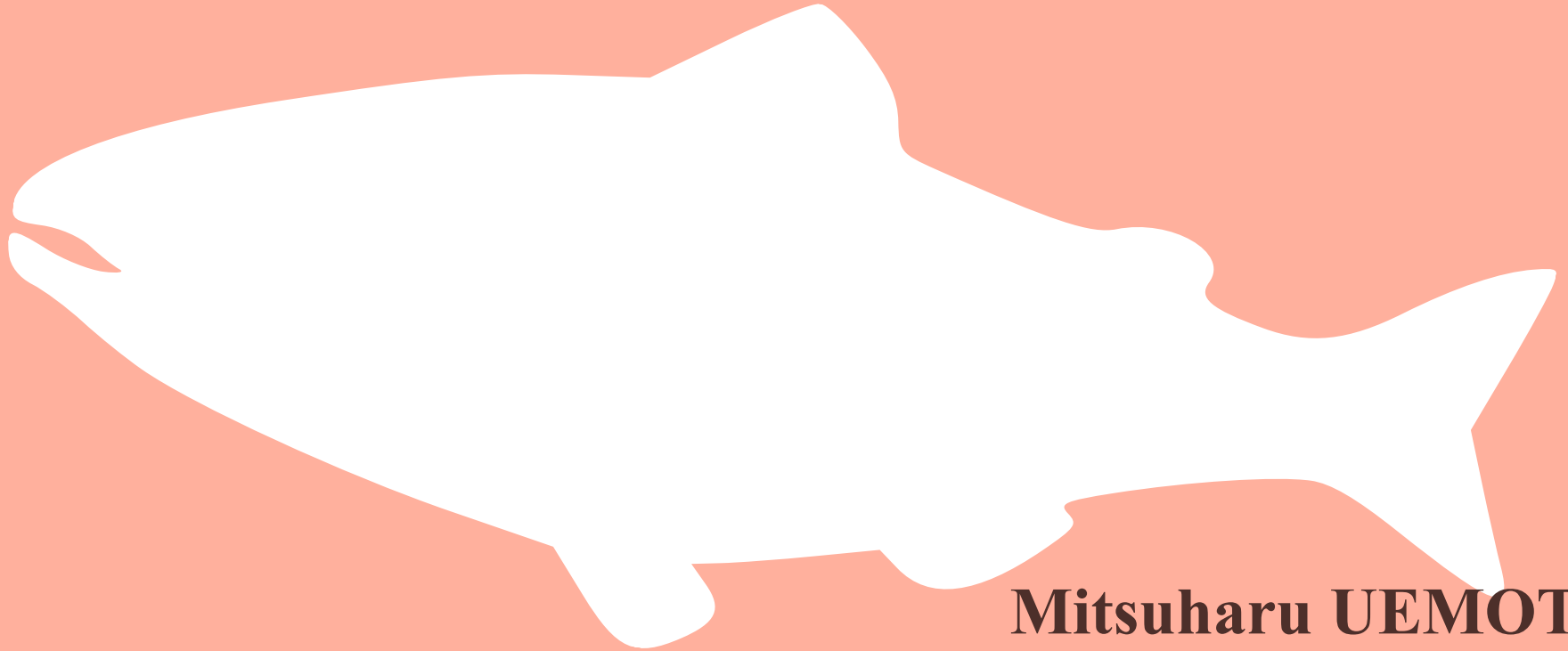


How to Use SALMON Multiscale Simulation

Exercise-4-2

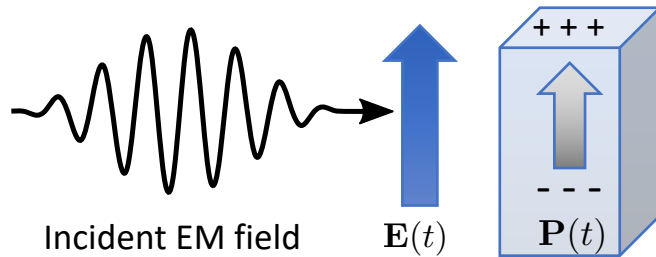


Mitsuharu UEMOTO

Center for Computational Sciences, University of Tsukuba

Light Propagation in Solid State Material

Light irradiation into the solid material,



$\mathbf{E}(t)$: Applied Electric Field
 $\mathbf{P}(t)$: Induced Polarization

Weak intensity light

- Light propagation in the solid media \rightarrow **Maxwell's wave equation.**

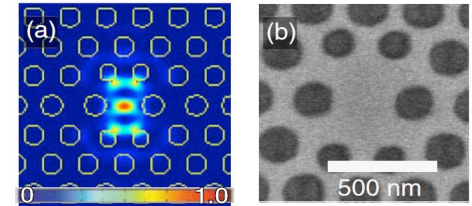
$$-\nabla \times \nabla \times \mathbf{A}(\mathbf{r}, t) - \frac{\epsilon}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{A}(\mathbf{r}, t) = 0$$

- Dielectric response to applied field \rightarrow **Linear Response**

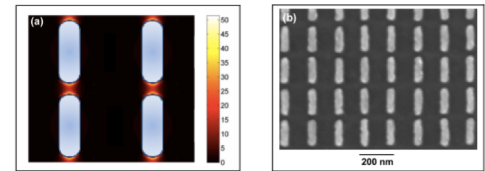
$$\mathbf{P} = \chi^{(1)} \mathbf{E} = (\epsilon - \epsilon_0) / 4\pi \cdot \mathbf{E}$$

Strong intensity light

