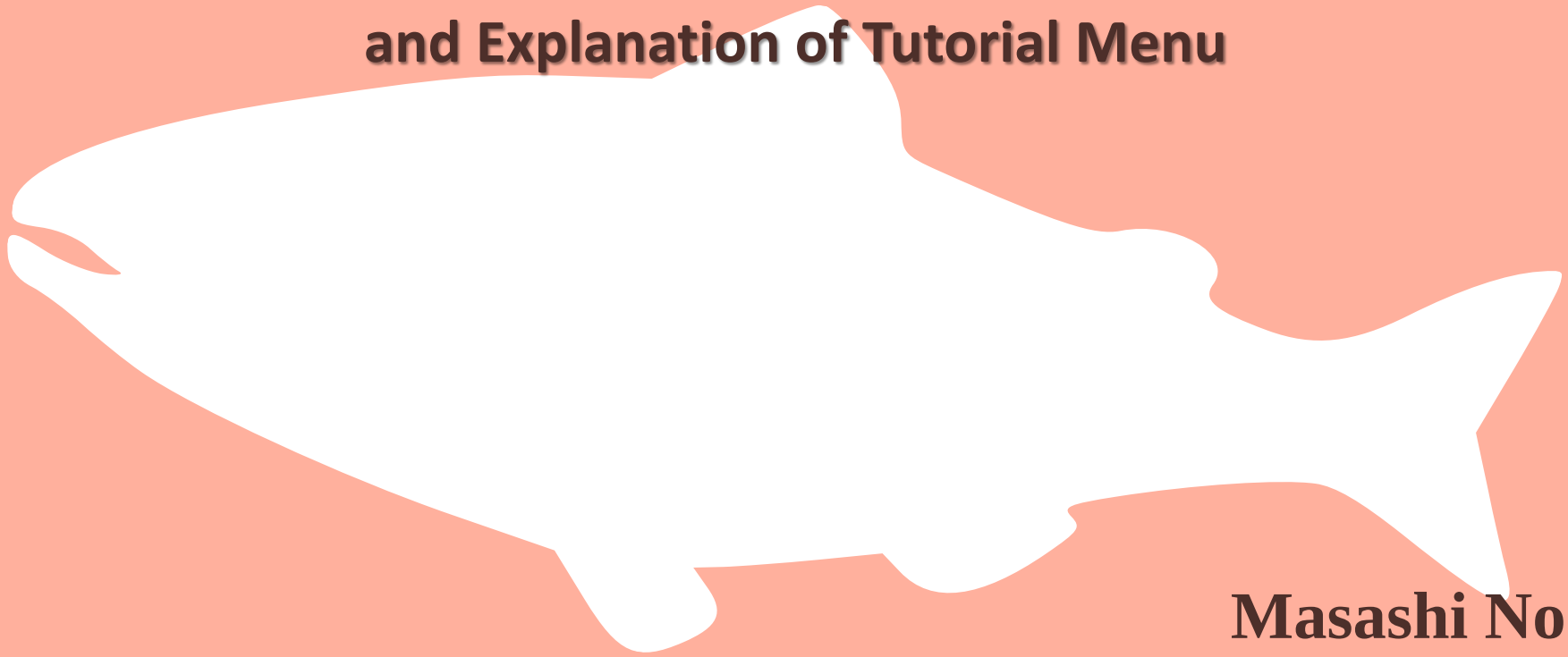
Introduction

About SALMON software package and Explanation of Tutorial Menu



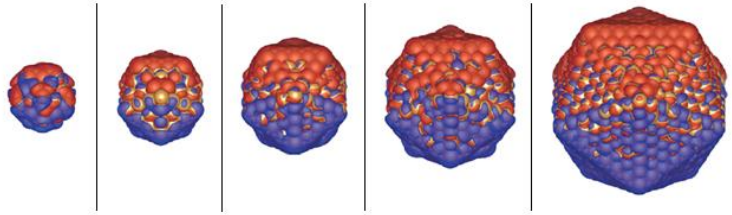
Masashi Noda

Center for Computer Science, University of Tsukuba

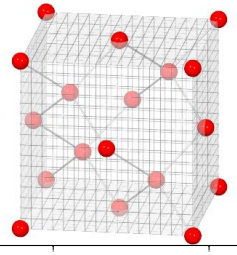
What is SALMON?

