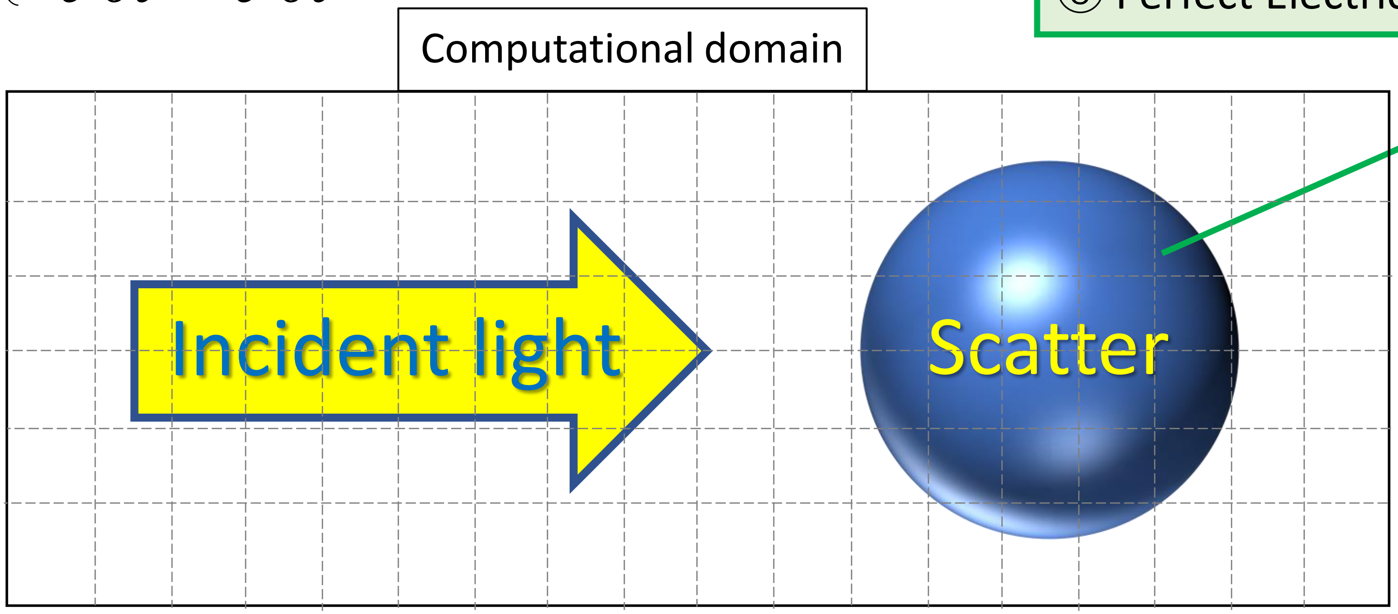


Demonstration of FDTD

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

$$\begin{cases} \dfrac{1}{c}\dfrac{\partial \mathbf{D}}{\partial t} = \dfrac{\epsilon}{c}\dfrac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \dfrac{4\pi\sigma}{c}\mathbf{E} - \dfrac{4\pi}{c}\mathbf{J} \\ \dfrac{1}{c}\dfrac{\partial \mathbf{B}}{\partial t} = \dfrac{\mu}{c}\dfrac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E} \end{cases}$$

Shape: arbitrary
Medium:
① Constant ϵ, μ, and σ
② Drude model
③ Perfect Electric Conductor(PEC)



Input keywords in fdtd.inp

- &units → 'A_eV_fs' is used now.
  ('au' and 'A_eV_fs' are available.)
- &calculation
- &control
- &system → In v.1.2.0, only iperiodic = 0 is allowed.
- &emfield → A y-polarized pulse(E_y component) is employed.
- &maxwell