- Optical Nonlinearity Induced by Intense Field**



Nature, 432, pp. 9–12, (2004).



Opt. Express, 15, 12 (2007)

Light Propagation in Solid State Material

Induced current density in matter

$$\mathbf{J}(t) = -\frac{e}{m} \sum_{b,\mathbf{k}} \frac{1}{\Omega} \int_{\Omega} \text{Re } u_{b,\mathbf{k}}^*(\mathbf{r}, t) \left(-i\hbar\nabla + \hbar\mathbf{k} + \frac{e}{c}\mathbf{A}(t) \right)^2 u_{b,\mathbf{k}}(\mathbf{r}, t) d\mathbf{r} + \mathbf{J}_{\text{NL}}$$



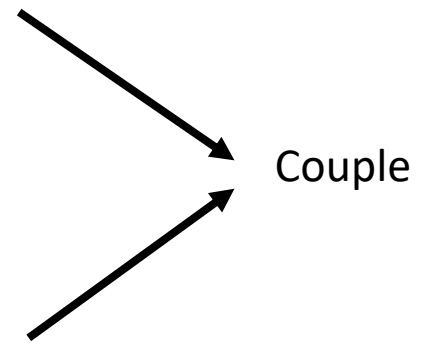
- “**Constitution Relation**” of Electromagnetics:
(Current density can be described as the functional of the EM field)

$$\mathbf{J} = \mathbf{J}[\mathbf{A}(t)]$$

Light propagation in the media

- Governing equation of EM field (Maxwell’s wave eq.)

$$-\nabla \times \nabla \times \mathbf{A} - \frac{1}{c^2} \frac{\partial}{\partial t^2} \mathbf{A} = -\frac{4\pi}{c} \mathbf{J}$$