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

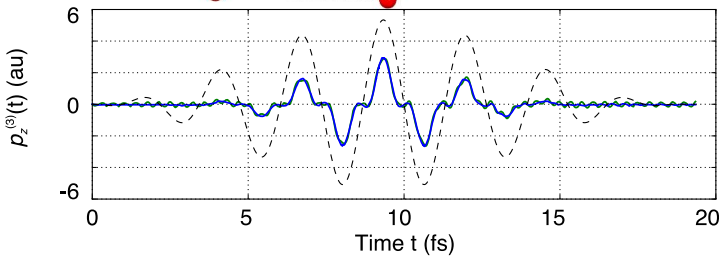
- Real-time electron dynamics



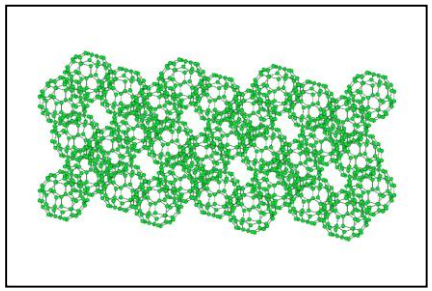
- Non-linear optical response

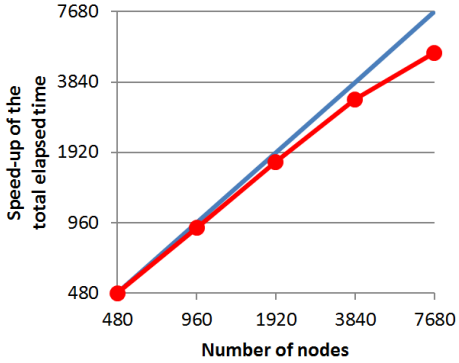


$\mathbf{p}^{(3)}(t)$

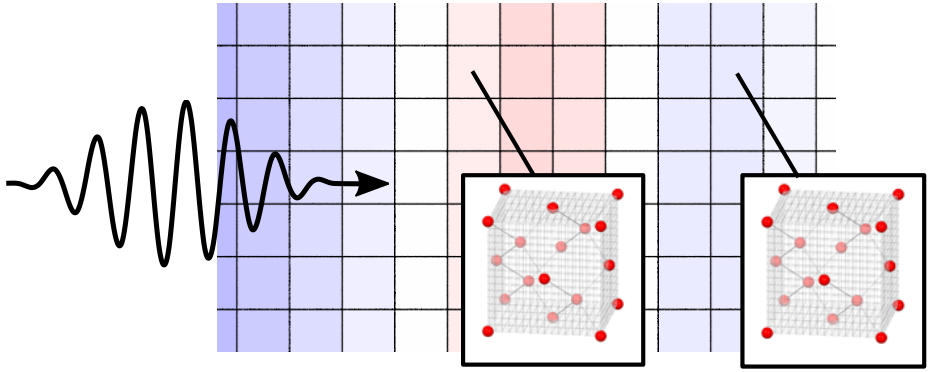


- Massive parallelization





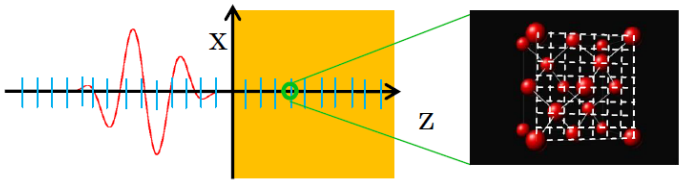
- Couple with Maxwell equation



Overview of SALMON

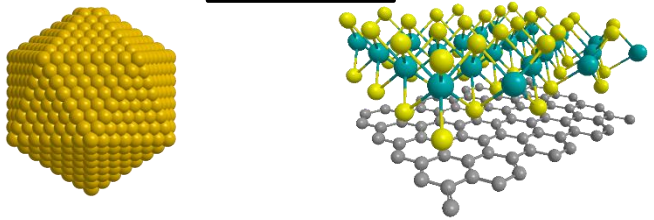
K. Yabana and G. F. Bertsch, Phys. Rev. B 54, 4484 (1996)

