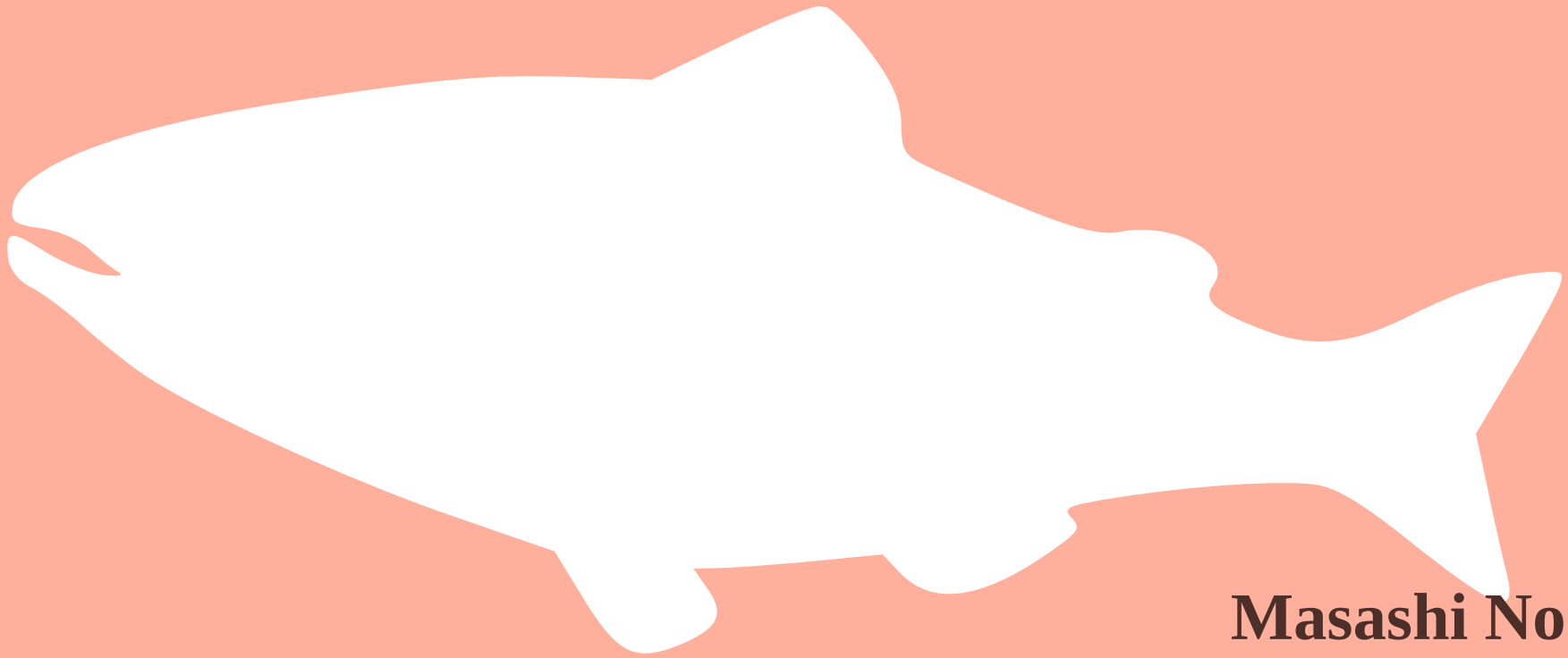
Basics of SALMON

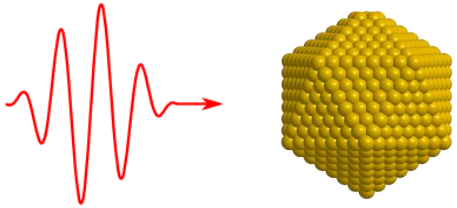


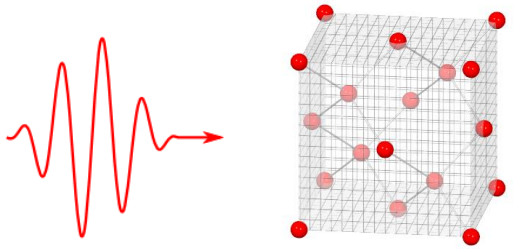
Masashi Noda
Institute for Molecular Science

What is SALMON?