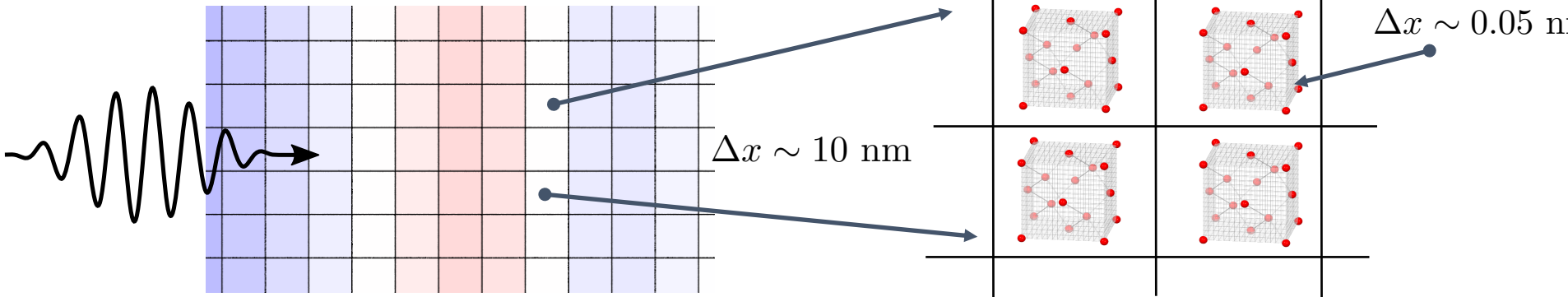


Multiscale Maxwell-TDDFT method

- A multiscale method treats light propagations in solid media, combining the macroscopic Maxwell equation and microscopic electron dynamics.

Macroscopic system (EM field)

Microscopic system (Electron dynamics)



Solve Maxwell's Eq. in Macroscopic grid:

$$\nabla \times \nabla \times \mathbf{A} + \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = \frac{4\pi}{c} \mathbf{J}$$

FDTD-based EM calculation:

$$\mathbf{J}(t - \Delta t_i) \rightarrow \mathbf{A}(t)$$

Solve TD-KS Eq. in Microscopic Grid

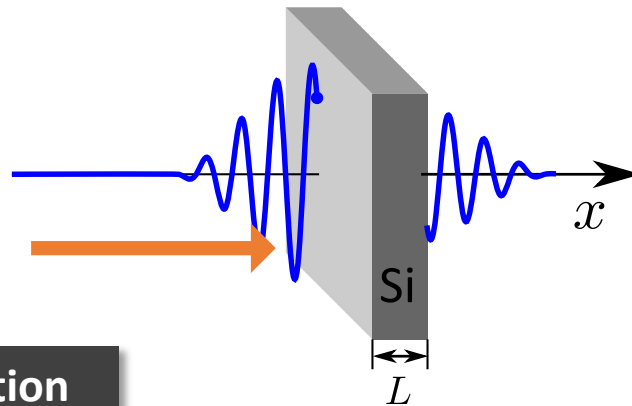
$$\hat{E}u_{n\mathbf{k}} = \hat{\mathcal{H}}(k)u_{n\mathbf{k}}$$

RT-TDDFT calculation:

$$\mathbf{A}(t - \Delta t_i) \rightarrow \mathbf{J}(t)$$

Exercise

- Short laser pulse propagation in a thin film silicon with a thickness L :



