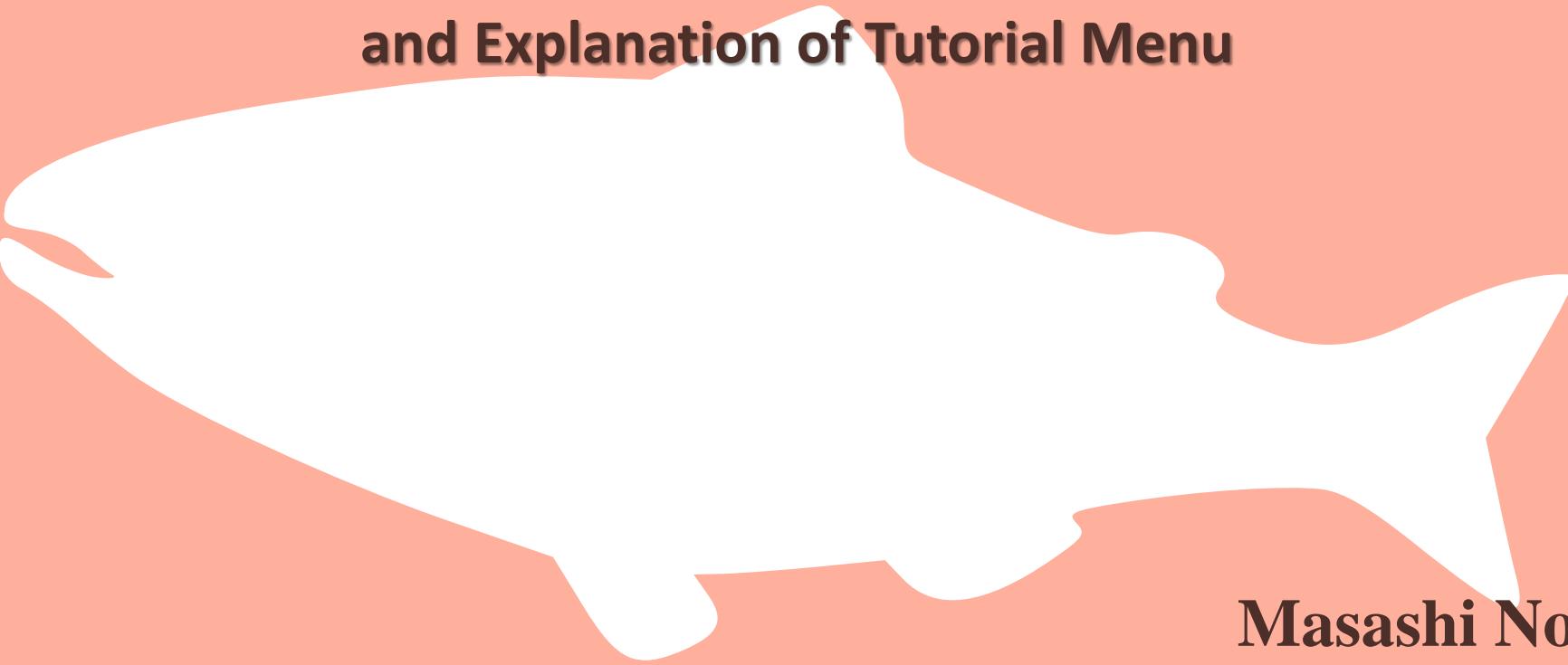


# Introduction

**About SALMON software package  
and Explanation of Tutorial Menu**

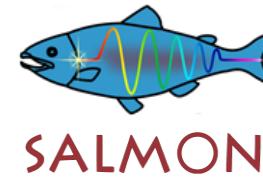


**Masashi Noda**

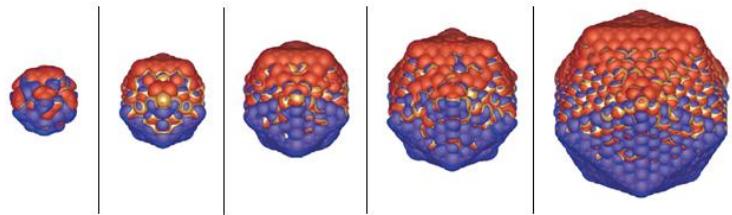
*Center for Computer Science, University of Tsukuba*