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

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



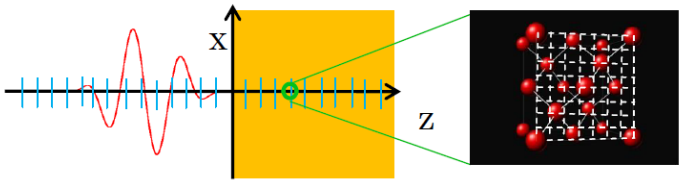


- Dielectric functions and polarizability

Overview of SALMON

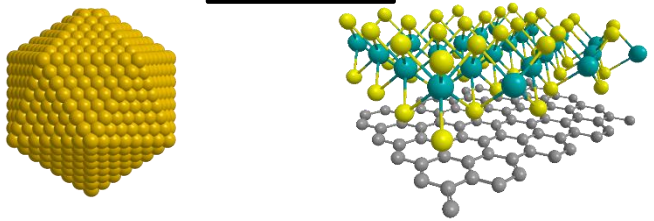
K. Yabana and G. F. Bertsch, Phys. Rev. B 54, 4484 (1996)

ARTED

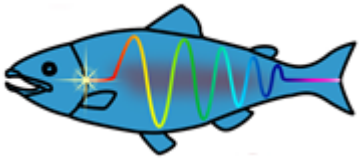


- solid/surface
- laser damage
- attosecond
- nanostructure (multiscale)

GCEED



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

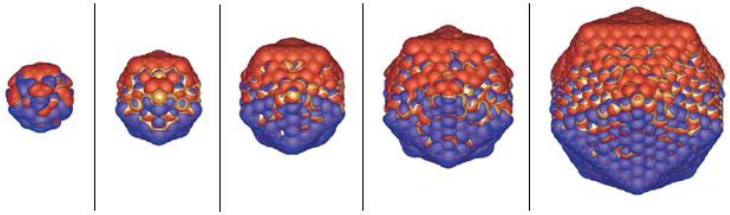


SALMON

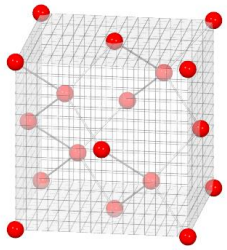
Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience

Characteristics of SALMON

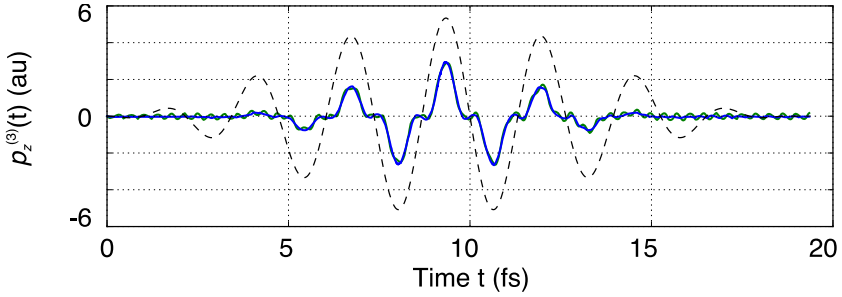
- Real-time electron dynamics



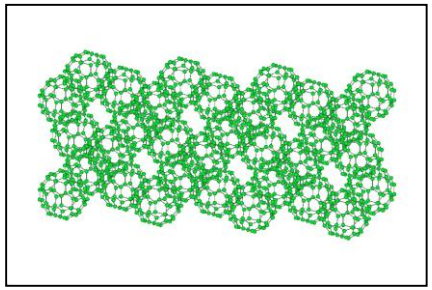
- Non-linear optical response

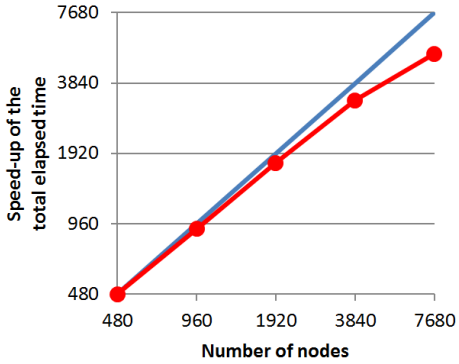


$$\mathbf{p}^{(3)}(t)$$

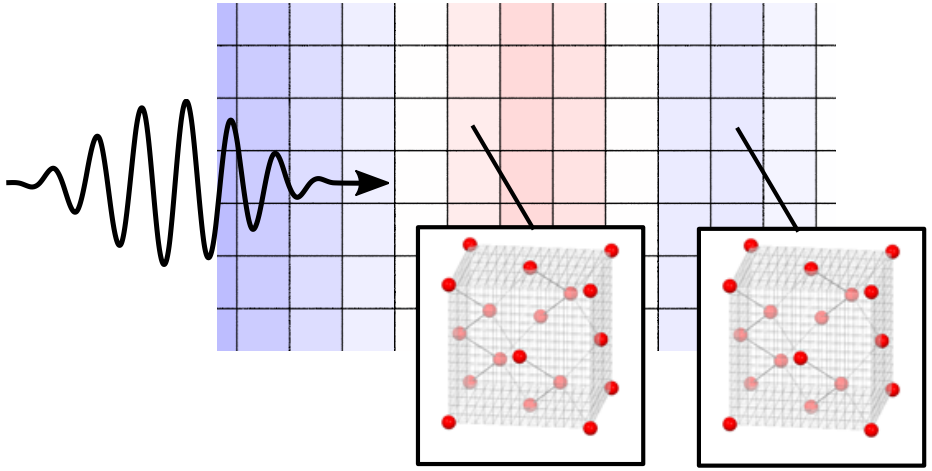


- Massive parallelization





- Couple with Maxwell equation



Development environment

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

- License: Apache 2.0
- Mailing list: 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)

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

ψ_n: Kohn-Sham orbital

V_H: Hartree potential

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

V_{xc}: Exchange-correlation potential

V_{ion}: Electron-nuclear interaction potential

- periodic system (velocity gauge)

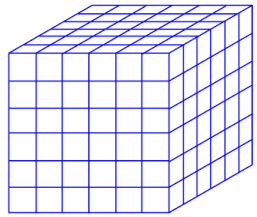
$$i\hbar\frac{\partial}{\partial t}u_{n\boldsymbol{k}}(\boldsymbol{r},t)=\left\{\frac{1}{2}\left(-i\hbar\nabla+\hbar\boldsymbol{k}+\frac{e}{c}\boldsymbol{A}(t)\right)^2+V_{ion}+V_H+V_{xc}\right\}u_{n\boldsymbol{k}}(\boldsymbol{r},t)$$

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

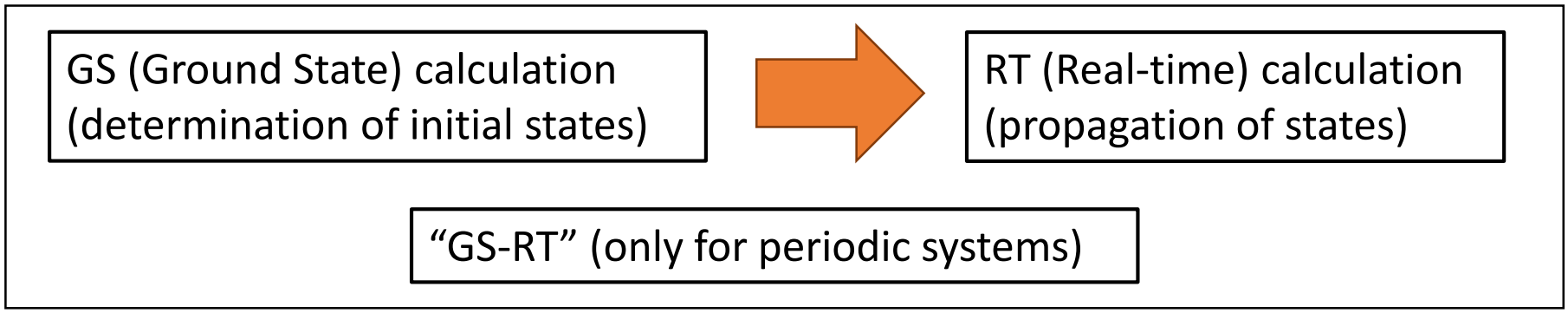
$\boldsymbol{k}$: wave vector

$\boldsymbol{A}(t)$: External vector potential

Physical quantities are expressed on grid.