Computation Condition

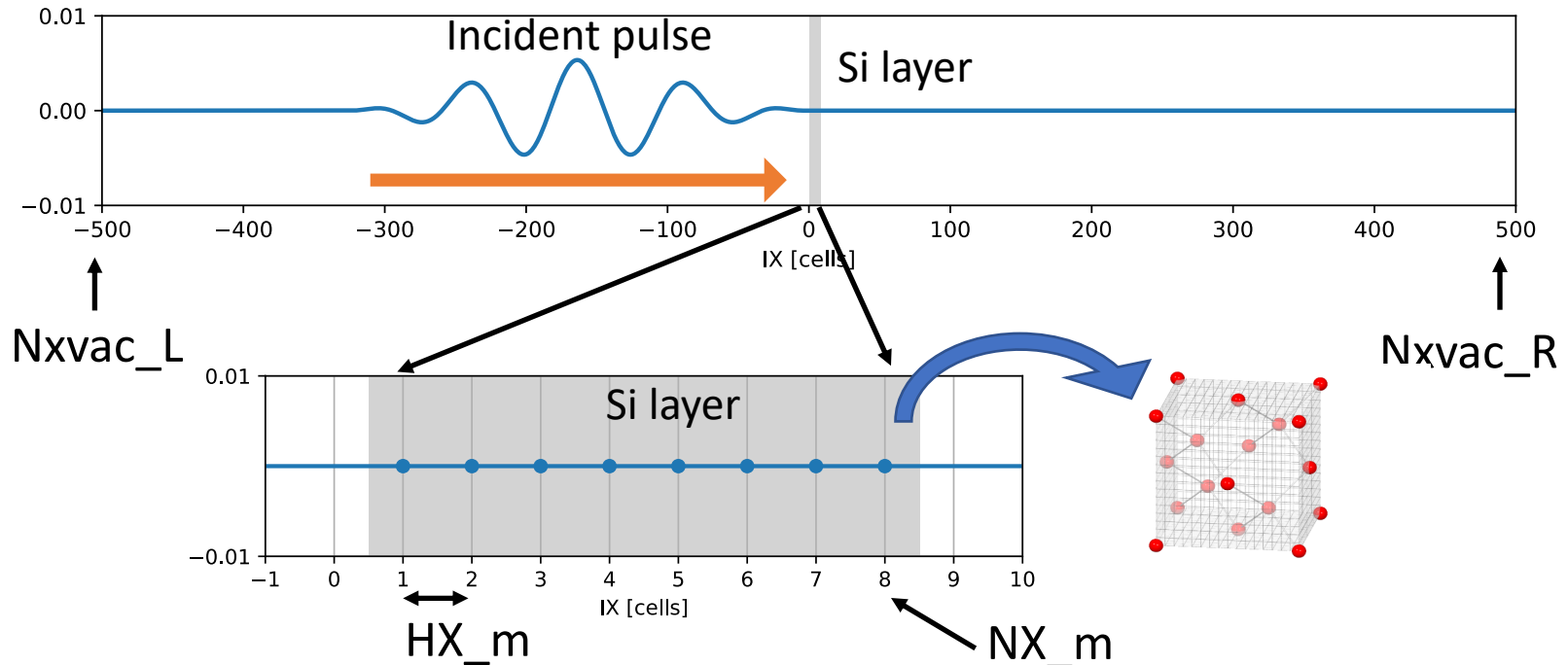
- Matter:
 - Silicon: $R=12^3$, $K=4^3$, $dt=0.16$ [au] (~ 3.8 [as])
 - Thickness $L=80$ [nm] ($\sim 1.5 \times 10^4$ [au])
- Laser Pulse
 - Central Frequency: 1.55 [eV]
 - Intensity: $I=10^{12}$ [W/cm²]
 - Pulse Length: $T=10.6$ [fs]

Results

- Matter Current Density
- Electromagnetic Field Profile
- Energy Absorption

Exercise

- Computation Model:



- Nxvac_L/R: Lower / upper-bound of computation domain
- NX_m: Upper bound of the matter region
- HX_m: Grid spacing