ARTED

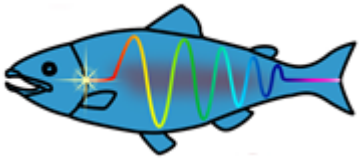


- solid/surface
- laser damage
- attosecond
- nanostructure (multiscale)

GCEED



- cluster/surface/interface
- optical near field
- bias voltage
- nanostructure (microscale)



SALMON

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

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

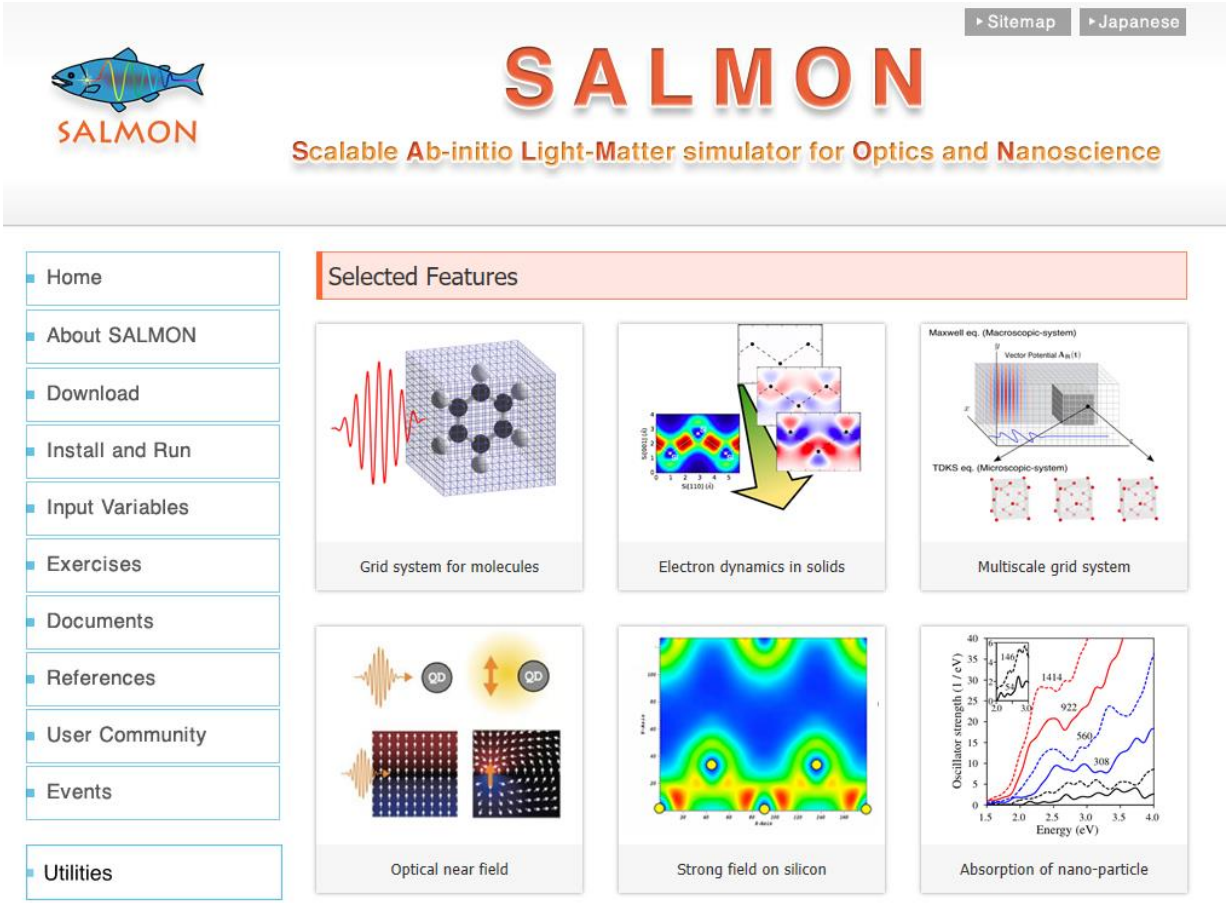
plane-wave first-principles code, a large-scale calculation

