SALMON

2022 CCS-KISTI Workshop
CCS, Univ. Tsukuba
Feb. 22, 2022

Development and applications of SALMON

- First-principles computations in optical science -

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計算科学研究センター
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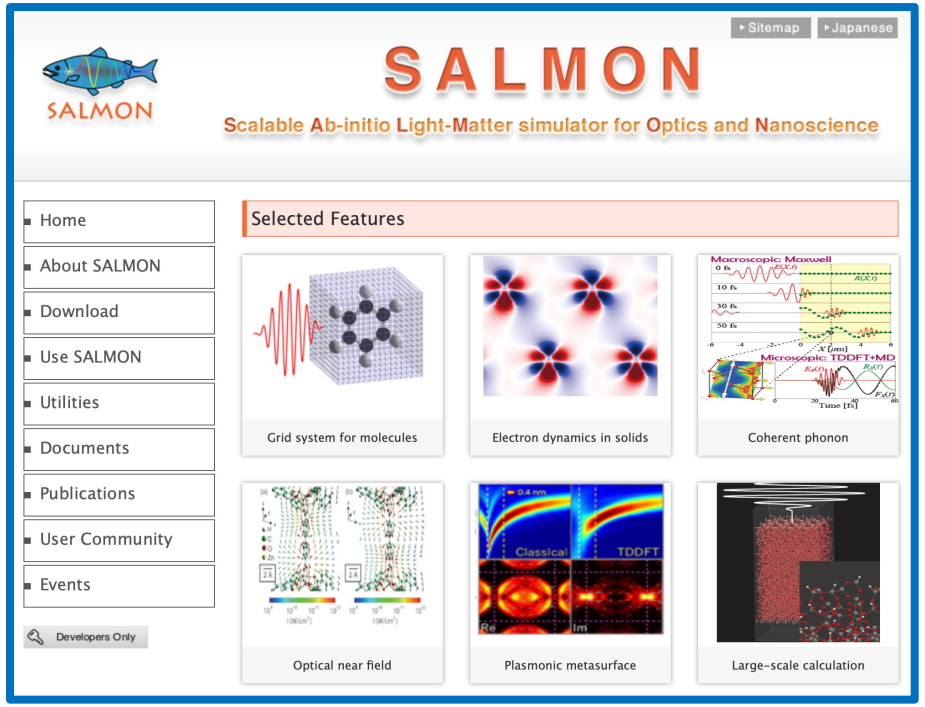
筑波大学
University of Tsukuba

Scalable Ab initio Light– Matter simulator for Optics and Nanoscience

Open-Source Software project:

https://salmon-tddft.jp



Computation of light-matter interaction from atomic scale using first-principles computational method in materials science

Contents

- (Self-) Interdisciplinary aspect in developing SALMON
- Light propagation from first-principles: hierarchy linkage in SALMON
- Co-design in developing SALMON and large-scale computation

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- (Self-) Interdisciplinary aspect in developing SALMON
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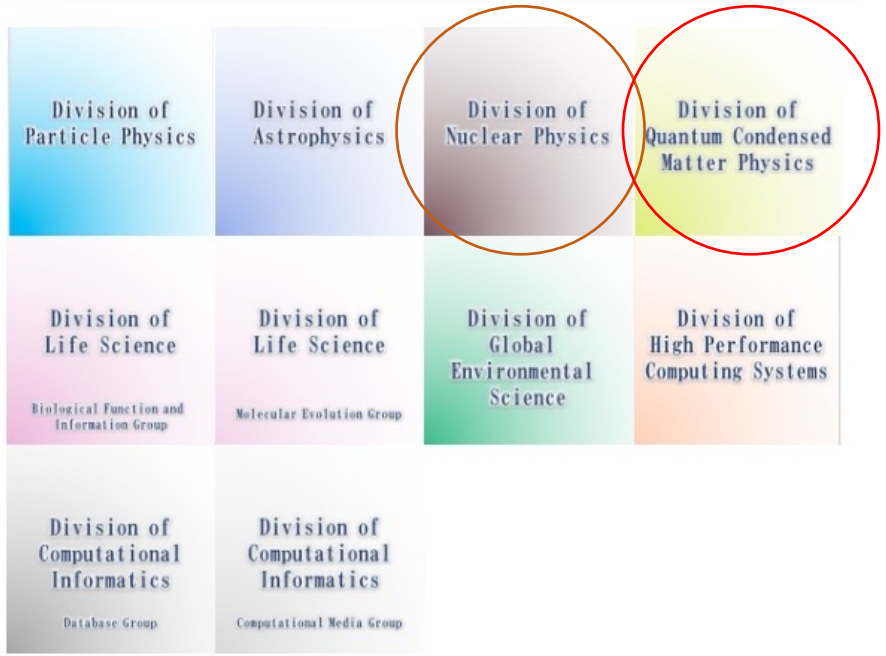
How did SALMON start?
(Self-) Interdisciplinary Computational Science

University of Tsukuba
Center for Computational Sciences
筑波大学　計算科学研究センター

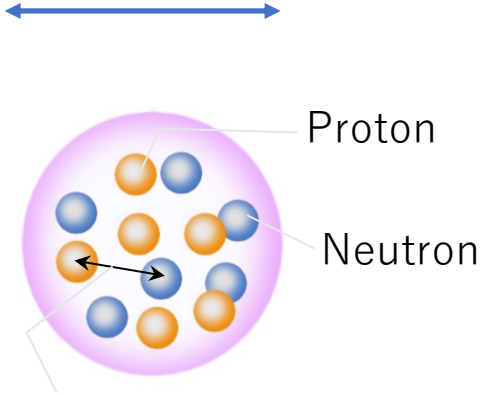
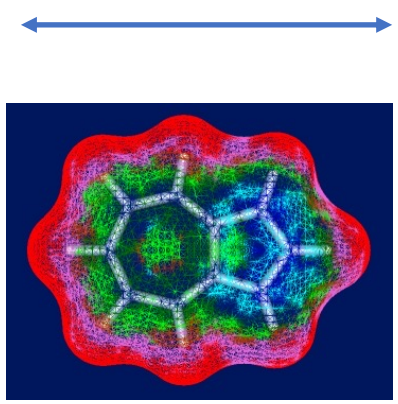
- Multidisciplinary Computational Science
- Co-Design by computational and computer scientists