# What is SALMON?

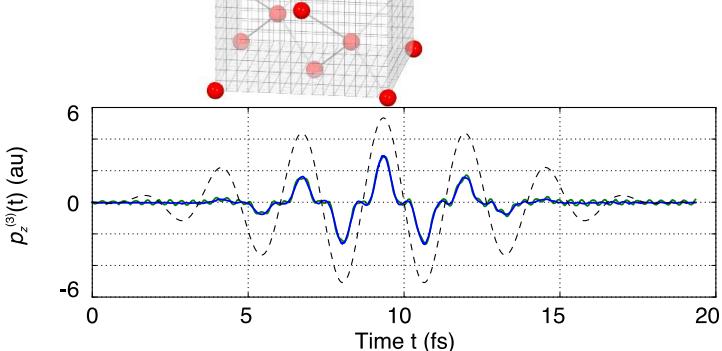
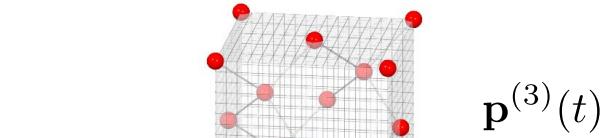
Scalable Ab-initio Light-Matter simulator  
for Optics and Nanoscience



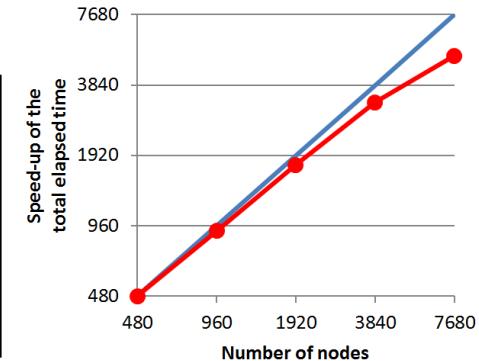
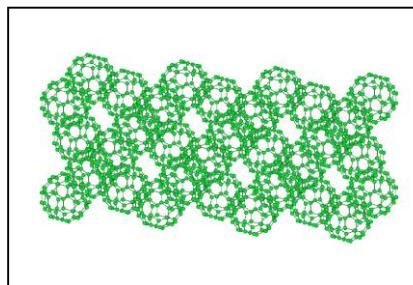
- Real-time electron dynamics