➢ SIESTA, Elk FP-LAPW

utilization of numerical atomic orbitals

License

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



- License: Apache 2.0
- Mailing list: 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:

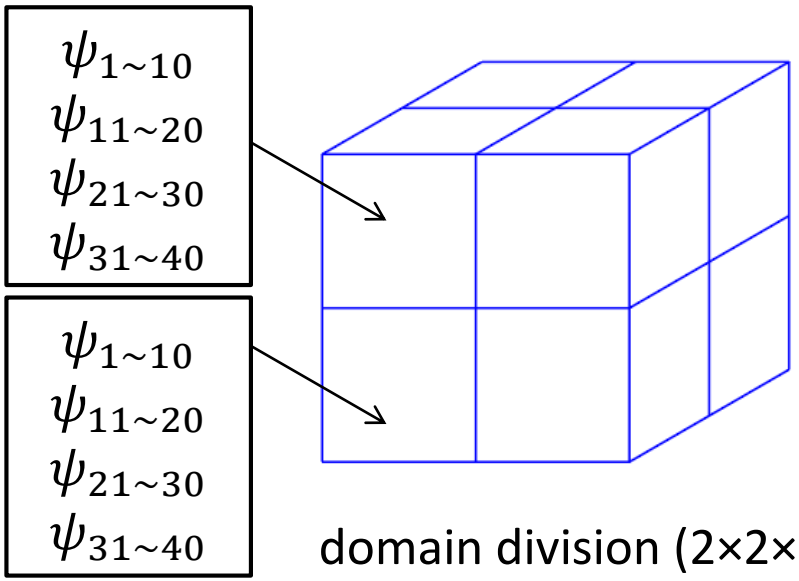
    https://www.abinit.org/sites/default/files/PrevAtomicData/psp-links/psp-links/lda_tm)
  - .cpi and .fhi (fhi98PP format:

    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

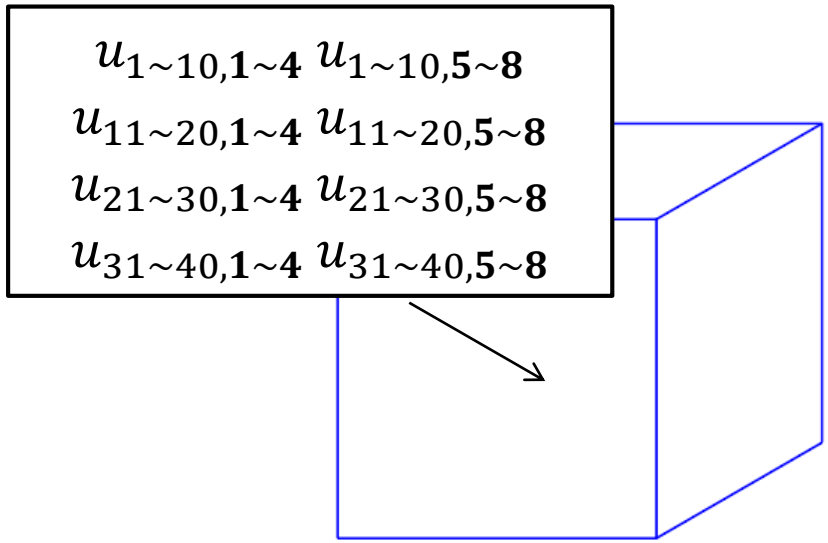
- isolated systems
  Kohn-Sham orbital: $\psi_n(\boldsymbol{r})$
  - ➢ MPI: orbital and domain



domain division (2×2×2)

  - ➢ OpenMP: domain

- periodic systems
  Bloch orbital: $u_{n\boldsymbol{k}}(\boldsymbol{r})$
  - ➢ MPI: k points

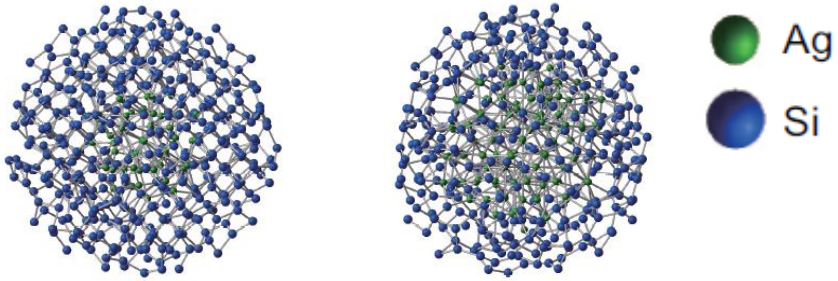


  - ➢ OpenMP: orbital and k points

This parallelization is done automatically.

