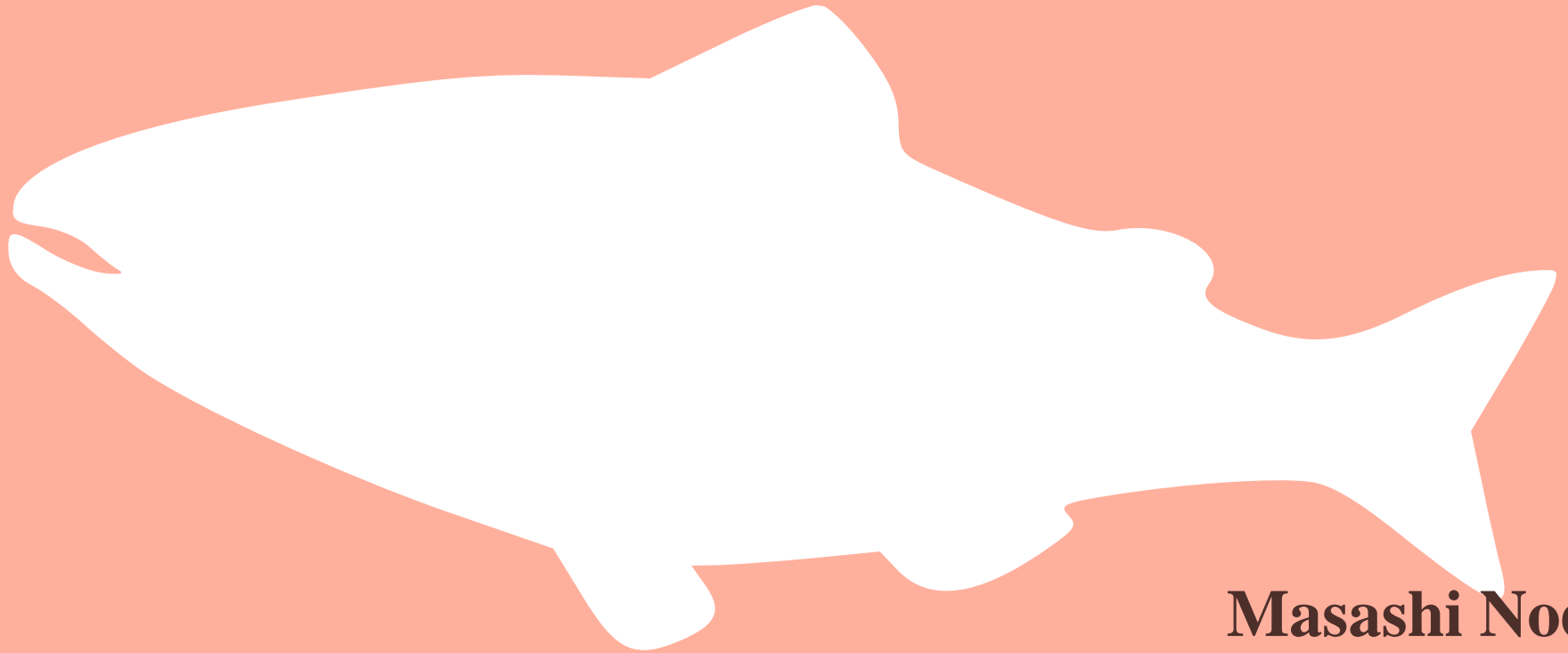


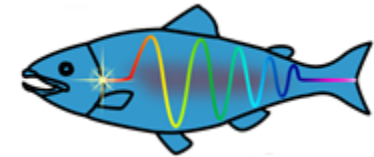
# Basics of SALMON



**Masashi Noda**  
*Institute for Molecular Science*

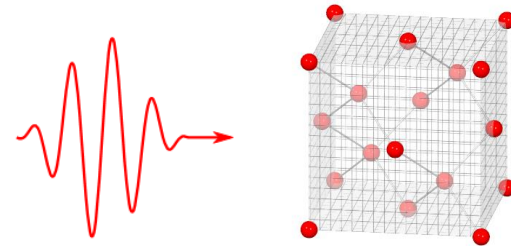
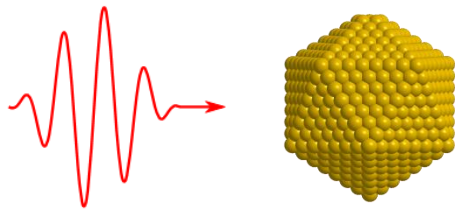
# What is SALMON?