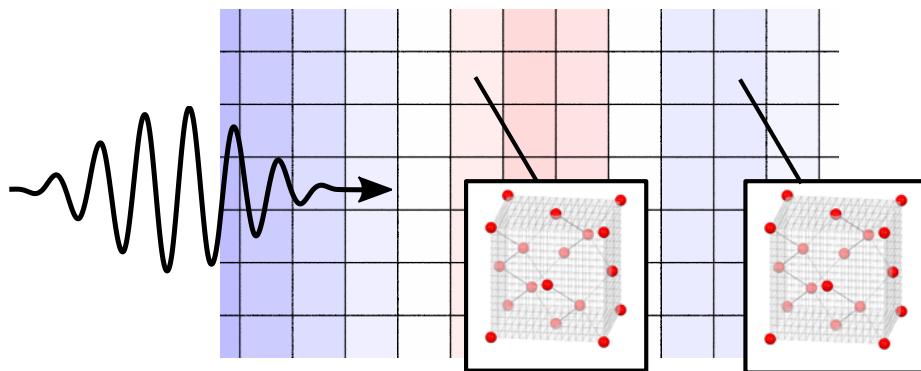
- Non-linear optical response



- Massive parallelization

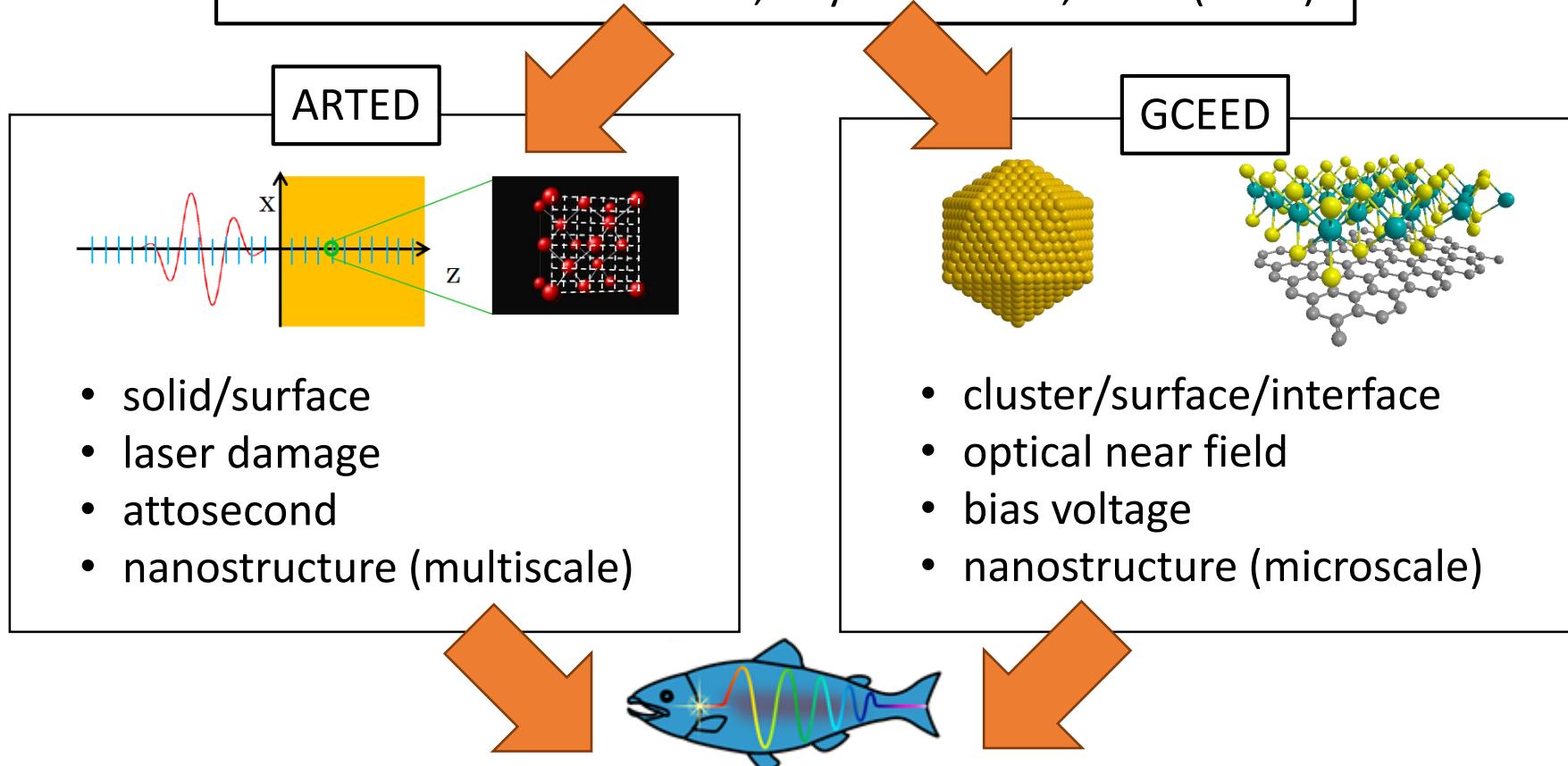


- Couple with Maxwell equation



# Overview of SALMON

K. Yabana and G. F. Bertsch, Phys. Rev. B 54, 4484 (1996)



**SALMON**

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

**SALMON**

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

<http://salmon-tddft.jp/>

SALMON TUTORIAL, TSUKUBA, 2018

# TDDFT codes

- TDDFT codes (frequency domain)

VASP, Quantum Espresso, Abinit, Gaussian, Q-Chem, GAMESS and so on ...