Division and Group



I am affiliated to two application-divisions:

- Quantum Condensed Matter Physics
- Nuclear Physics

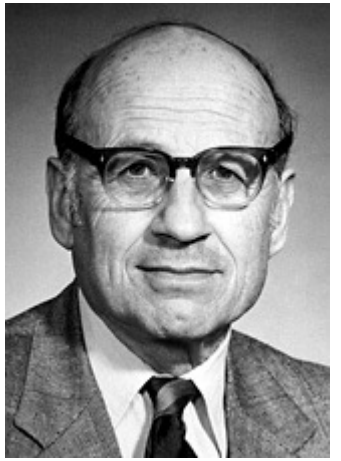
	Nuclei	Atoms, Molecules, Solids
Different scale	10^{-14} m 	10^{-9} m 
Different interaction	Nuclear force between protons and neutrons	Coulomb force between electrons and nuclei
Common physics law	**Quantum mechanics for the dynamics of fermions (protons and neutrons in nuclei, electrons in atoms, molecules, and solids).**	

Common theories are useful: (Time-Dependent) Density Functional Theory

In electronic systems, Density Functional Theory (DFT) has been quite successful (Novel prize awarded). But only for static problem.

$$\varepsilon_i \phi_i(r) = \left[\frac{1}{2m}p^2 + V_{ion}(r) + V_H(r) + V_{xc}(r)\right]\phi_i(r)$$

Static (eigenvalue) problem, Kohn-Sham equation



W. Kohn
Initiate DFT in electronic systems
1998 Nobel prize in chemistry

Extension to dynamics: Time-Dependent Density Functional Theory (TDDFT)

$$i\hbar\frac{\partial}{\partial t}\psi_i(r,t) = \left[\frac{1}{2m}p^2 + V_{ion}(r) + V_H(r,t) + V_{xc}(r,t) + V_{ext}(r,t)\right]\psi_i(r,t)$$

Popular method in nuclear physics, from 70's.

TDDFT simulation for nucleus-nucleus collisions

Before I entered graduate course in 1982.

H. Flocard, S.E. Koonin, M.S. Weiss,
Phys. Rev. 17(1978)1682.

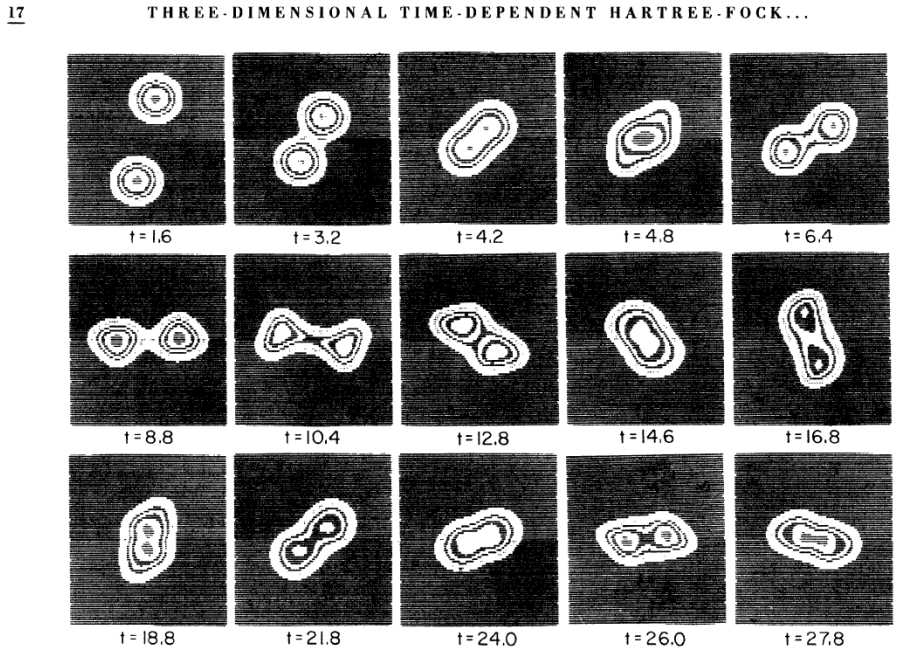


FIG. 2. Contour lines of the density integrated over the coordinate normal to the scattering plane for an $^{16}O+^{16}O$ collision at $E_{lab}=105$ MeV and incident angular momentum $L=13\hbar$. The times t are given in units of 10^{-22} sec.

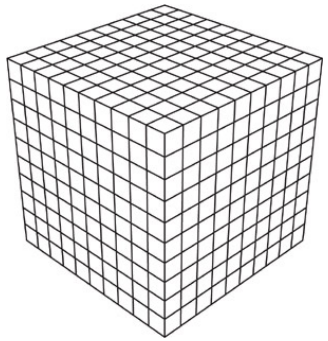
^{16}O-^{16}O collision

Time evolution of proton and neutron orbitals.

$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)=h[n(\vec{r},t)]\psi_i(\vec{r},t)$$