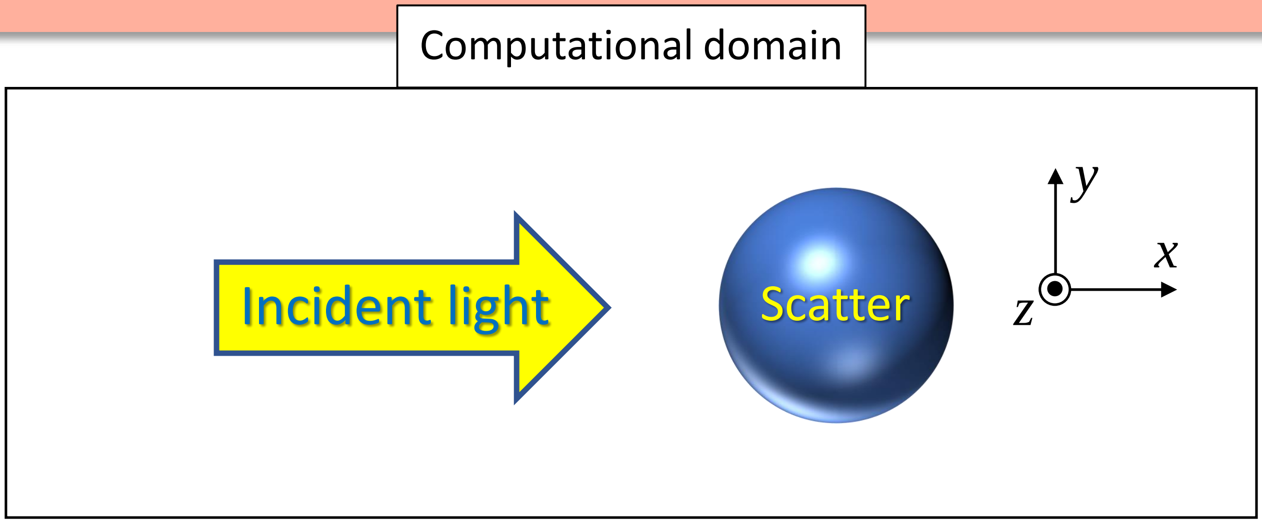
Input keywords in fdtd.inp

- &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 fdtd.inp

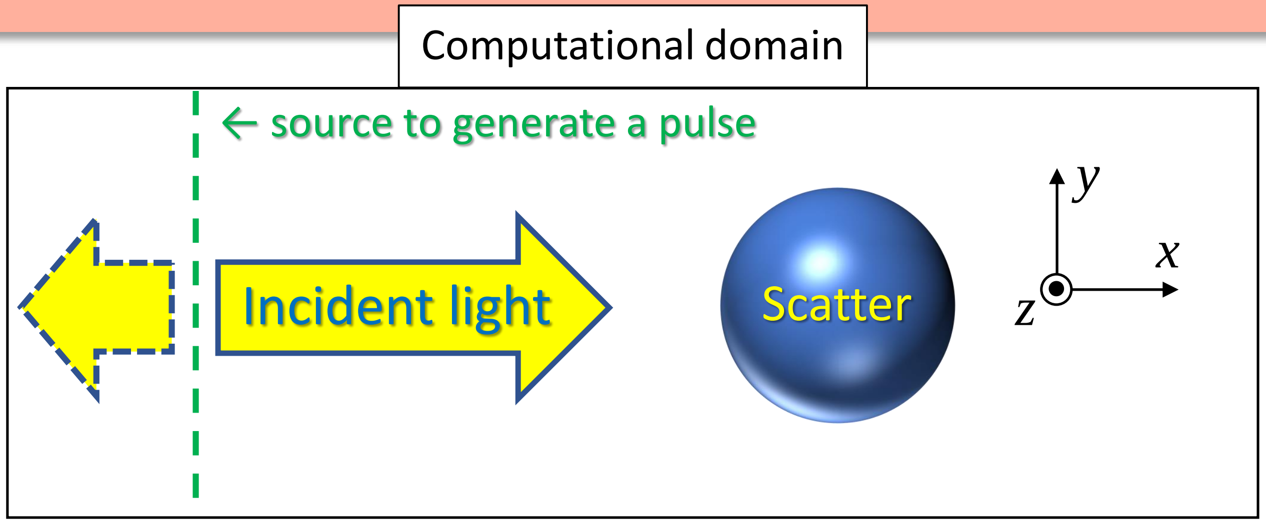


- &units
- &calculation
- &control
- &system
- &emfield
- **&maxwell**

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 fdtd.inp

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



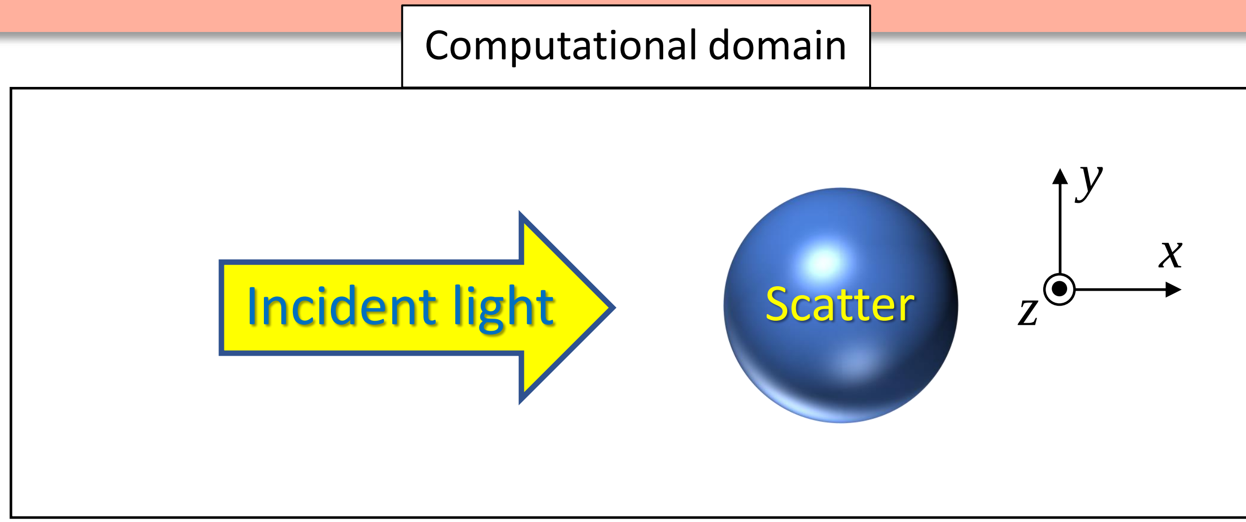
wave_input = 'source'
→ Type how to generate pulse.
→ In v.1.2.0, this is 'source' only.

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 fdtd.inp

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



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

Sitemap | Japanese

SALMON

SALMON

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

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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.

→usage: ./make_shape.py

- FDTD_make_figani - by T. Takeuchi at University of Tsukuba. This package is a figure and animation maker for FDTD program in SALMON.