Flowchart of SALMON



GS calculation

- Isolated system (length gauge)

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

ϵ_n: 1-particle energy

- periodic system (velocity gauge)

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

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

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

Exchange-correlation functions

- Adiabatic approximation
- Exchange-correlation potential

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

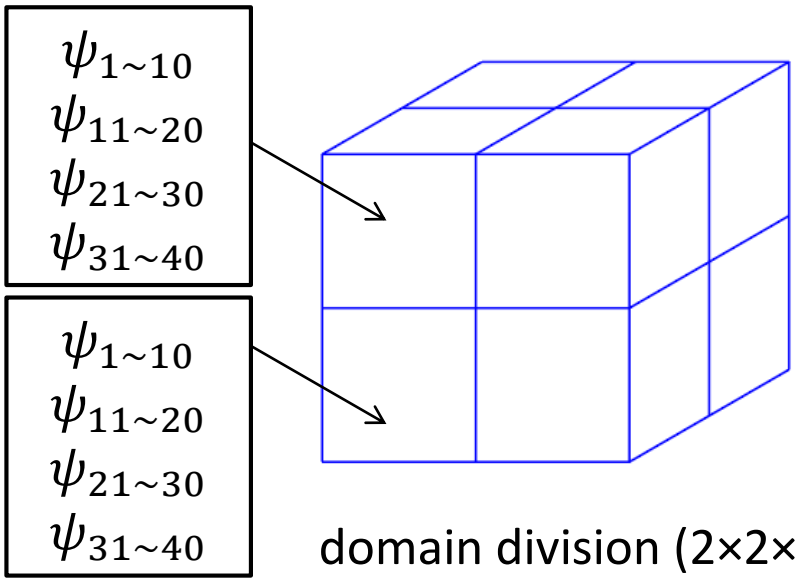
ϵ_{xc}: energy per electron n: electron density

- 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)

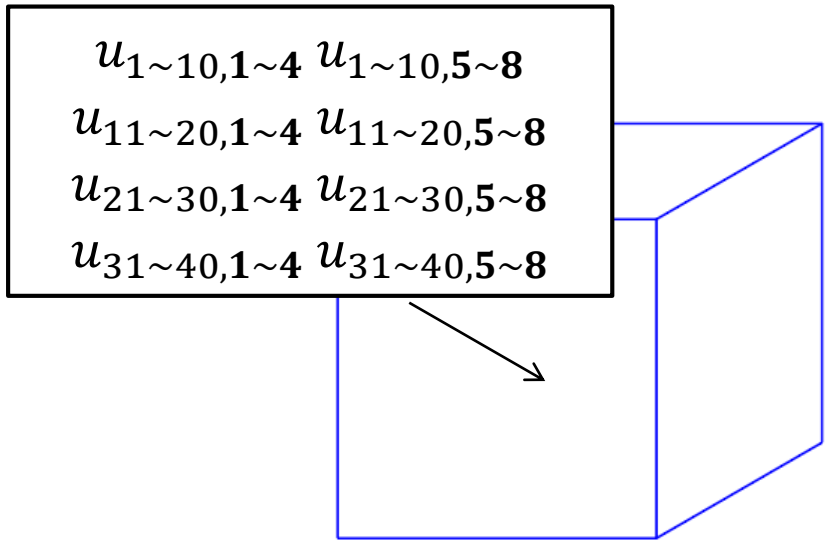
- isolated systems
  Kohn-Sham orbital: $\psi_n(\boldsymbol{r})$
  - ➢ MPI: orbital and domain



domain division (2×2×2)