- Real-time TDDFT codes

➤ Octopus

code widely used to describe electron dynamics

➤ FPSID

utilization of plane-wave basis, calculation for molecular dynamics

➤ Qbox

plane-wave first-principles code, a large-scale calculation

➤ SIESTA, Elk FP-LAPW

utilization of numerical atomic orbitals

# License

- Web page:
- <http://salmon-tddft.jp>

The screenshot shows the official website for SALMON. At the top right are links for "Sitemap" and "Japanese". The main title "SALMON" is in large red letters, with the subtitle "Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience" in smaller orange text below it. On the left is a sidebar with a salmon icon and a list of navigation links: Home, About SALMON, Download, Install and Run, Input Variables, Exercises, Documents, References, User Community, Events, and Utilities. The main content area is titled "Selected Features" and contains six sub-sections with corresponding images:

- Grid system for molecules: Shows a 3D grid with atoms and a red wavefunction plot.
- Electron dynamics in solids: Shows a 2D grid with electron density plots and a 3D grid with a green arrow pointing to a specific feature.
- Multiscale grid system: Shows a 3D grid with labels for Maxwell eq. (Macroscopic-system) and TDKS eq. (Microscopic-system).
- Optical near field: Shows two 2D grids with arrows indicating energy transfer between quantum dots (QD).
- Strong field on silicon: Shows a 2D heatmap of electric field intensity on a silicon surface.
- Absorption of nano-particle: Shows a line graph of oscillator strength versus energy (eV), with several peaks labeled: 146, 313, 1414, 922, 569, 308, and 161.

- License: Apache 2.0
- Mailing list: [salmon-user@salmon-tddft.jp](mailto:salmon-user@salmon-tddft.jp) (contact address for inquiry)

# Developers

- Isabella Floss (TU Wien, Austria)
- Yuta Hirokawa (University of Tsukuba, Japan)
- Kenji Iida (Institute for Molecular Science, Japan)
- Kazuya Ishimura (Institute for Molecular Science, Japan)
- Kyung-Min Lee (Max Planck Institute for the Structure and Dynamics of Matter, Germany)
- Katsuyuki Nobusada (Institute for Molecular Science, Japan)
- Masashi Noda (University of Tsukuba, Japan)
- Tomohito Otobe (National Institutes for Quantum and Radiological Science and Technology, Japan)
- Shunsuke Sato (Max Planck Institute for the Structure and Dynamics of Matter, Germany)
- Yasushi Shinohara (University of Tokyo, Japan)
- Takashi Takeuchi (University of TsukubaInstitute for Molecular Science, Japan)
- Xiao-Min Tong (University of Tsukuba, Japan)
- Mitsuharu Uemoto (University of Tsukuba, Japan)
- Kazuhiro Yabana (University of Tsukuba, Japan)
- Atsushi Yamada (University of Tsukuba, Japan)
- Shunsuke Yamada (University of Tsukuba, Japan)
- Maiku Yamaguchi (University of Tokyo, Japan)

(Alphabetic order)

# Pseudopotential and Functional

- pseudopotential files
  - Yabana-Bertsch format
  - .pspnc (ABINIT format:  
[https://www.abinit.org/sites/default/files/PrevAtomicData/psp-links/psp-links/lda\\_tm](https://www.abinit.org/sites/default/files/PrevAtomicData/psp-links/psp-links/lda_tm))
  - .cpi and .fhi (fhi98PP format:  
[https://www.abinit.org/sites/default/files/PrevAtomicData/psp-links/psp-links/lda\\_fhi](https://www.abinit.org/sites/default/files/PrevAtomicData/psp-links/psp-links/lda_fhi))
- Exchange-Correlation functions

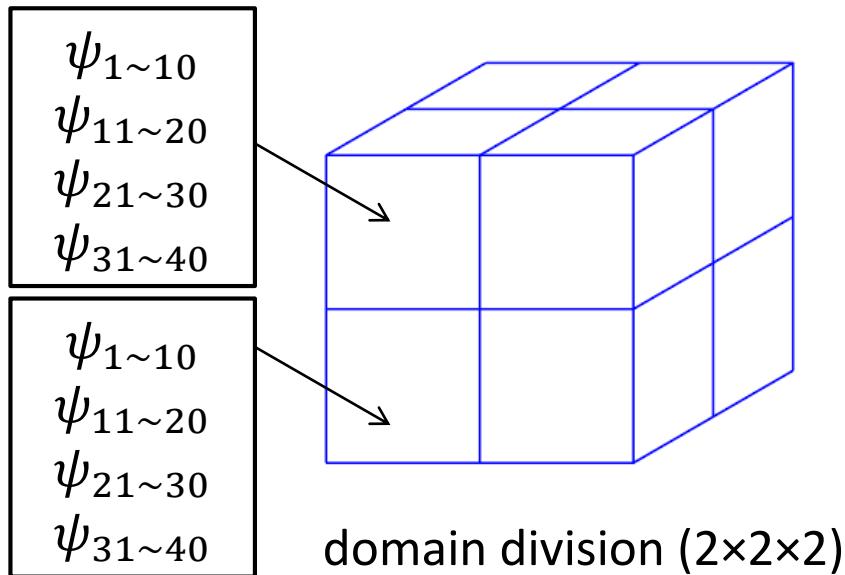
	Isolated systems	Periodic systems
LDA-PZ (Perdew-Zunger LDA)	✓	✓
LSDA-PZ (Perdew-Zunger LSDA)	✓	
PAM (Perdew-Zunger LDA with modification)		✓
TBmBJ (Tran-Blaha meta-GGA exchange with Perdew-Wang correlation)		✓
LibXC without kinetic terms	✓	✓