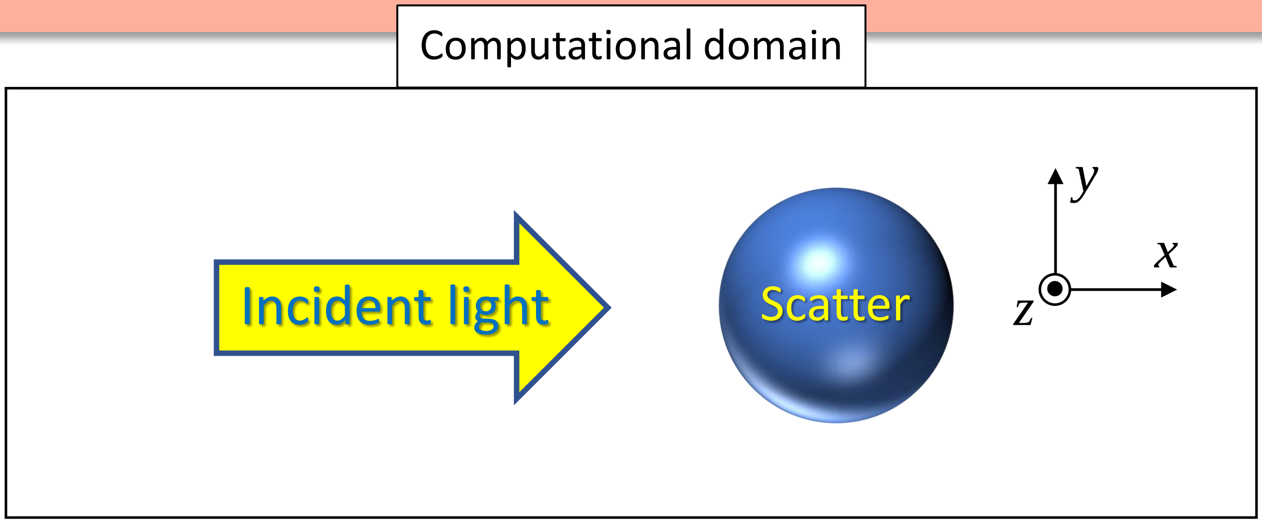
Post-Processing

Data Visualization

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

FDTD simulation by fdtd.inp

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

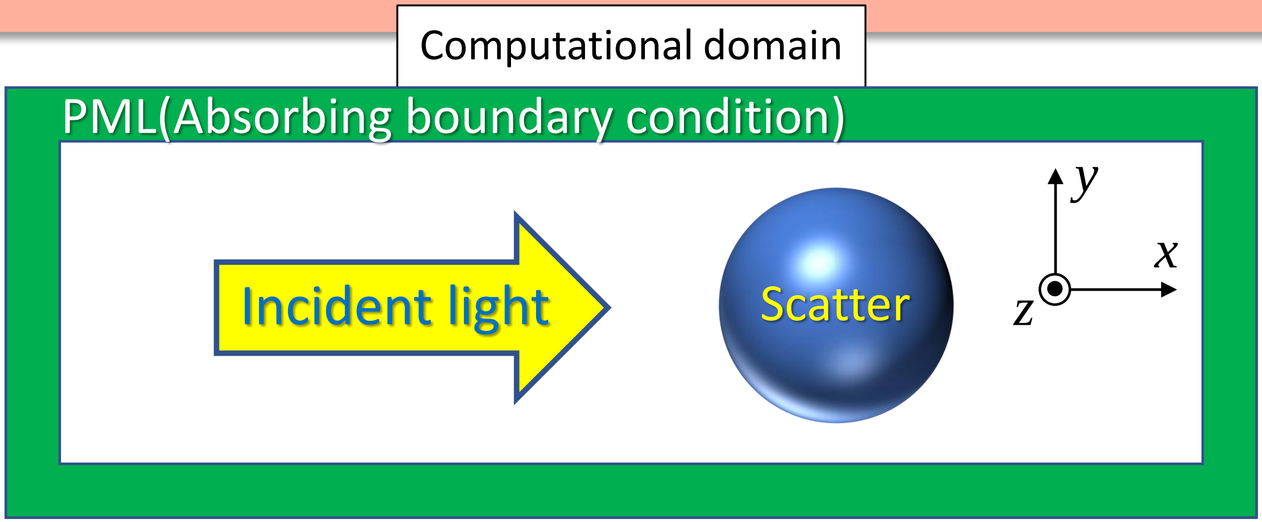


iobs_num_em = 1
→ **Number of observation points.**

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 fdtd.inp