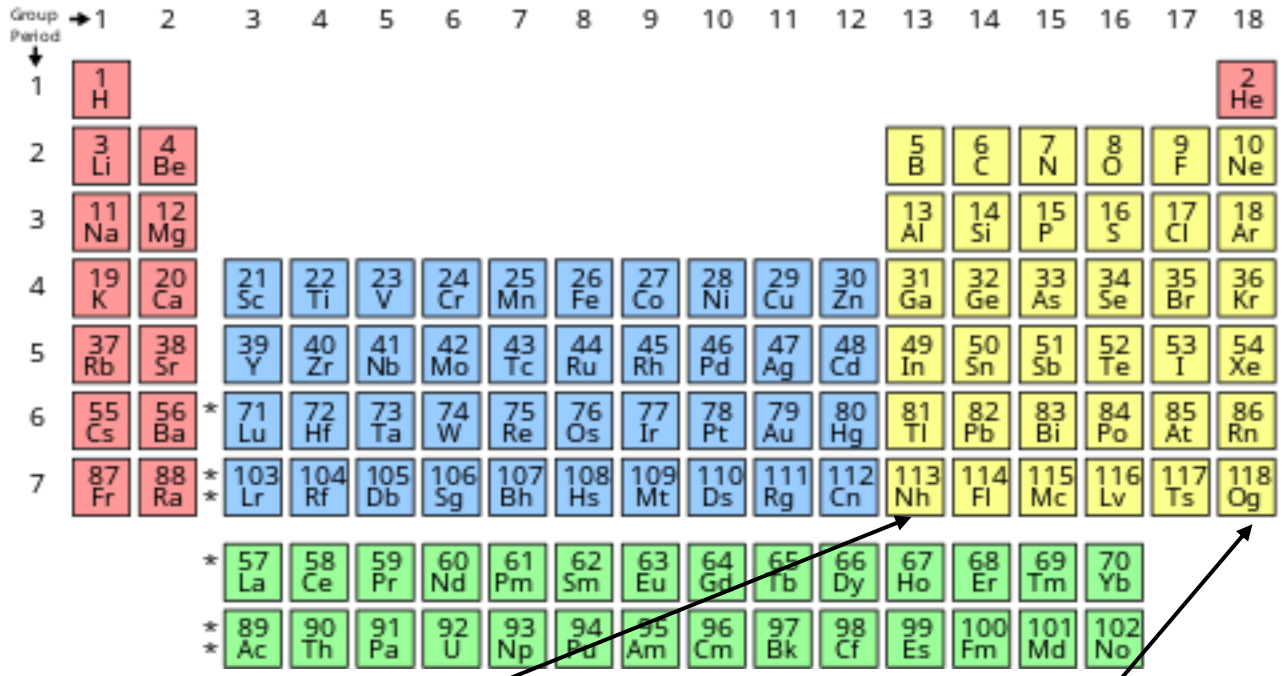
$$n(\vec{r},t)=\sum_i|\psi_i(\vec{r},t)|^2$$

$$\psi(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N,t)=A\{\psi_1(\vec{r}_1,t)\psi_2(\vec{r}_2,t)\cdots\psi_N(\vec{r}_N,t)\}$$



Spatial grid 30x28x16, time step 4×10^2
using CRAY-1 (80MFLOPS)

Synthesis of superheavy elements



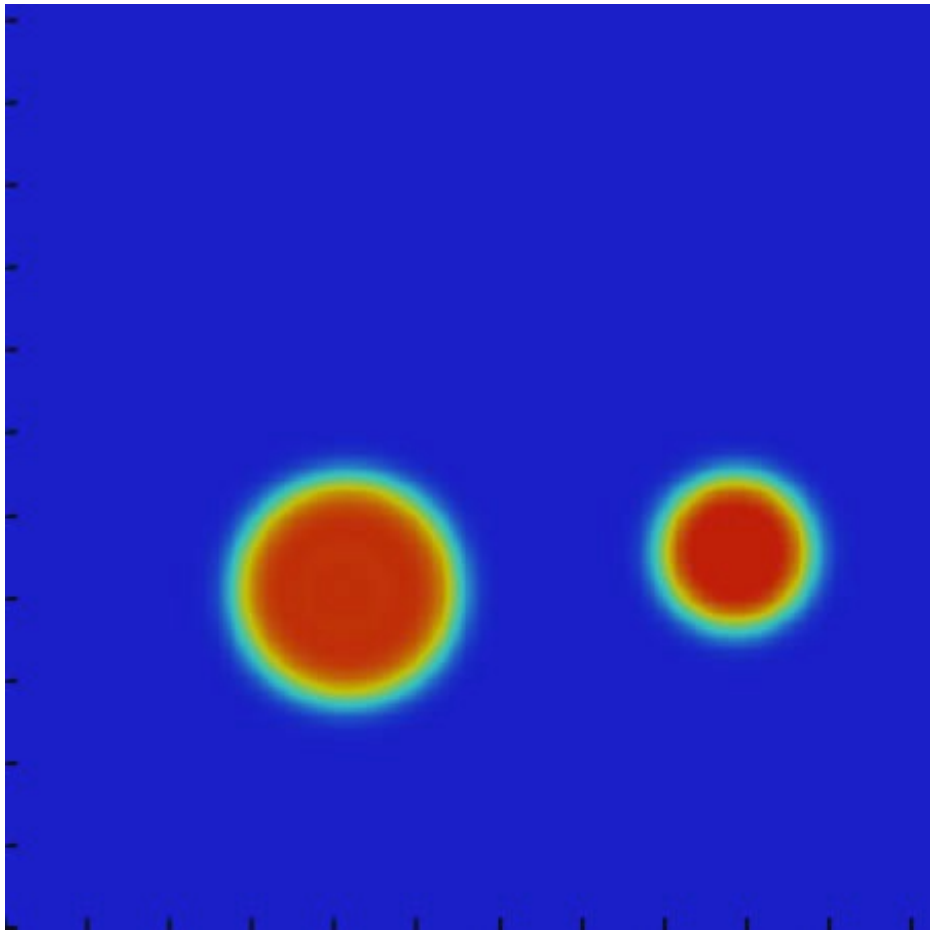
Nh=Nihonium
Discovered by Japanese team, 2004.

Z=118:
Largest element at present

TDDFT simulation to produce Z=120 element

K. Sekizawa, K. Yabana, Phys. Rev. C93, 054616 (2016)

$^{238}U + {}^{64}Ni$ (proton number: 92 + 28 = 120)



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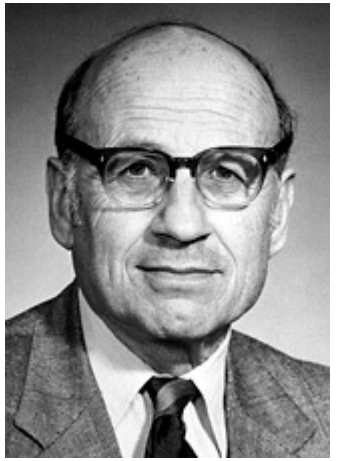
$$\varepsilon_i \phi_i(r) = \left[\frac{1}{2m}p^2 + V_{ion}(r) + V_H(r) + V_{xc}(r)\right]\phi_i(r)$$

Static (eigenvalue) problem, Kohn-Sham equation



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Popular method in nuclear physics, from 70's.