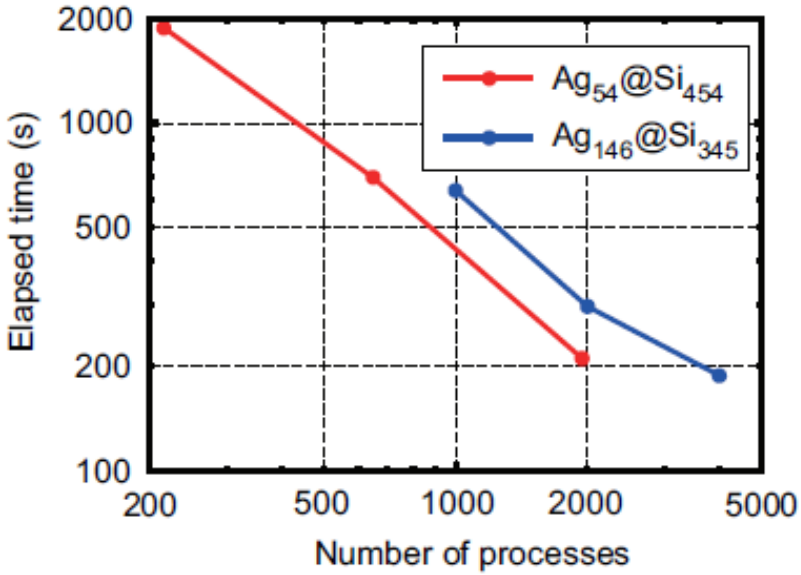
Performance (1)

$Ag_{54}@Si_{454}$ $Ag_{146}@Si_{345}$



Diameter: 2.5nm

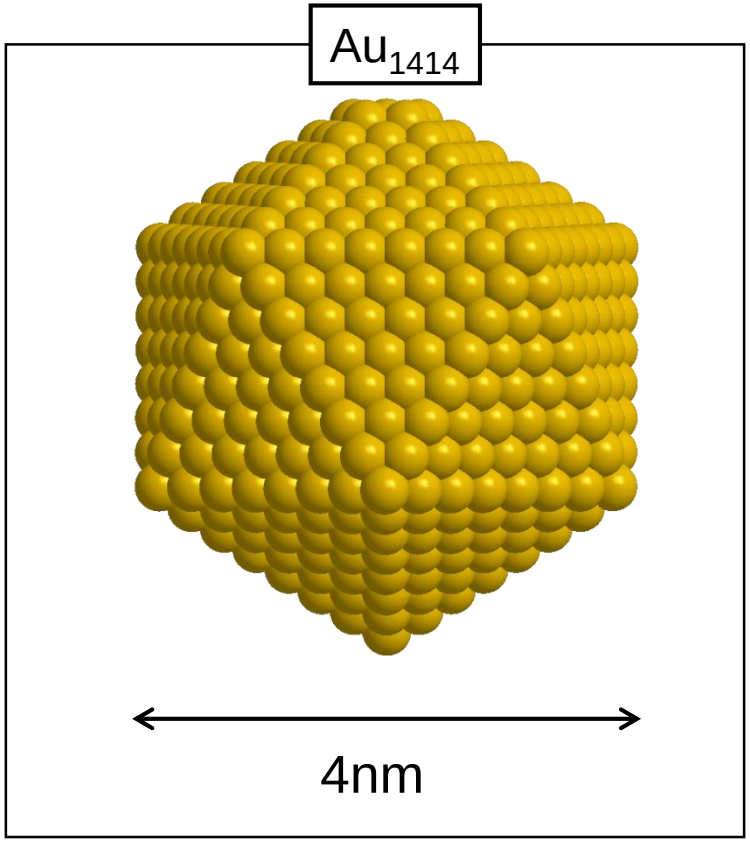
The K computer (RIKEN)
Time steps: 1000



System	CPU performance
$Ag_{54}@Si_{454}$	12.1% (1,944 processes)
$Ag_{146}@Si_{345}$	9.2% (4,000 processes)

Calculations for product runs end in 1.4 hours.