# Parallelization

- isolated systems

Kohn-Sham orbital:  $\psi_n(\mathbf{r})$

➤ MPI: orbital and domain

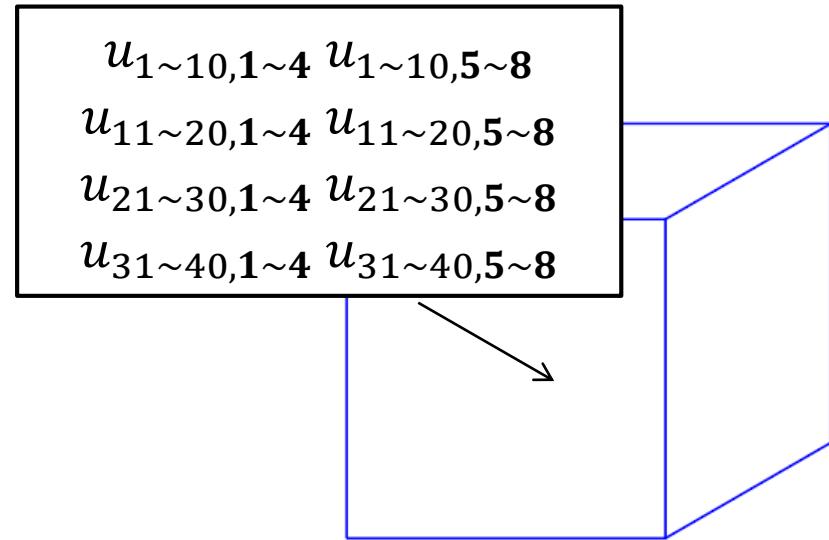


➤ OpenMP: domain

- periodic systems

Bloch orbital:  $u_{n\mathbf{k}}(\mathbf{r})$

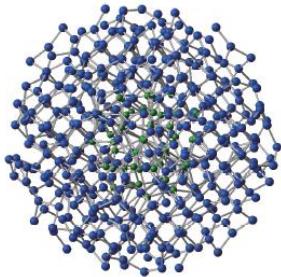
➤ MPI: k points



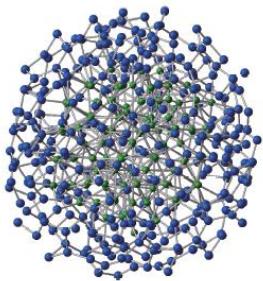
This parallelization is done automatically.