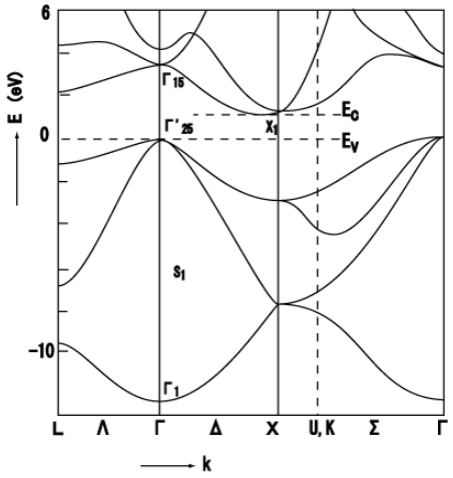
We extended static DFT in material science to electronic dynamics using nuclear-theory method.

Quantum electronic dynamics in a unit cell of silicon crystal

$$\varepsilon_i \phi_i(r) = \left[\frac{1}{2m}p^2 + V_{ion}(r) + V_H(r) + V_{xc}(r)\right]\phi_i(r)$$

eigenvalue -> energy band

Energy band of silicon



First-principles DFT
Band calculation

middle 90's

Time-dependent Kohn-Sham equation

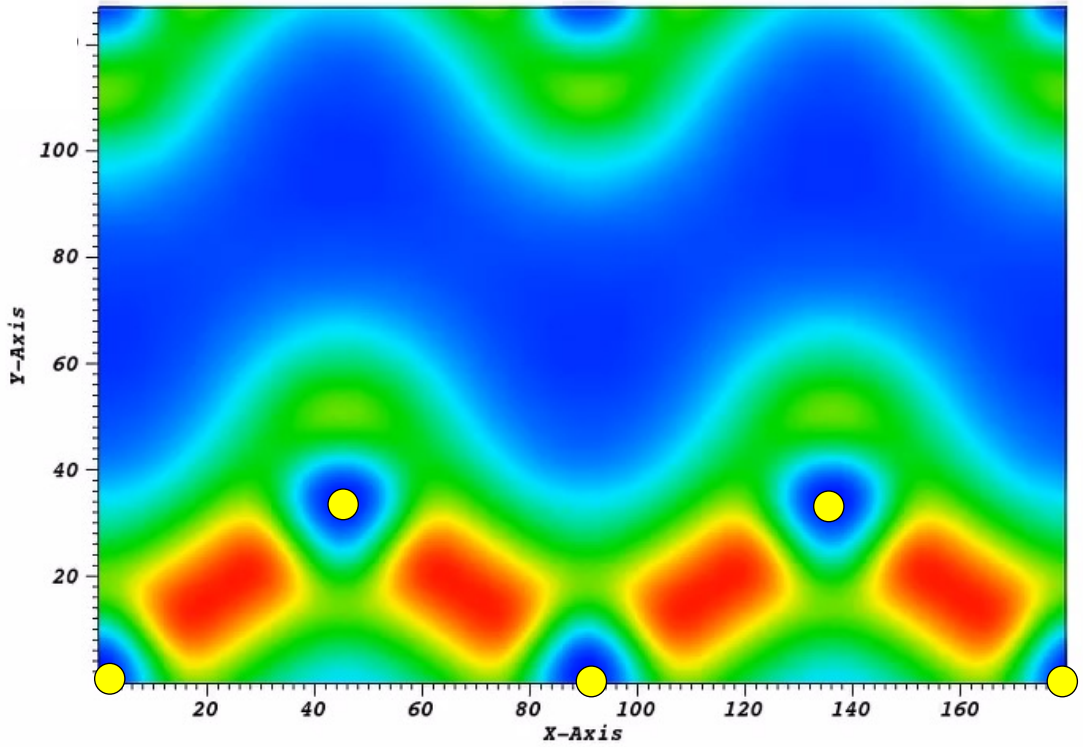
$$i\hbar\frac{\partial}{\partial t}u_{nk}(r,t) = \left[\frac{1}{2m}\left(p + \hbar k + \frac{e}{c}A(t)\right)^2 + V_H(r,t) + V_{xc}(r,t)\right]u_{nk}(r,t)$$

$$A(t) = -c\int^t E(t')\mathrm{d}t'$$

Electron density under pulsed light

$\hbar\omega = 1.55\,\mathrm{eV}$

$I = 1.0\times10^{14}\ \mathrm{W/cm^2}$



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Traditional computational methods in optical science

ELECTROMAGNETISM (EM)

Light propagation solving Maxwell's equations

$$\nabla \cdot \boldsymbol{B} = 0$$
$$\nabla \times \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} = \boldsymbol{0}$$
$$\nabla \cdot \boldsymbol{D} = \rho$$
$$\nabla \times \boldsymbol{H} - \frac{\partial \boldsymbol{D}}{\partial t} = \boldsymbol{j}$$

e.g, FDTD (Finite-difference time-domain method)

Linear and local constitutive relation

$$\mathbf{D}(\mathbf{r},t) = \int dt' \epsilon(t-t')\mathbf{E}(\mathbf{r},t')$$

QUANTUM MECHANICS (QM)

First-principles quantum mechanics calculations of optical constants

$$\varepsilon_r = 1 + \frac{2Ne^2}{\varepsilon_0 \hbar} \sum_j \frac{\omega_{j0} \left| \langle 0|x|j \rangle \right|^2}{\omega_{j0}^2 - (\omega + i\gamma)^2}$$

e.g, GW-BS, TDDFT

They are not sufficient in current optics frontier.

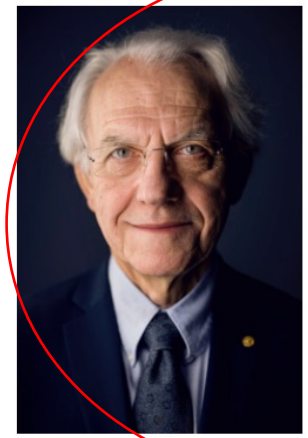
One of directions in current optics:

Generate and Utilize Intense and Ultrashort Laser Pulse

Nobel Prize in Physics 2018

Ill. Niklas Elmehed. © Nobel Media

Arthur Ashkin



© Nobel Media AB. Photo: A. Mahmoud

Gérard Mourou

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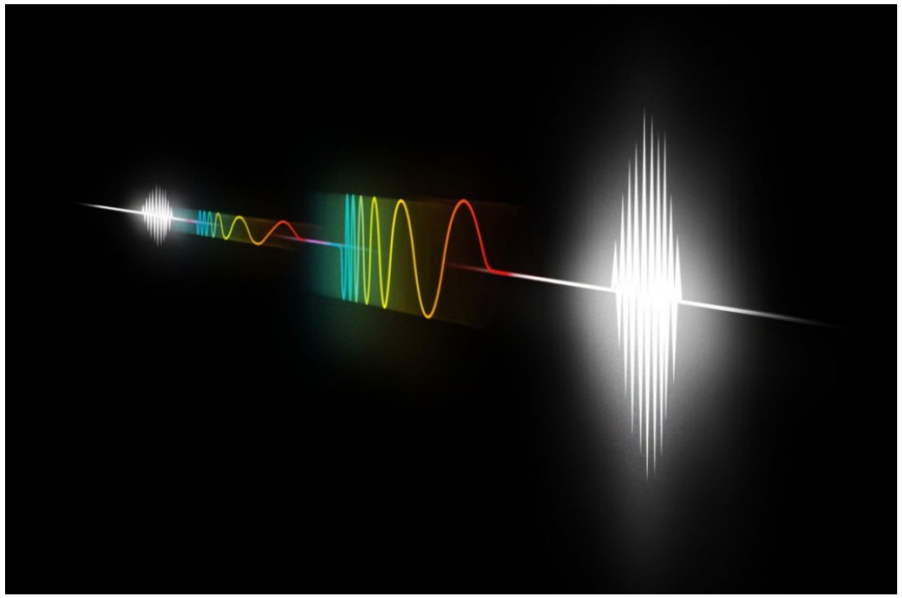
Donna Strickland



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In SALMON, we combine Maxwell and TDDFT

Light propagation solving Maxwell's equations (Classical)

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

Electron dynamics by TDDFT

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

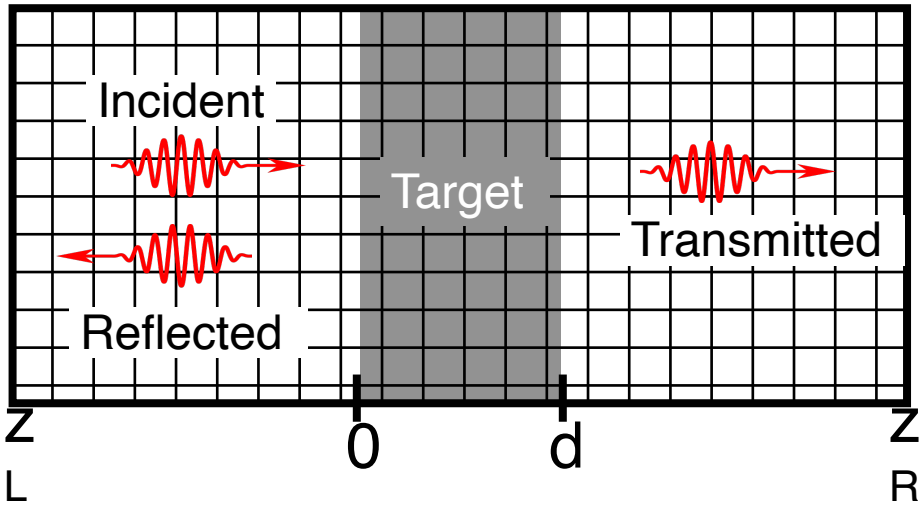
$$\mathbf{j} = -\frac{e}{2m}\left\{\psi_i^*\left(-i\hbar\nabla + \frac{e}{c}\mathbf{A}\right)\psi_i + c.c.\right\}$$

Two frameworks connecting two descriptions

Microscopic (single-grid) vs Macroscopic (multi-grid)

Microscopic (Single-scale) vs. Macroscopic (Multi-scale)

Microscopic Maxwell+TDDFT



$$i\frac{\partial}{\partial t}u_{n\mathbf{k}} = \hat{H}_{\mathbf{k}+\frac{1}{c}A(\mathbf{r},t)}u_{n\mathbf{k}}$$

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\mathbf{A}(\mathbf{r},t) + \frac{1}{c}\nabla\dot{\phi}(\mathbf{r},t) = -\frac{4\pi}{c}\mathbf{j}_e(\mathbf{r},t)$$

$$\nabla^2\phi(\mathbf{r},t) = 4\pi n_e(\mathbf{r},t)$$

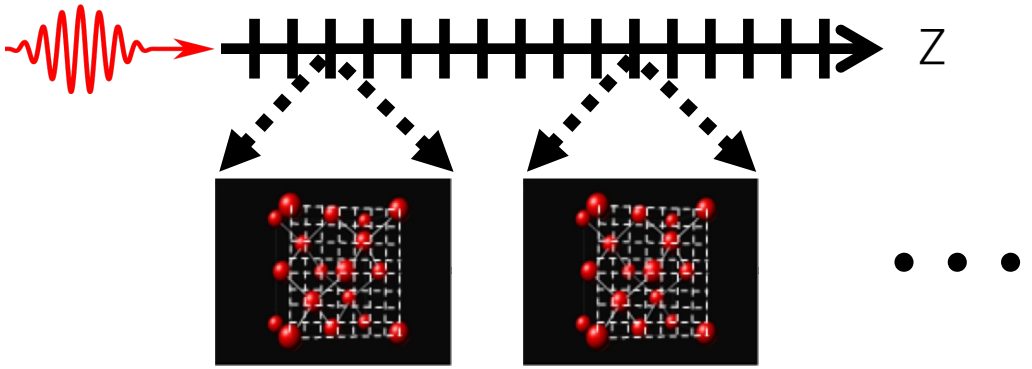
Single-scale approach using a **common** spatial grid

S. Yamada *et al*, PRB **98**, 245147 (2018).

Macroscopic Maxwell+TDDFT

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial Z^2}\right)\mathbf{A}_Z(t) = \frac{4\pi}{c}\mathbf{J}_Z(t)$$

10nm-scale grid



nm-scale grid #1 nm-scale grid #2

$$i\frac{\partial}{\partial t}u_{n\mathbf{k},Z} = \hat{H}_{\mathbf{k}+\frac{1}{c}A_Z(t)}u_{n\mathbf{k},Z}$$

$$i\frac{\partial}{\partial t}u_{n\mathbf{k},Z} = \hat{H}_{\mathbf{k}+\frac{1}{c}A_Z(t)}u_{n\mathbf{k},Z}$$