Performance (2)



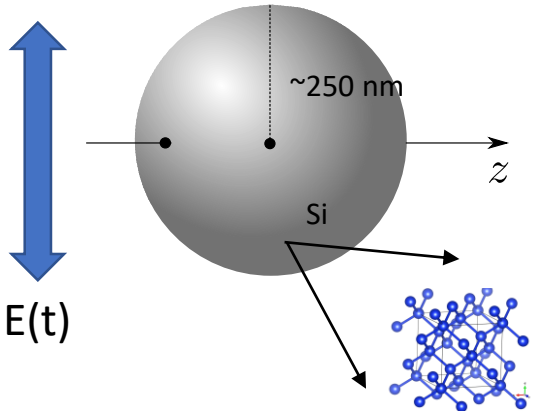
The K computer (RIKEN)

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

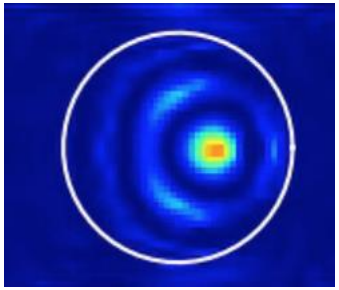
Calculations for product runs end in 7 hours with 15,600 processes.

Performance (3)

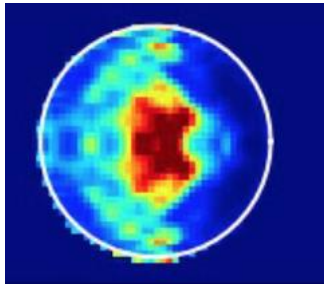
Laser Excitation Silicon Nanosphere



EM Energy



Excitation Energy



~ 24,000 [Node Hours] for Computation

Computation

- World-class many-core supercomputer **"Oakforest-PACS" (OFP)**
  - Processer:
    - 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

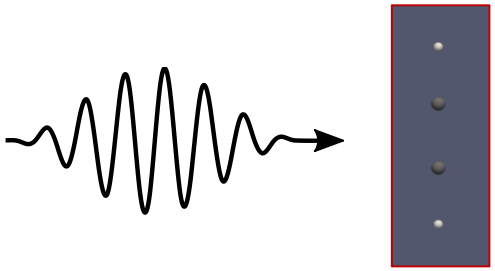
- Log-in to Super-computer
- Build and Install
- Submit Job

Program: Exercise-2 & Exercise-3

16:30-17:30, November 12

Exercise-2. How to use SALMON – Isolated Systems

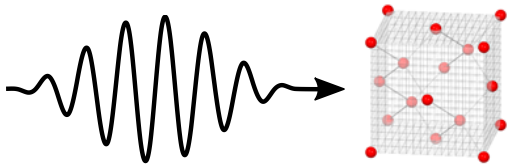
- Input file format
- Calculations of the ground state, polarizability and photoabsorption of C_2H_2 molecule
- Calculation of electron dynamics in C_2H_2 molecule under a pulsed electric field