  - ➢ OpenMP: domain

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

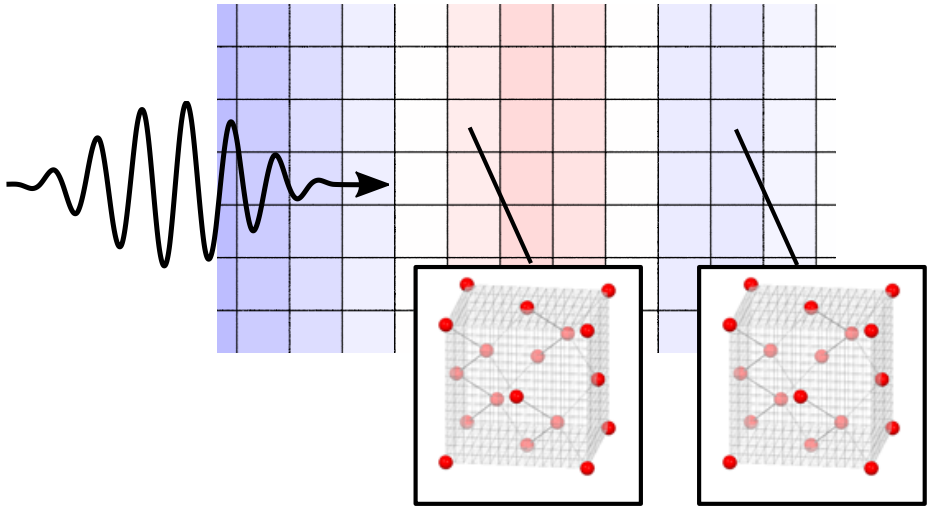


  - ➢ OpenMP: orbital and k points

This parallelization is done automatically.

Parallelization (2)

- multiscale calculation



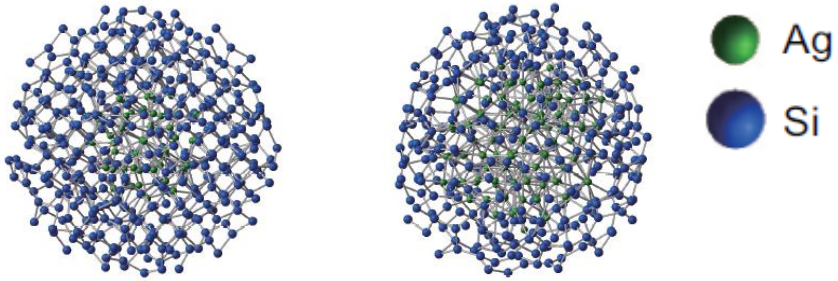
➢ MPI:
macroscopic grids
orbital and k points ($u_{nk}(\boldsymbol{r})$)
in microscopic cell

➢ OpenMP:
orbital and k points ($u_{nk}(\boldsymbol{r})$)
in microscopic cell

This parallelization is done automatically.

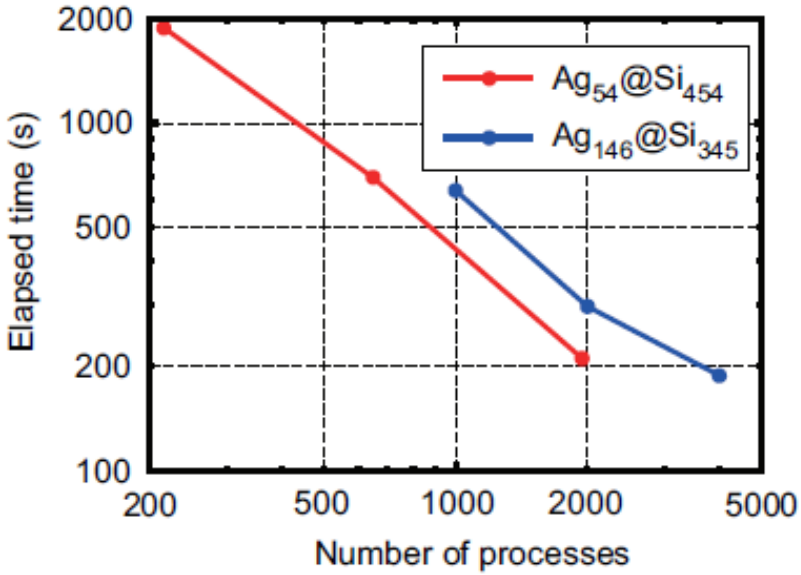
Performance (1)