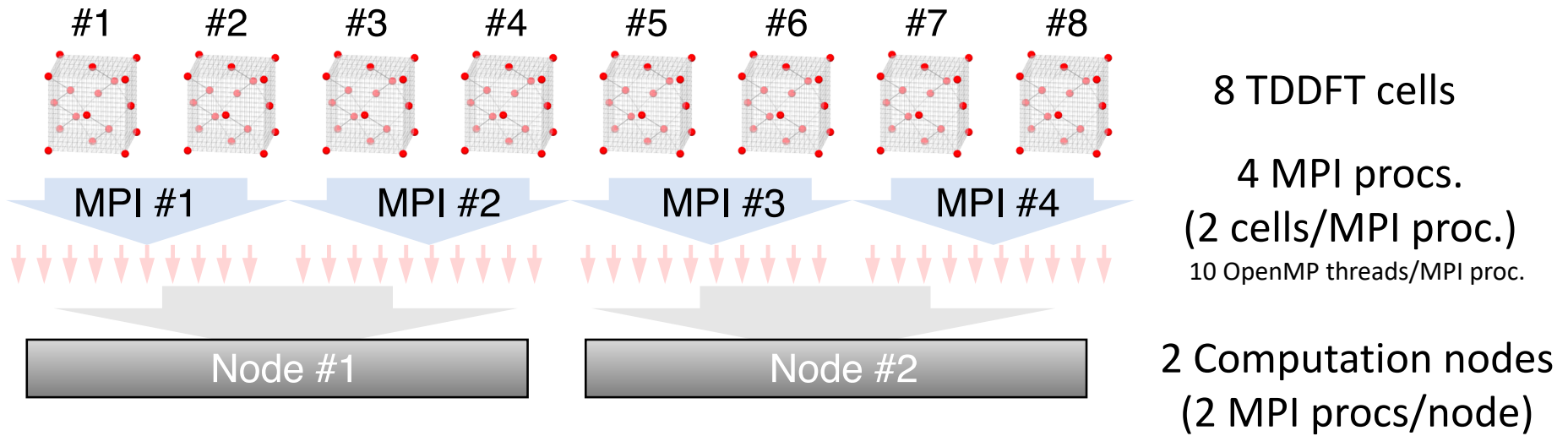
$$\text{Thickness} = \text{NX}_m * \text{HX}_m = 80 \text{ [nm]}$$

Job Submission

- Enter your working directory and submit the job script:

```
$ cd ~/work/exercise4-2_ms  
$ sbatch job.sh
```

- Parallelization scheme of the job (Hybrid MPI and OpenMP execution):



Input File

```
$ less Si_multiscale.inp
```

LIST1: Si_multiscale.inp

```
&calculation
  calc_mode = 'GS_RT'
  use_ms_maxwell = 'y'
/
&control
  sysname = 'Si'
/
...
```

- “**use_ms_maxwell**”
Enable the multiscale calculation mode

Input File

LIST: Si_multiscale.inp

```
&emfield
  ae_shape1 = 'Acos2'
  r_laser_int_wcm2_1 = 1d12
  pulse_tw1 = 441.195136248d0
  omega1 = 0.05696145187d0
  ekdir_re1 = 0.,0.,1.
/
```

- “pulse_tw1”
Incident pulse length: 441 [au] (~ 10.6 [fs])
- “r_laser_int_wcm2_1”
Intensity of the incident pulse: 10^{12} [W/cm²]
- “omega1”
Central frequency of the incident pulse: 0.056.. [au] (~ 1.55 [eV])

Input File

LIST: Si_multiscale.inp

```
&multiscale
  fdtddim = '1D'
  twod_shape = 'periodic'
  NX_m = 8
  HX_m = 188.97
  NXvacL_m = -500
  NXvacR_m = +500
/
```

- **NX_m**: Number of the macroscopic grid points; 8 [macro-points]
- **HX_m**: Grid spacing; 188.97 [au/cell] = 10 [nm/cell]
- **NXVac(L|R)_m**: Upper/lower bound of computation domain; -500 ~ +500 [cell] = -5000 ~ +5000 [nm]