Scalable **A**b-initio **L**ight-**M**atter simulator  
for **O**ptics and **N**anoscience



**SALMON**

- A software to calculate electron dynamics and optical responses
- Real-time and real-space
- Treatment of light-matter interaction

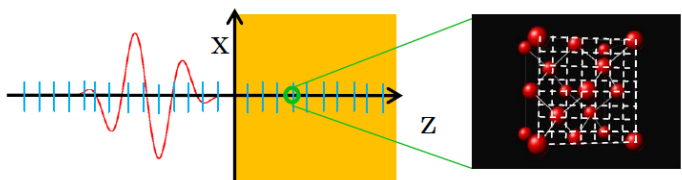


- Dielectric functions and polarizability

# Overview of SALMON

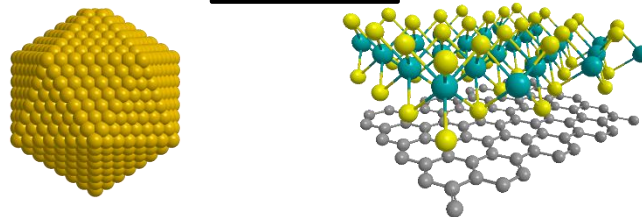
K. Yabana and G. F. Bertsch, Phys. Rev. B 54, 4484 (1996)

ARTED

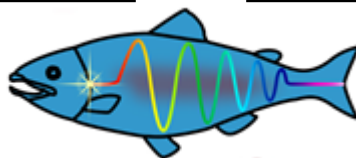


- solid/surface
- laser damage
- attosecond
- nanostructure (multiscale)

GCEED



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



## SALMON

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

# SALMON

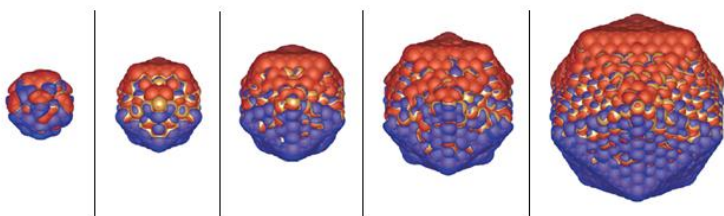
Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience