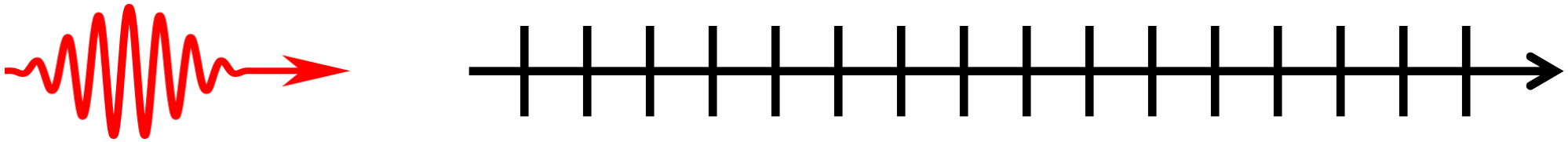
Multiscale approach using **different** spatial grid

K. Yabana *et al.*, PRB **85**, 045134 (2012).

Nonlinear light propagation: multiscale Maxwell-TDDFT simulation

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial Z^2}\right)\mathbf{A}_Z(t) = \frac{4\pi}{c}\mathbf{J}_Z(t)$$

Grid points for light propagation



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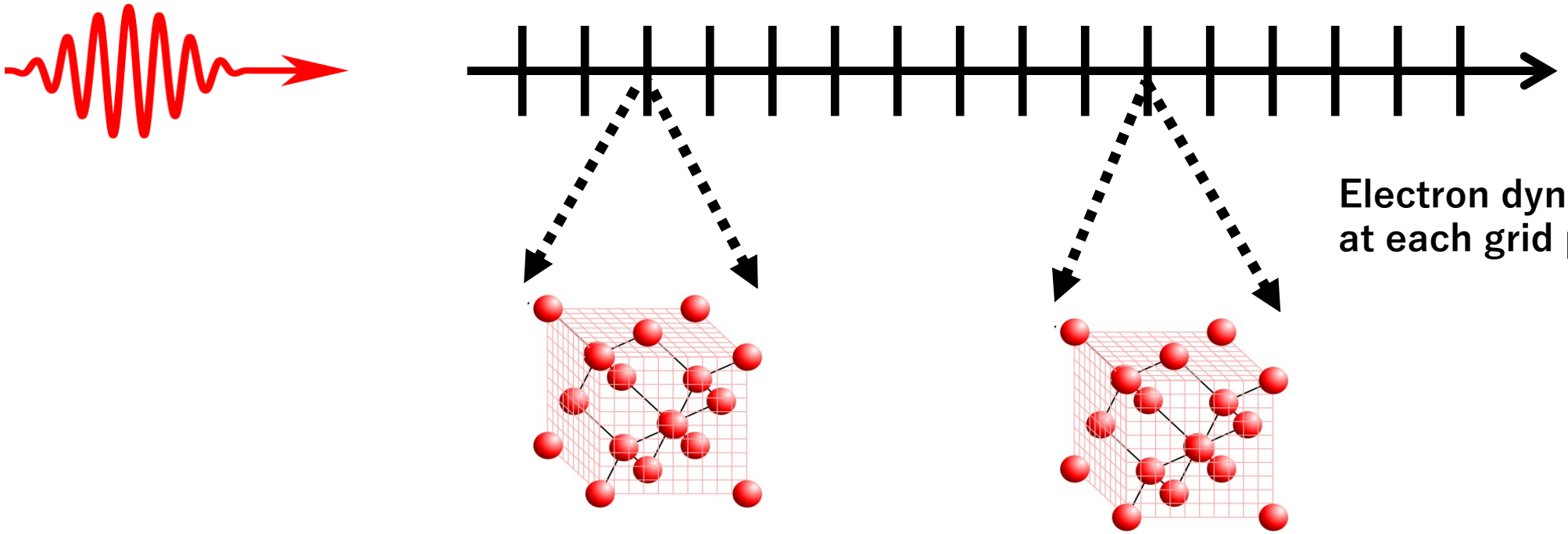
Grid points for light propagation



Electron dynamics calculation at each grid point

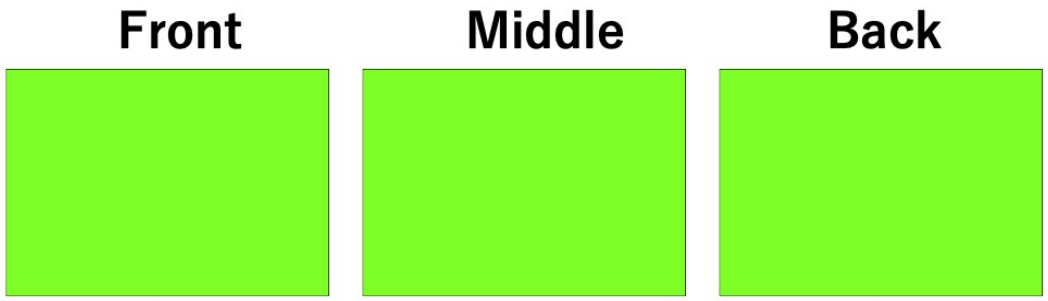
$$i\hbar\frac{\partial}{\partial t}u_{n\mathbf{k},Z_1} = H_{\mathbf{k}+\frac{\mathbf{e}}{\mathbf{c}}\mathbf{A}_{\mathbf{Z_1}}(\mathbf{t})}u_{n\mathbf{k},Z_1} \qquad i\hbar\frac{\partial}{\partial t}u_{n\mathbf{k},Z_2} = H_{\mathbf{k}+\frac{\mathbf{e}}{\mathbf{c}}\mathbf{A}_{\mathbf{Z_2}}(\mathbf{t})}u_{n\mathbf{k},Z_2} \qquad \cdots$$

K. Yabana, T. Sugiyama, Y. Shinohara, T. Otobe, G.F. Bertsch,
"Time-dependent density functional theory of strong electromagnetic fields in crystalline solids", Phys. Rev. B85, 045134 (2012).