# Performance (1)

$\text{Ag}_{54}@\text{Si}_{454}$

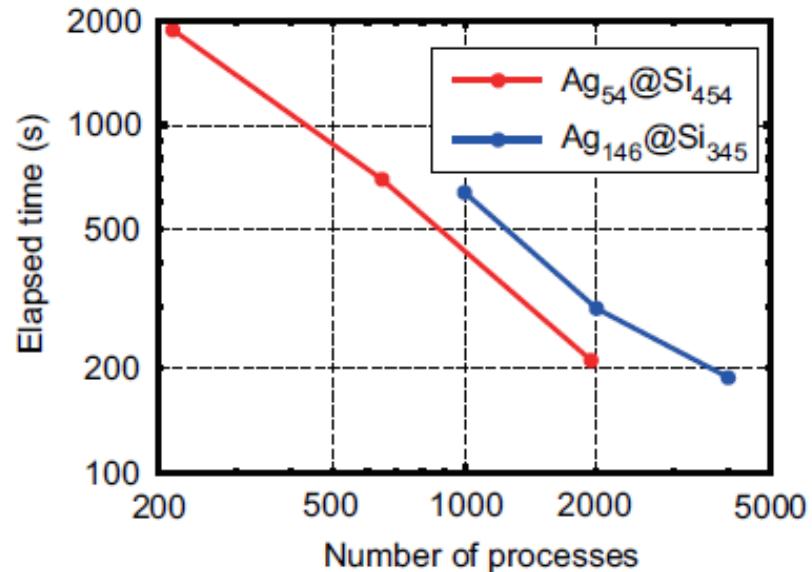


$\text{Ag}_{146}@\text{Si}_{345}$



Diameter: 2.5nm

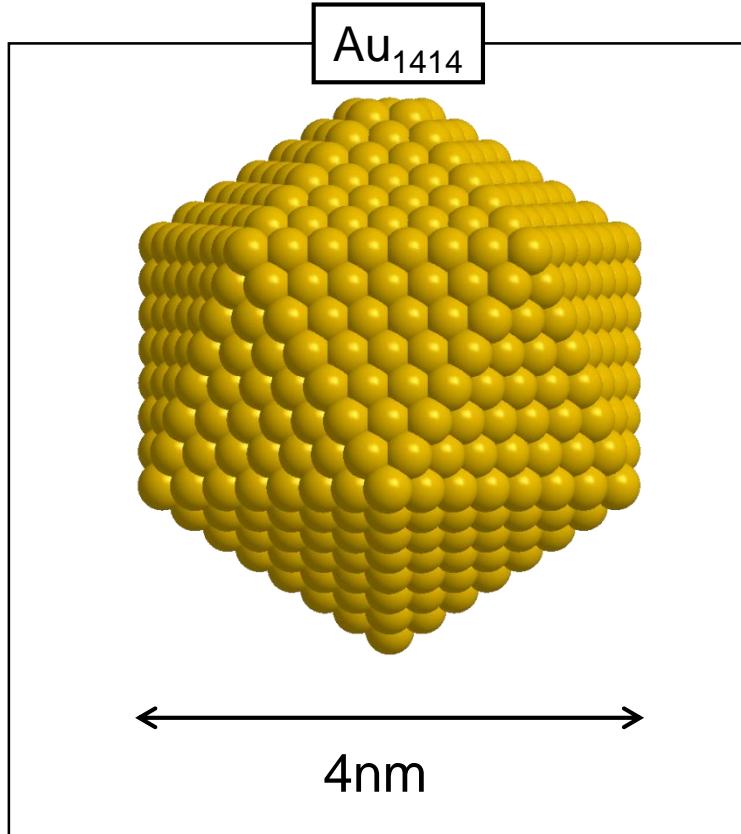
The K computer (RIKEN)  
Time steps: 1000



System	CPU performance
$\text{Ag}_{54}@\text{Si}_{454}$	12.1% (1,944 processes)
$\text{Ag}_{146}@\text{Si}_{345}$	9.2% (4,000 processes)

Calculations for product runs end in 1.4 hours.

# Performance (2)



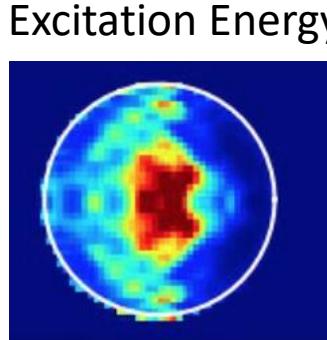
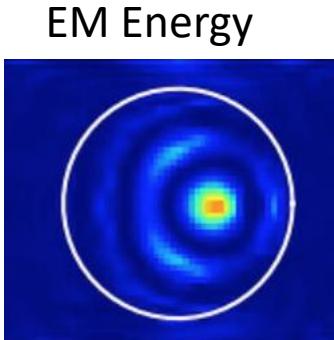
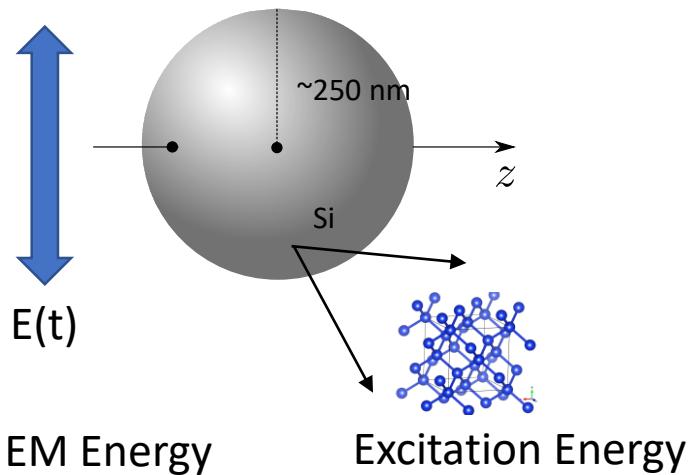
The K computer (RIKEN)