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

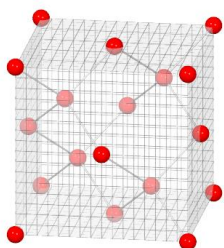
SALMON TUTORIAL, TSUKUBA, 2017

# Characteristics of SALMON

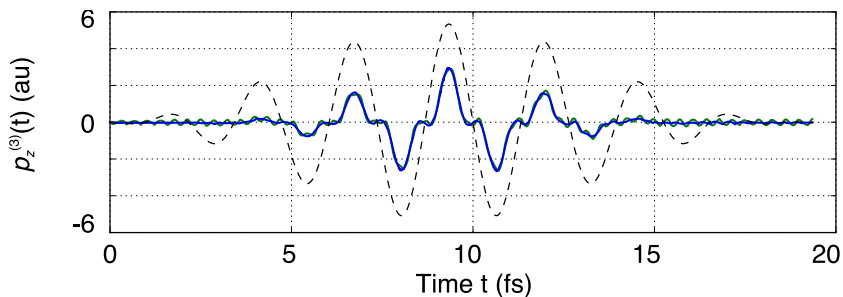
- Real-time electron dynamics



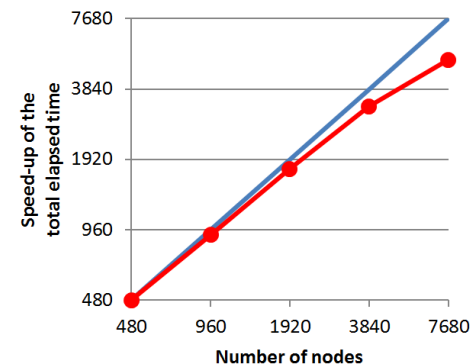
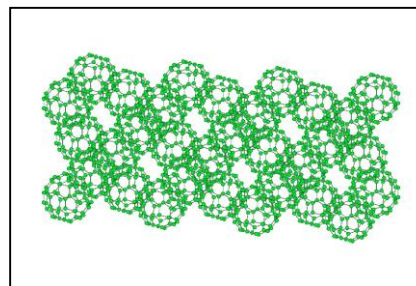
- Non-linear optical response



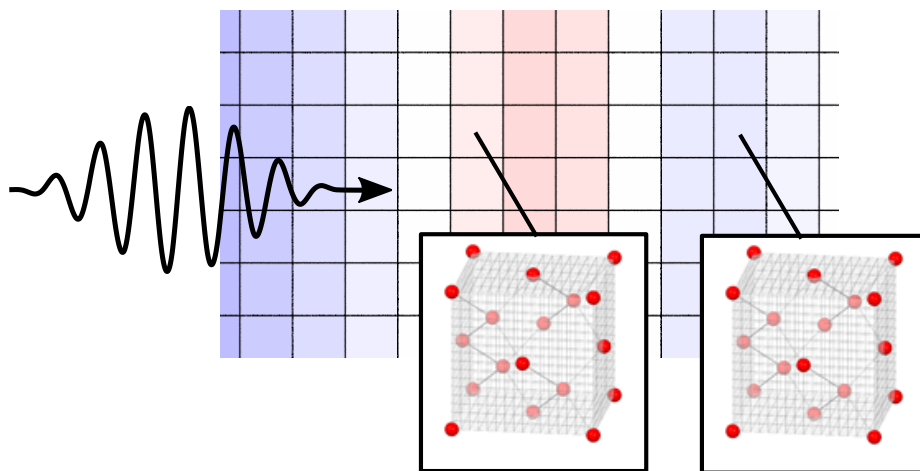
$$p^{(3)}(t)$$



- Massive parallelization




- Couple with Maxwell equation



# Development environment

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



The screenshot shows the main page of the SALMON project website. At the top left is a logo featuring a blue fish with a rainbow-like pattern, with the word "SALMON" in red below it. To the right of the logo are navigation tabs for "Main page" (selected) and "Discussion", and a search bar containing "Search salmon". Below the logo is a vertical menu with links for "About SALMON", "download", "Documents", "Samples", "References", "Development", "User Information", and "Events". Further down are "Navigation" links (Main page, Recent changes, Random page, Help) and "Tools" links (What links here, Related changes, Special pages, Printable version, Permanent link, Page information). The main content area has a heading "Main Page" and a paragraph: "SALMON (Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience) is an open-source software based on first-principles time-dependent density functional theory to describe optical responses and electron dynamics in matters induced by light electromagnetic fields. At present, SALMON is under a trial release. We plan to release an official version by the end of October, 2017." Below this is a bulleted list of links: "About SALMON", "Download", "Documents", "Samples", "References", "Development", "User Information", and "Events". At the bottom of the page, it states "This page was last modified on 16 October 2017, at 08:46." and includes links for "Privacy policy", "About salmon", and "Disclaimers". A "Powered By MediaWiki" logo is in the bottom right corner.