Macroscopic (multi-scale) Maxwell-TDDFT: pulsed light on Si nano-film

Change of electron density from ground state

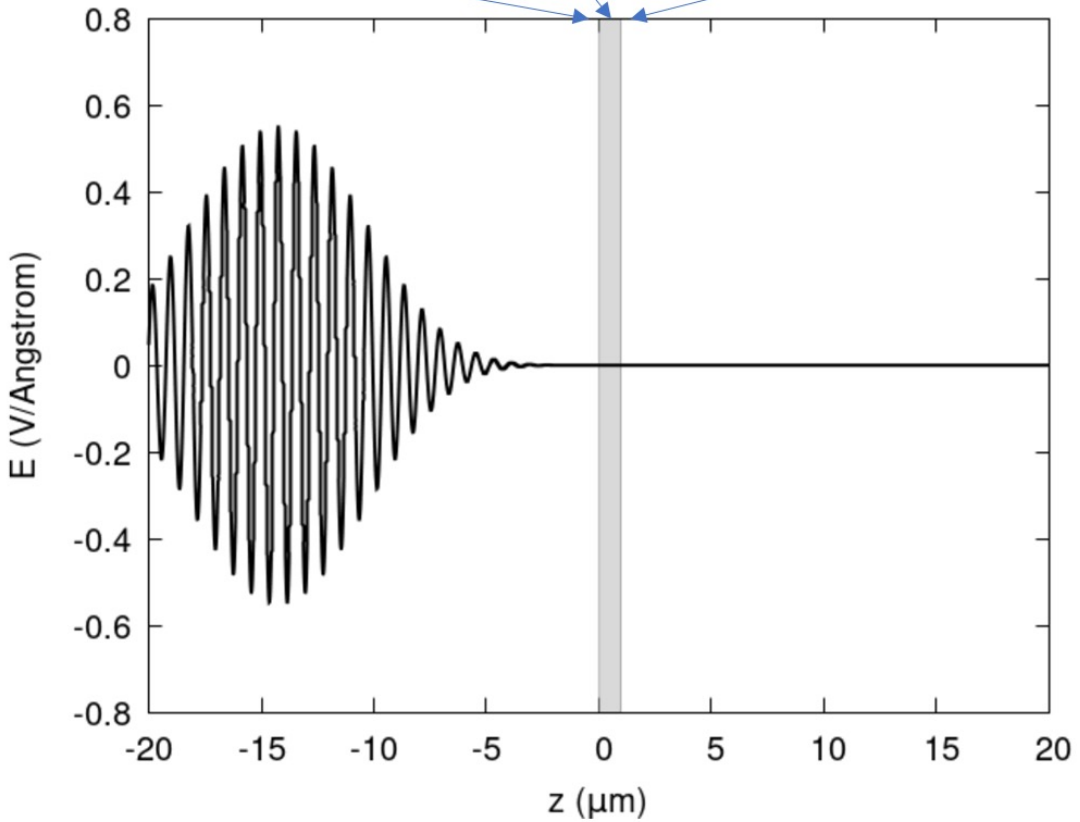
$$\Delta n(\mathbf{r},t) = n(\mathbf{r},t) - n_{GS}(\mathbf{r})$$



~200 grid points for 1μm film

Thin film
Silicon, 1 μm thick

Laser pulse
800nm (1.55eV=below gap)
4×10^{12}W/cm^2



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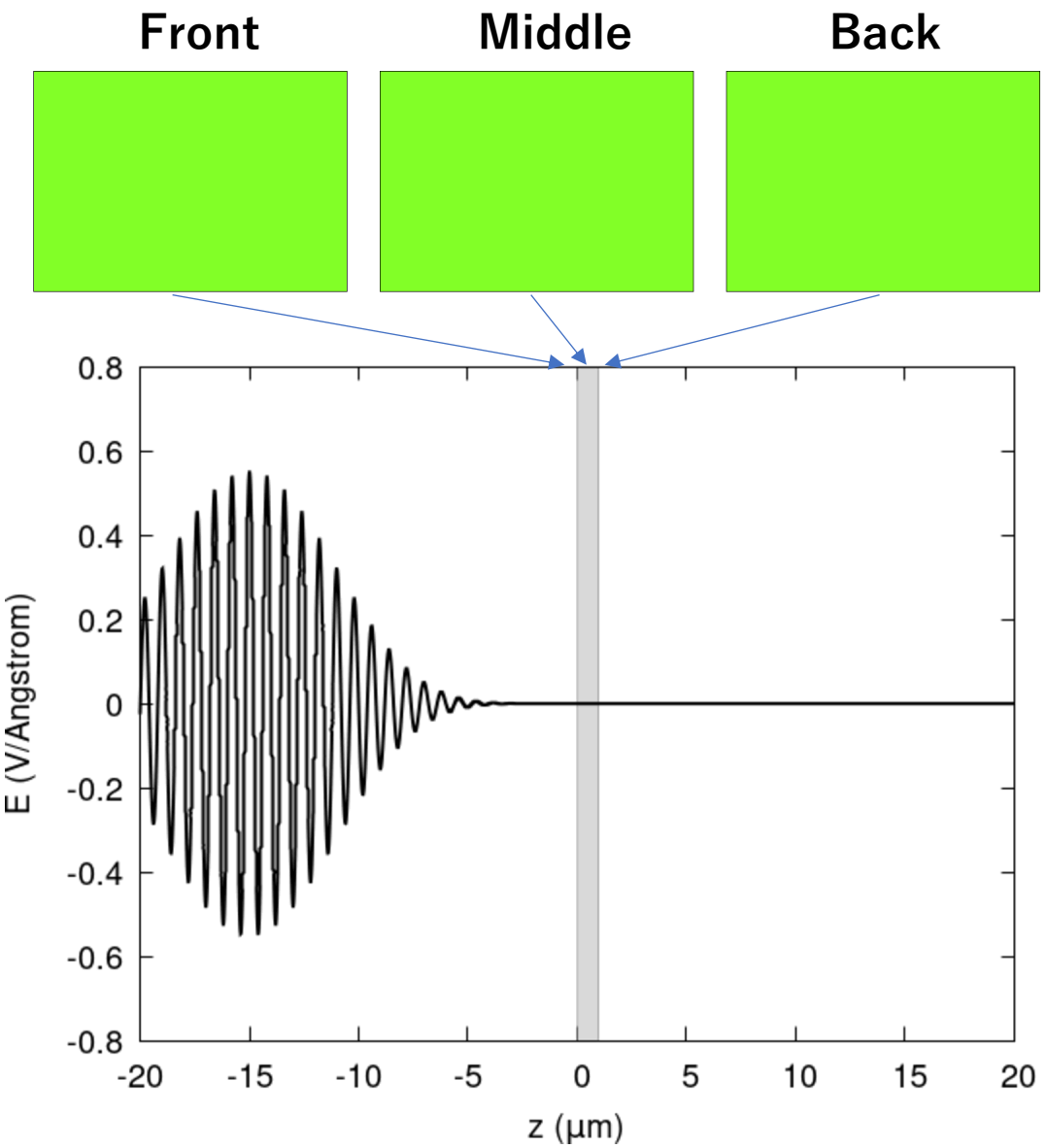