Output Files

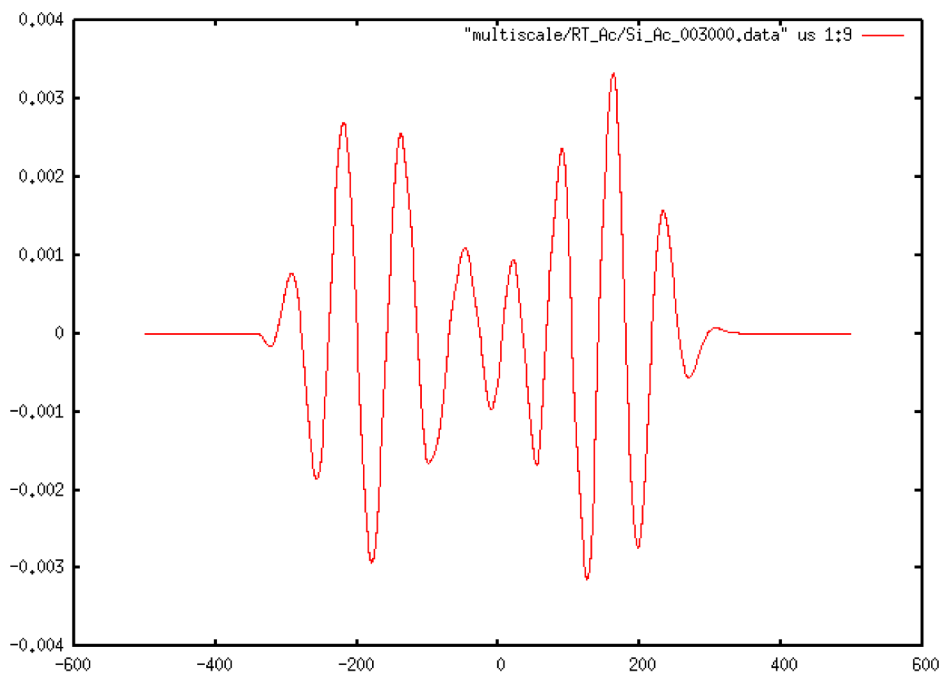
- multiscale/RT_Ac/Si_Ac_XXXXXX.data (XXXXXX: Timestep)
 - Electromagnetic field and energy distributions at each timesteps

Column		Detail
1,2,3	IX,IY,IZ	Index coordinates of macroscopic grid
4,5,6	Acx, Acy, Acz	Vector potential
7,8,9	Ex, Ey, Ez	Electric field
10,11,12	Bx, By, Bz	Magnetic field
13,14,15	Jmx, Jmy, Jmz	Matter current density
16	E_ex	Excitation energy
17	E_abs	Absorbed energy
18	E_em	Total EM energy

Ez Field Plotting (GNU PLOT)

LIST: Operation to visualize E_z distribution:

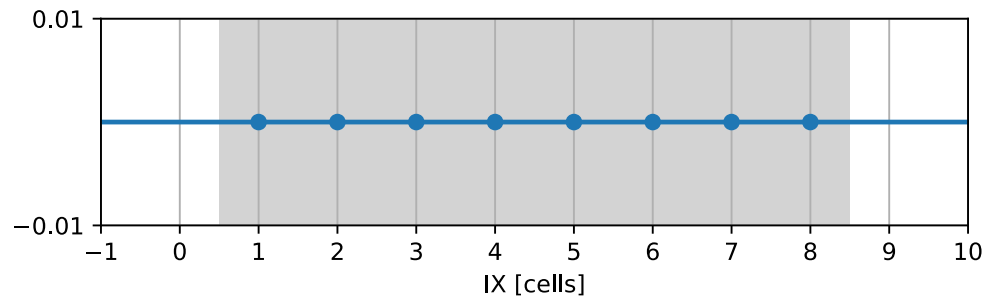
```
$ gnuplot  
> plot "multiscale/RT_Ac/Si_Ac_003000.data" us 1:9 w l
```



Example: E_z field profile at Timestep=3000 ($t=11.6$ [fs]).

Output Files

- multiscale/Mxxxxx/Si_Ac_M.data (xxxxxx: Macro-point index)
 - Current densities and vector potential at each macro-points



Column	Detail	
1	Time	
2,3,4	Acx, Acy, Acz	Vector potential at xxxxxx-th macro-point
5,6,7	Jmx, Jmy, Jmz	Matter current density

```
$ gnuplot  
> plot "multiscale/M000004/Si_Ac_M.data" us 1:7 w l
```