- License: Apache 2.0
- Mailing list: [salmon-users@salmon-tddft.jp](mailto:salmon-users@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 (Institute for Molecular Science, 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 (Institute 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)

# Time-dependent Kohn-Sham equations

- isolated system (length gauge)

$$i\hbar \frac{\partial}{\partial t} \psi_n(\mathbf{r}, t) = \left\{ -\frac{1}{2} \nabla^2 + V_{ext}(\mathbf{r}, t) + V_{ion} + V_H + V_{xc} \right\} \psi_n(\mathbf{r}, t)$$

$\psi_n$ : Kohn-Sham orbital

$V_H$ : Hartree potential

$V_{ext}(\mathbf{r}, t)$ : External scalar potential

$V_{xc}$ : Exchange-correlation potential

$V_{ion}$ : Electron-nuclear interaction potential

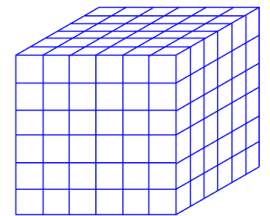
- periodic system (velocity gauge)

$$i\hbar \frac{\partial}{\partial t} u_{n\mathbf{k}}(\mathbf{r}, t) = \left\{ \frac{1}{2} \left( -i\hbar \nabla + \hbar \mathbf{k} + \frac{e}{c} \mathbf{A}(t) \right)^2 + V_{ion} + V_H + V_{xc} \right\} u_{n\mathbf{k}}(\mathbf{r}, t)$$

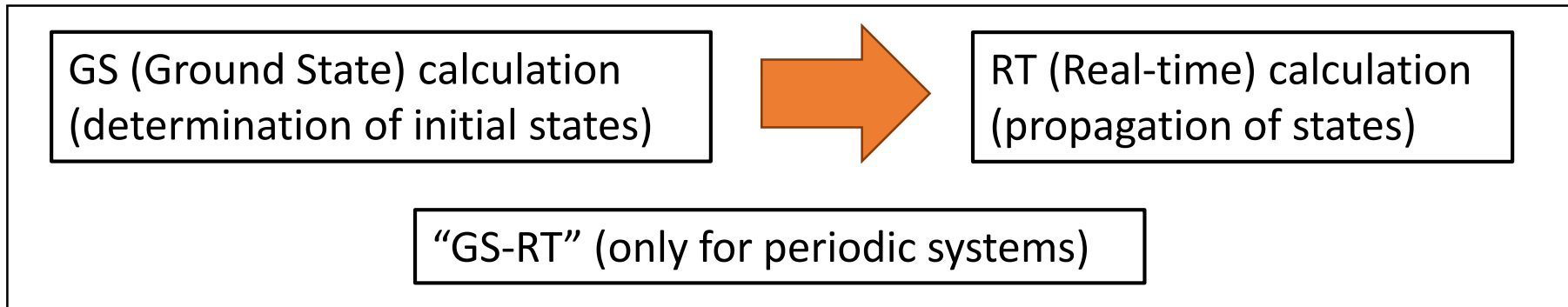
$u_{n\mathbf{k}}$ : Bloch orbital

$\mathbf{k}$ : wave vector       $\mathbf{A}(t)$ : External vector potential

Physical quantities are expressed on grid.



# Flowchart of SALMON



## GS calculation

- Isolated system (length gauge)

$$\left\{ -\frac{1}{2} \nabla^2 + V_{ion} + V_H + V_{xc} \right\} \psi_n(\mathbf{r}) = \epsilon_n \psi_n(\mathbf{r})$$

$\epsilon_n$ : 1-particle energy

- periodic system (velocity gauge)

$$\left\{ \frac{1}{2} (-i\hbar\nabla + \hbar\mathbf{k})^2 + V_{ion} + V_H + V_{xc} \right\} u_{nk}(\mathbf{r}) = \epsilon_{nk} u_{nk}(\mathbf{r})$$



# Pseudopotential

- Norm-conserving pseudopotential (Kleiman and Bylander separable form)

$$V_{ion} = V_{local} + \sum_{lm} \frac{|\psi_{lm}^{PS} v_l\rangle \langle v_l \psi_{lm}^{PS}|}{\langle \psi_{lm}^{PS} | v_l | \psi_{lm}^{PS} \rangle}$$

$V_{local}$ : local part of pseudopotential

$v_l$ : non-local part of pseudopotential

$\psi_{lm}^{PS}$ : pseudowavefunction

- pseudopotential files treated by SALMON

➤ 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

- Adiabatic approximation
- Exchange-correlation potential

$$V_{xc}(\mathbf{r}) = \epsilon_{xc}([n], \mathbf{r}) + n(\mathbf{r}) \frac{\delta \epsilon_{xc}([n], \mathbf{r})}{\delta n(\mathbf{r})}$$