Number of processes	CPU performance
7,800	11.0%
15,600	9.3%

Calculations for product runs end in 7 hours with 15,600 processes.

# Performance (3)

## Laser Excitation Silicon Nanosphere



~ 24,000 [Node Hours] for Computation

## Computation



- World-class many-core supercomputer  
**"Oakforest-PACS" (OFP)**
  - Processor:
    - Intel Xeon Phi 7250 (68 cores 1.4GHz base clock)
  - Number of Nodes:
    - **8208 nodes (use up to 8192)**
  - Theoretical Peak Performance
    - 25 PFLOPS

# Program: Exercise-1

14:15-16:15, November 12

## Exercise-1. Installation of SALMON

- Log-in to Super-computer
- Build and Install
- Submit Job

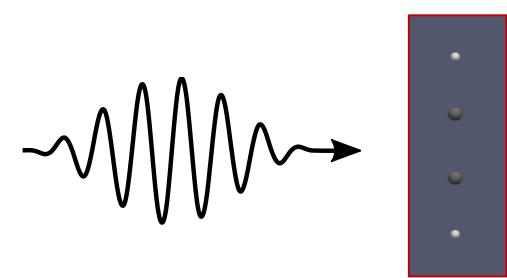


# Program: Exercise-2 & Exercise-3

16:30-17:30, November 12

## Exercise-2. How to use SALMON – Isolated Systems

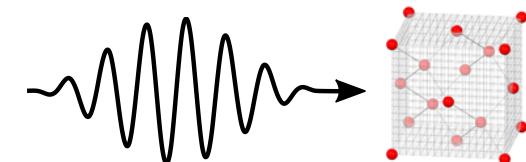
- Input file format
- Calculations of the ground state, polarizability and photoabsorption of  $C_2H_2$  molecule
- Calculation of electron dynamics in  $C_2H_2$  molecule under a pulsed electric field



14:00-15:00, November 13

## Exercise-3. How to use SALMON – Periodic Systems

- Calculation of the ground state
- Calculations of dielectric function of crystalline silicon
- Calculations of electron dynamics in crystalline silicon under a pulsed electric field