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

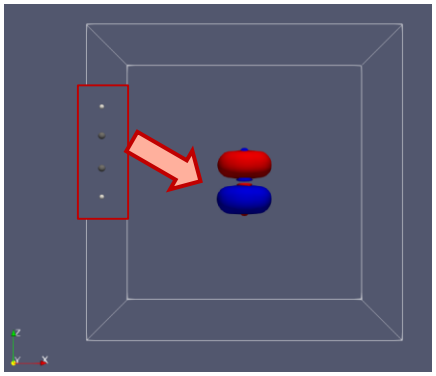


Program: Exercise-4

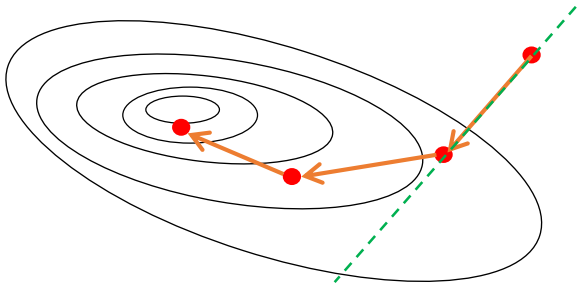
15:15-17:15, November 13

Exercise-4. How to use SALMON – Advanced Options

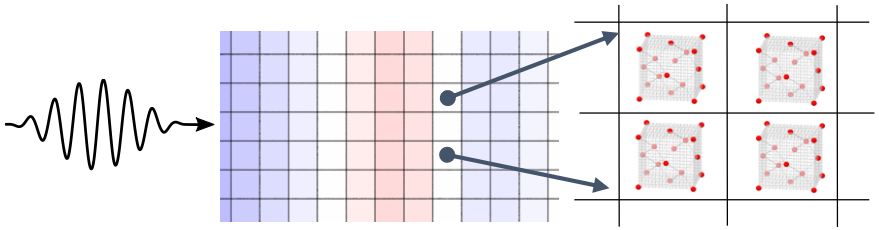
4-1 Visualization



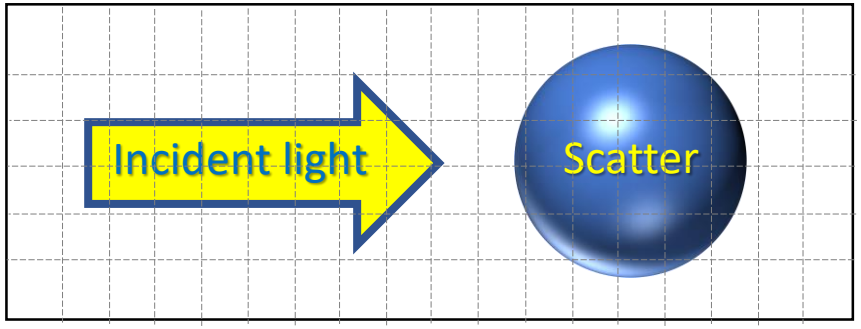
4-3 Optimization and
Nonadiabatic Molecular Dynamics