$\epsilon_{xc}$ : energy per electron       $n$ : electron density

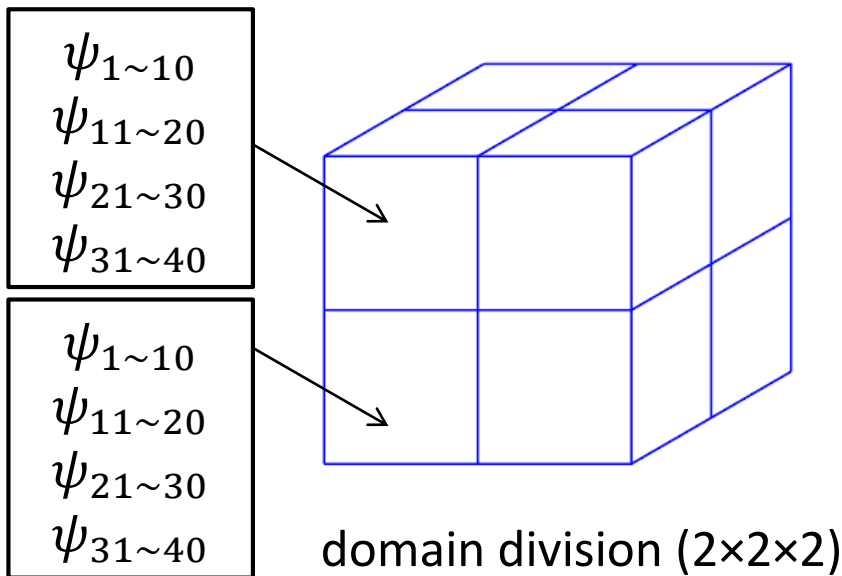
- Exchange-Correlation functions

	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)		✓

# Parallelization (1)

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

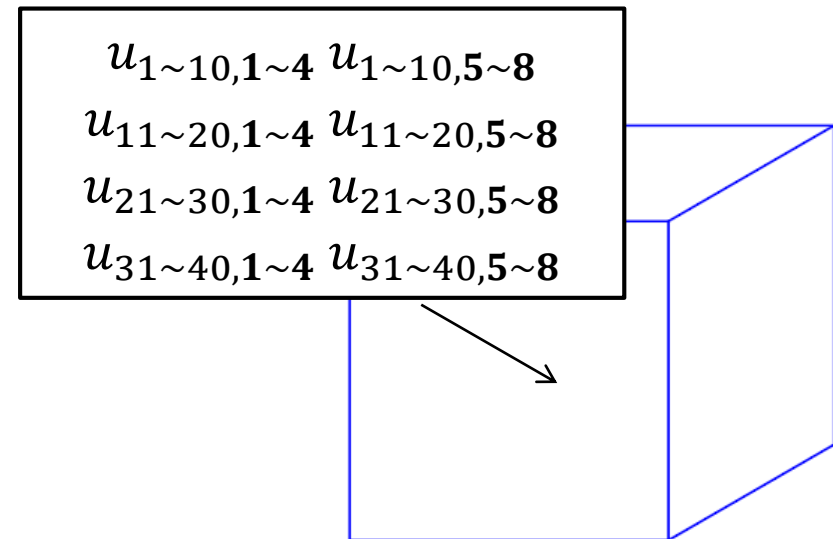
➤ MPI: orbital and domain



➤ OpenMP: domain

- periodic systems  
Bloch orbital:  $u_{nk}(\mathbf{r})$

➤ MPI: orbital and k points