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



Diameter: 2.5nm

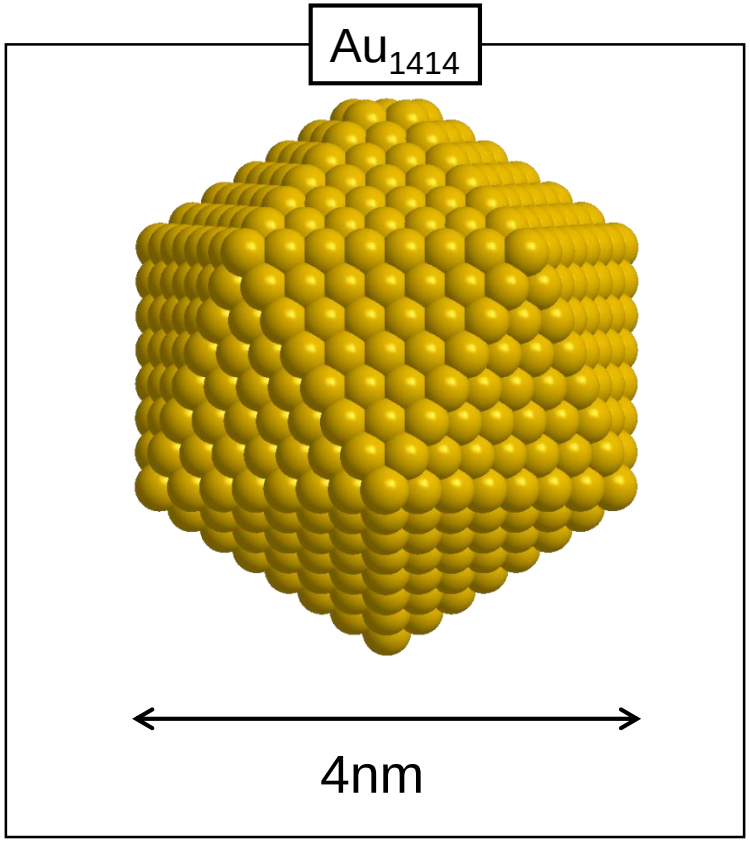
Used computer: K computer (RIKEN)
Time steps: 1000



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)



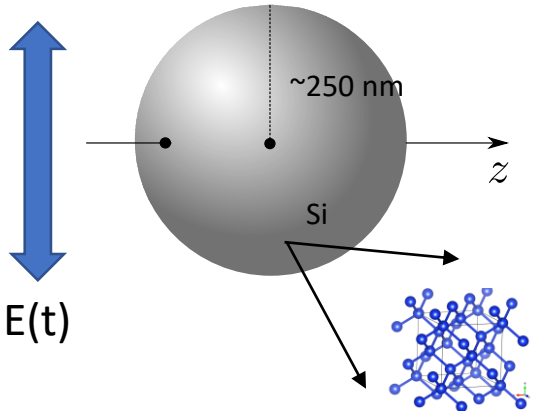
Used computer: K computer (RIKEN)

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

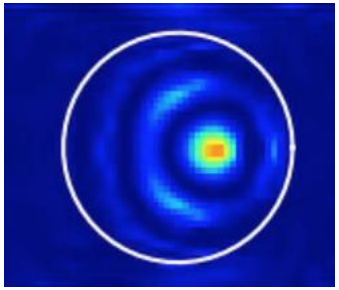
Calculations for product runs end in 7 hours with 15,600 processes.

Performance (3)

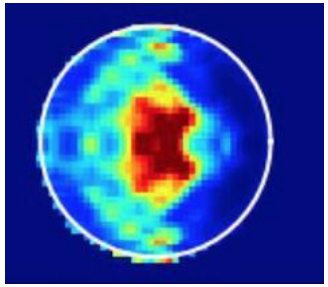
Laser Excitation Silicon Nanosphere



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