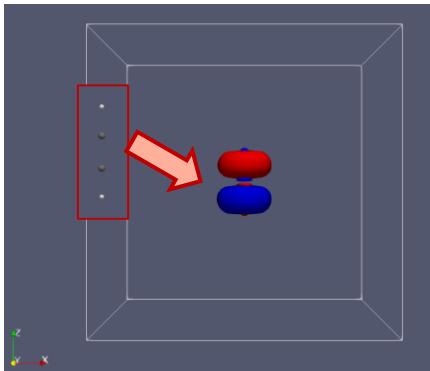


# Program: Exercise-4

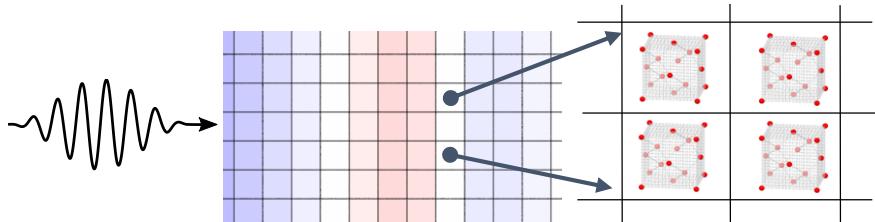
15:15-17:15, November 13

## Exercise-4. How to use SALMON – Advanced Options

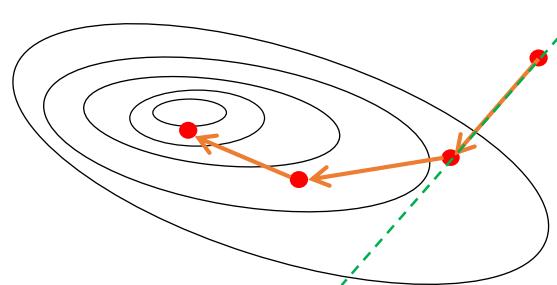
### 4-1 Visualization



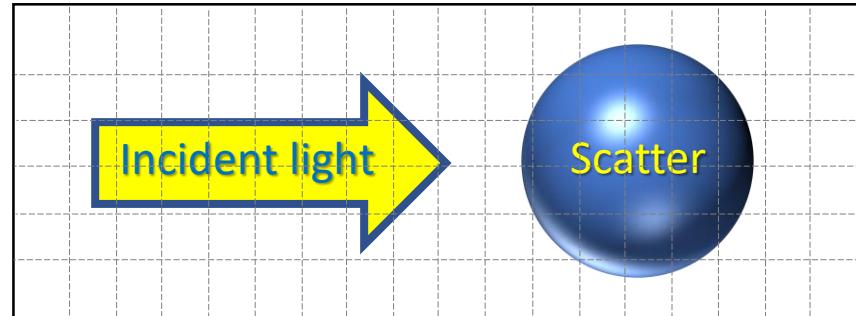
### 4-2 Multi-scale simulation



### 4-3 Optimization and Nonadiabatic Molecular Dynamics



### 4-4 FDTD simulation



# Information

Download the PDF files  
of the tutorial slide → <http://salmon-tddft.jp/download/tutorial2018-pdf.zip>

<https://salmon-tddft.jp>

Download of a source  
and a manual

Web manual

The screenshot shows the SALMON website's main page. On the left, a sidebar menu lists various sections: Home, About SALMON, Download (circled in yellow), Install and Run, Input Variables, Exercises, Documents (circled in yellow), References, User Community, Events, and Utilities. To the right, there is a large section titled "Selected Features" containing six sub-sections with corresponding images: "Grid system for molecules" (a 3D grid with atoms), "Electron dynamics in solids" (two 2D plots showing electron density), "Multiscale grid system" (a 3D grid with different resolutions), "Optical near field" (two 2D plots showing optical fields), "Strong field on silicon" (a 2D heatmap of electric field intensity on a silicon surface), and "Absorption of nano-particle" (a plot of oscillator strength vs energy with peaks labeled at 1467, 1414, 922, 569, 308 eV).

# SALMON

Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience  
<http://salmon-tddft.jp/>

SALMON TUTORIAL, TSUKUBA, 2018

# Information (continued)

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

Download of  
a source file

Download				
Latest Release (1.2.0)				
	Date	Filetype	Download link	MD5 check sum
<b>Unix/Linux Source</b>	2018-10-25	Tarball (gzip)	<a href="#">SALMON-v.1.2.0.tar.gz (602k)</a>	a1ff15cf0f7c39c43b9ae81c30b9bac6
<b>Manual</b>	2018-10-25	pdf	<a href="#">Manual_SALMON-v.1.2.0_simple.pdf</a>	

Web manual

Documents	
Manual for SALMON	
Contents	PDF file
Manual for SALMON-v.1.2.0	<a href="#">Manual_SALMON-v.1.2.0_20181025.pdf</a>
Manual for SALMON-v.1.1.0	<a href="#">Manual_SALMON-v.1.1.0_20180929.pdf</a>
Manual for SALMON-v.1.0.0	<a href="#">Manual_SALMON-v1.0.0.pdf</a>
Web Manual for SALMON	
Contents	
<a href="#">Web Manual for SALMON-v.1.2.0</a>	
<a href="#">Web Manual for SALMON-v.1.1.0</a>	
Documents of past events	
A tutorial seminar with hands-on session, Nov. 24, 2017 at Univ. of Tsukuba	
Contents	PDF file