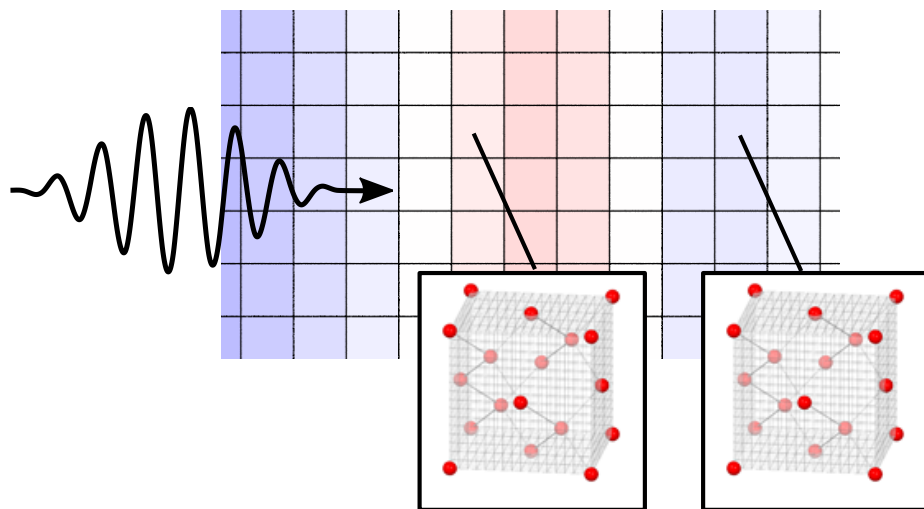


➤ OpenMP: orbital and k points

This parallelization is done automatically.

# Parallelization (2)

- multiscale calculation

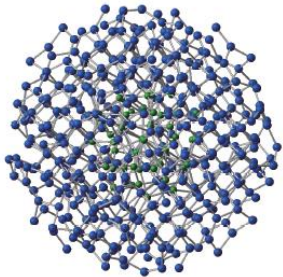


- MPI:  
macroscopic grids  
orbital and k points ( $u_{nk}(\mathbf{r})$ )  
in microscopic cell
- OpenMP:  
orbital and k points ( $u_{nk}(\mathbf{r})$ )  
in microscopic cell

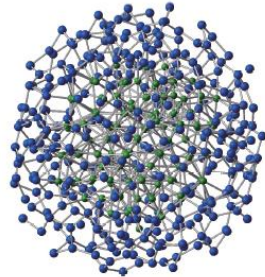
This parallelization is done automatically.