4-2 Multi-scale simulation



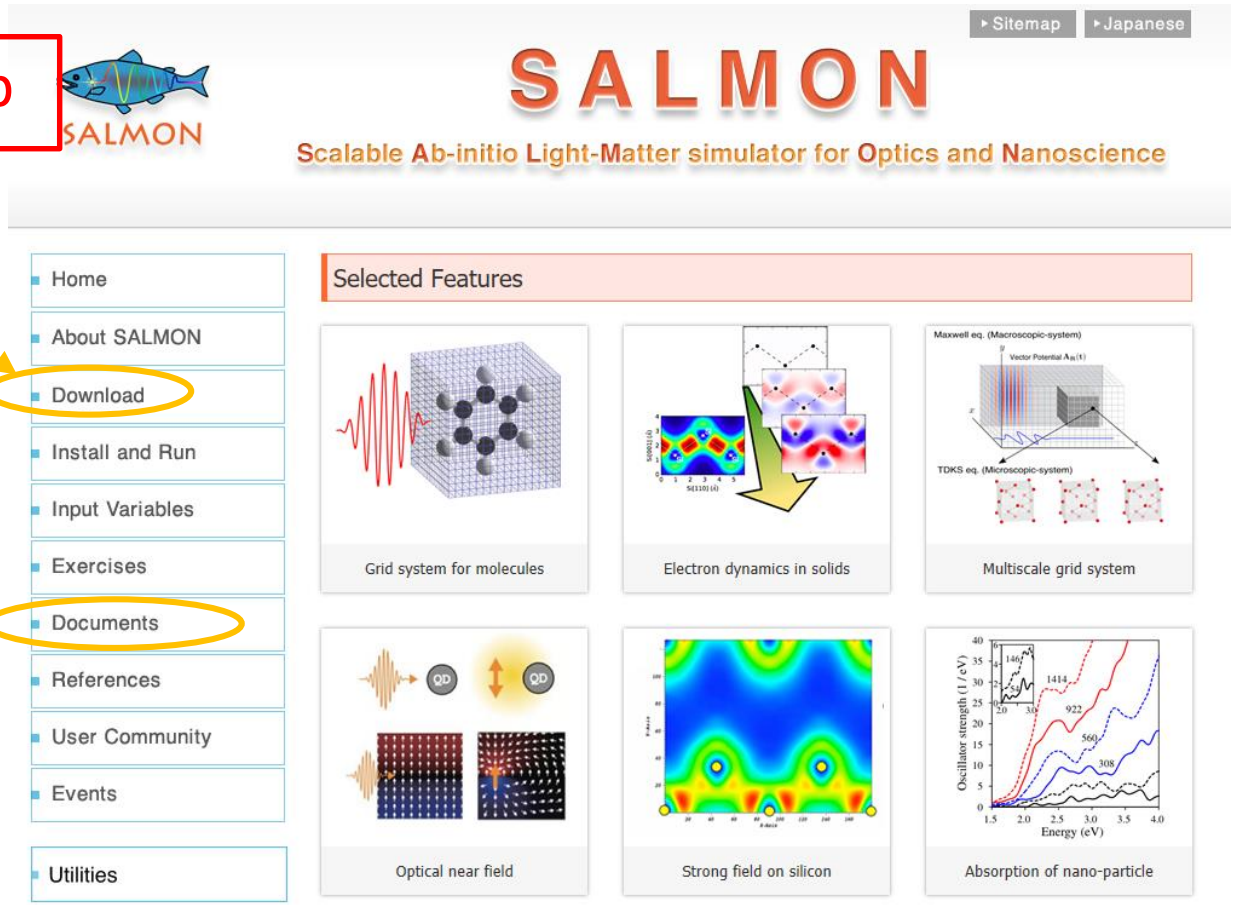
4-4 FDTD simulation



Information

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

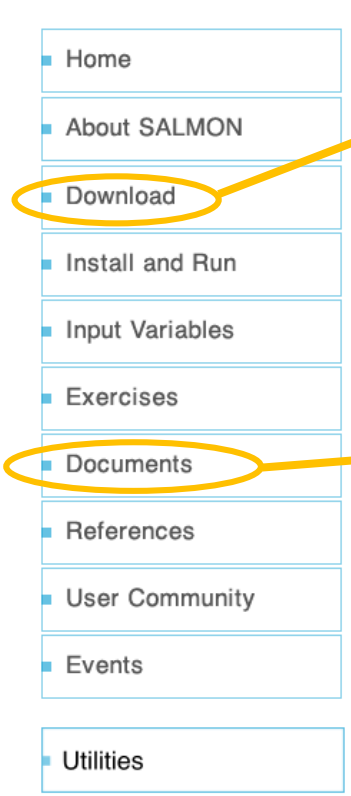
https://salmon-tddft.jp



Download of a source and a manual

Web manual

Information (continued)



Download of a source file

Web manual

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Latest Release (1.2.0)

	Date	Filetype	Download link	MD5 check sum
Unix/Linux Source	2018-10-25	Tarball (gzip)	SALMON-v.1.2.0.tar.gz (602k)	a1ff15cf0f7c39c43b9ae81c30b9bac6
Manual	2018-10-25	pdf	Manual_SALMON-v.1.2.0_simple.pdf	

Documents

Manual for SALMON

Contents	PDF file
Manual for SALMON-v.1.2.0	Manual_SALMON-v.1.2.0_20181025.pdf
Manual for SALMON-v.1.1.0	Manual_SALMON-v.1.1.0_20180929.pdf
Manual for SALMON-v.1.0.0	Manual_SALMON-v1.0.0.pdf

Web Manual for SALMON

Contents
Web Manual for SALMON-v.1.2.0
Web Manual for SALMON-v.1.1.0

Documents of past events

A tutorial seminar with hands-on session, Nov. 24, 2017 at Univ. of Tsukuba

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