- out_fdtd.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.
**************************
```

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→usage: ./make_figani.py

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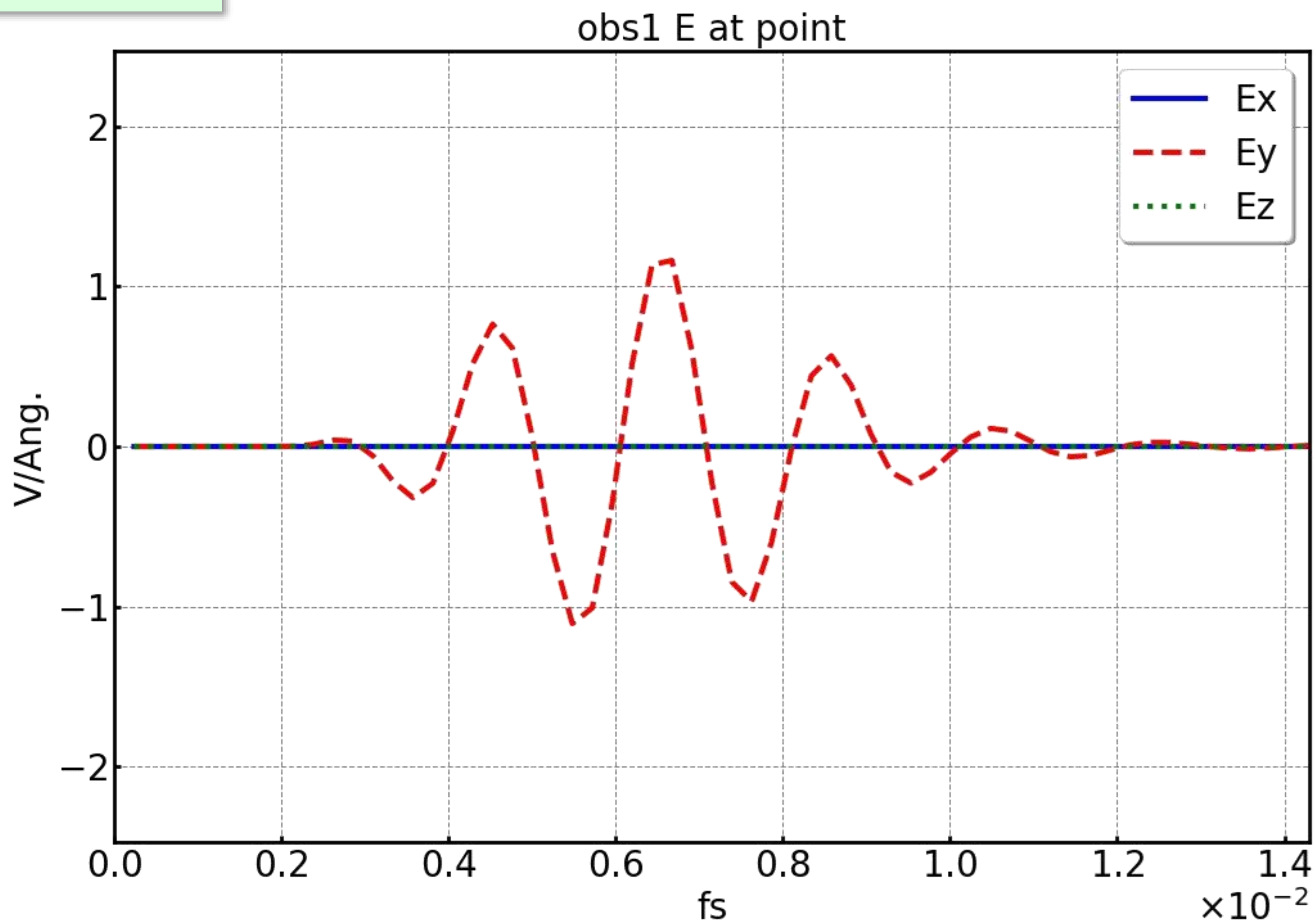
Result: Temporal profile of E by fdtd.inp

./make_figani.py



Result: Temporal profile of H by fdtd.inp

./make_figani.py