# Performance (1)

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

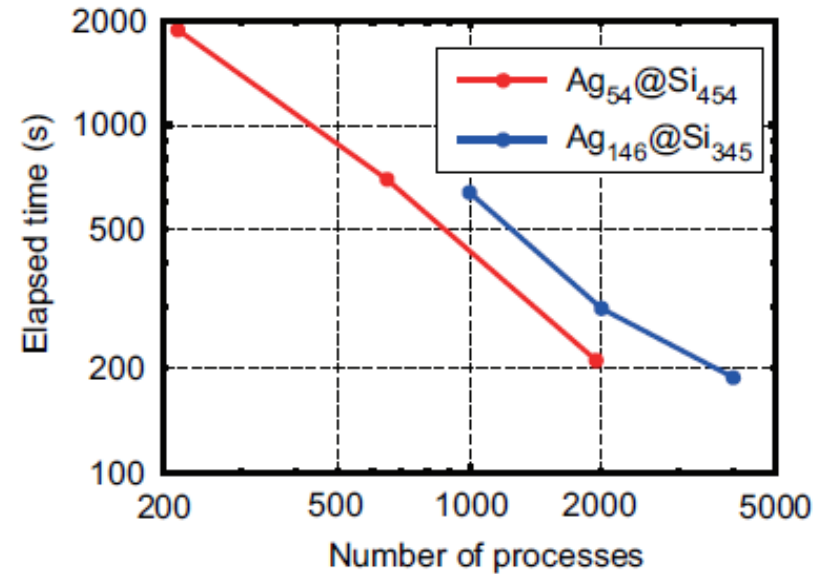


$\text{Ag}_{146}@\text{Si}_{345}$



Diameter: 2.5nm

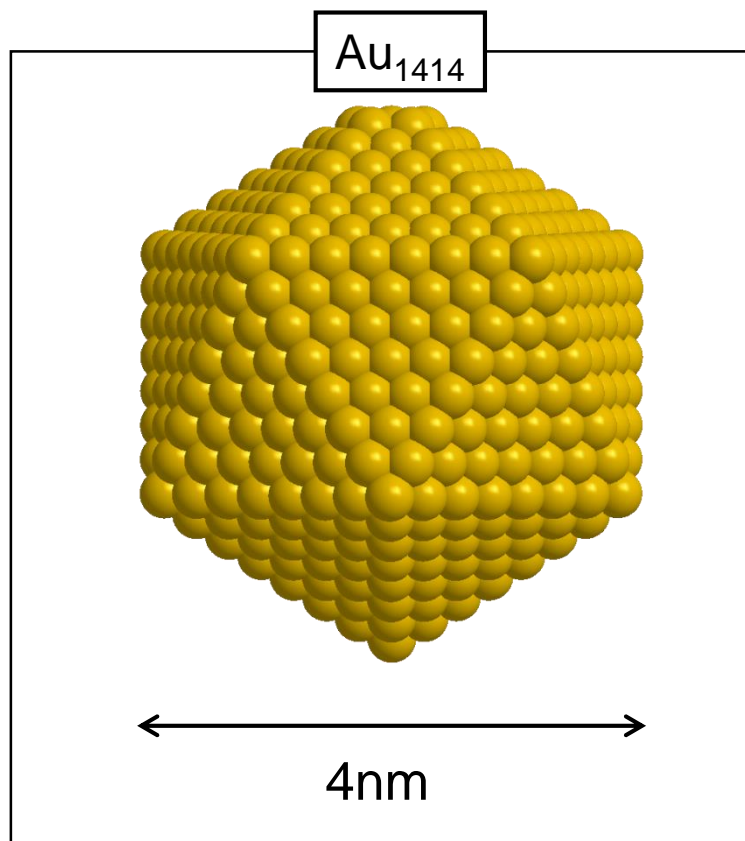
Used computer: K computer (RIKEN)  
Time steps: 1000



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)



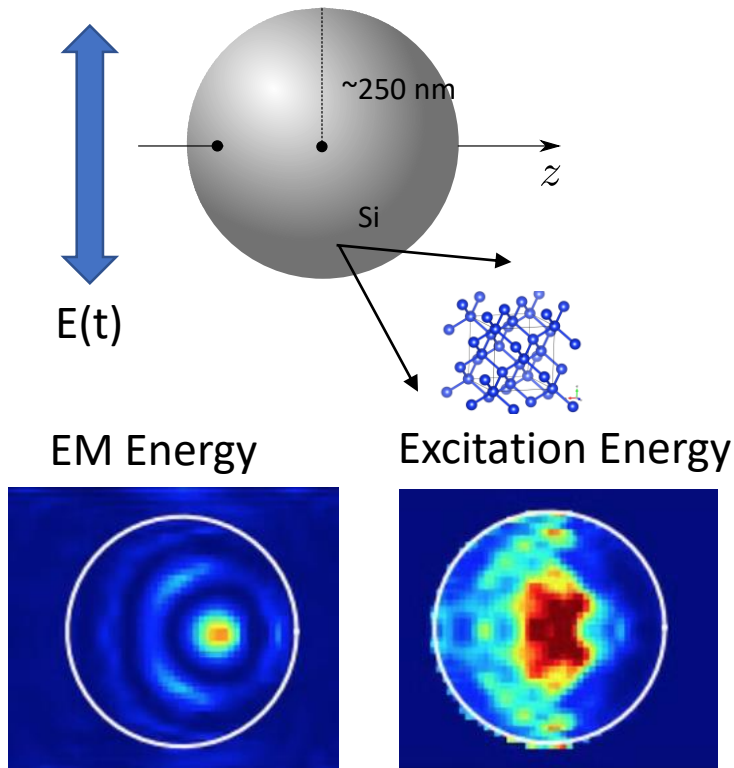
Used computer: K computer (RIKEN)

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