~200 grid points for 1μm film

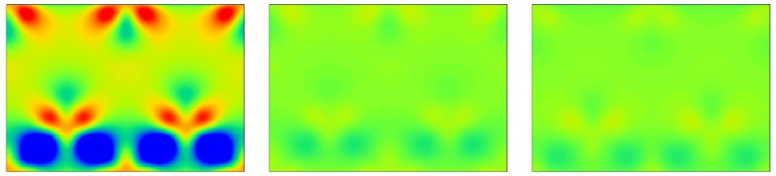
Thin film
Silicon, 1 μm thick

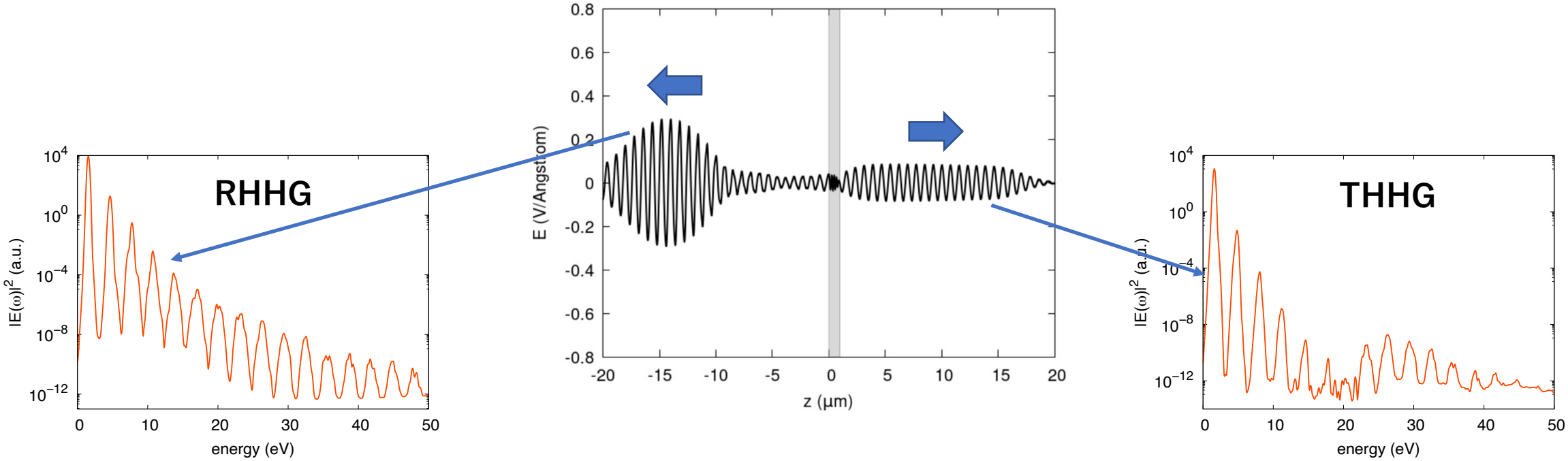
Laser pulse
800nm (1.55eV=below gap)
$4 \times 10^{12} W/cm^2$

High harmonic generation in reflection/transmission waves

Thin film
Silicon, 1 μm thick

Laser pulse
800nm (1.55eV=below gap)
4×10^{12}W/cm^2





S. Yamada et.al, Phys. Rev. B107, 035132 (2023)

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Development of SALMON
Co-Design

University of Tsukuba
Center for Computational Sciences
筑波大学　計算科学研究センター

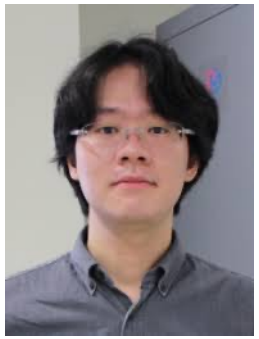
- Multidisciplinary Computational Science
- Co-Design by computational and computer scientists

Division and Group

Code development:

- **Physics researchers in Quantum Condensed Matter Physics**
- **Computer researchers in High Performance Computing Systems**

In-house collaboration between computational and computer scientists.



Dr. Yuta Hirokawa

2014.04-2018.09 Univ. Tsukuba, Grad. Student, Department of Computer Science
supervised by Prof. Boku.
Ph.D thesis
"Co-design for first-principles electronic dynamics simulation
in cutting-edge high performance computing systems"
2018.10-2020.10 Researcher, CCS, University of Tsukuba
2020.11- Private company

Compile options in SALMON

```
$ python ../configure.py --arch=ARCHITECTURE --prefix=../
$ make
$ make install
```

In executing the python script, you need to specify `ARCHITECTURE` that indicates the architecture of the CPU in your computer system such as `intel-avx`. The options of the `ARCHITECUTRE` are as follows:

arch	Detail	Compiler	Numerical Library
intel-knl	Intel Knights Landing	Intel Compiler	Intel MKL
intel-knc	Intel Knights Corner	Intel Compiler	Intel MKL
intel-avx	Intel Processer (Ivy-, Sandy-Bridge)	Intel Compiler	Intel MKL
intel-avx2	Intel Processer (Haswell, Broadwell ..)	Intel Compiler	Intel MKL
intel-avx512	Intel Processer (Skylake-SP)	Intel Compiler	Intel MKL
fujitsu-fx100	FX100 Supercomputer	Fujitsu Compiler	SSL-II
fujitsu-a64fx-ea	A64FX processor (Fugaku, FX1000, FX700)	Fujitsu Compiler	SSL-II
nvhpc-openmp	NVHPC OpenMP (CPU)	Nvidia HPC Compiler	Nvidia HPC SDK
nvhpc-openacc	NVHPC OpenACC (GPU)	Nvidia HPC Compiler	Nvidia HPC SDK
nvhpc-openacc-cuda	NVHPC OpenACC+CUDA (GPU)	Nvidia HPC Compiler	Nvidia HPC SDK

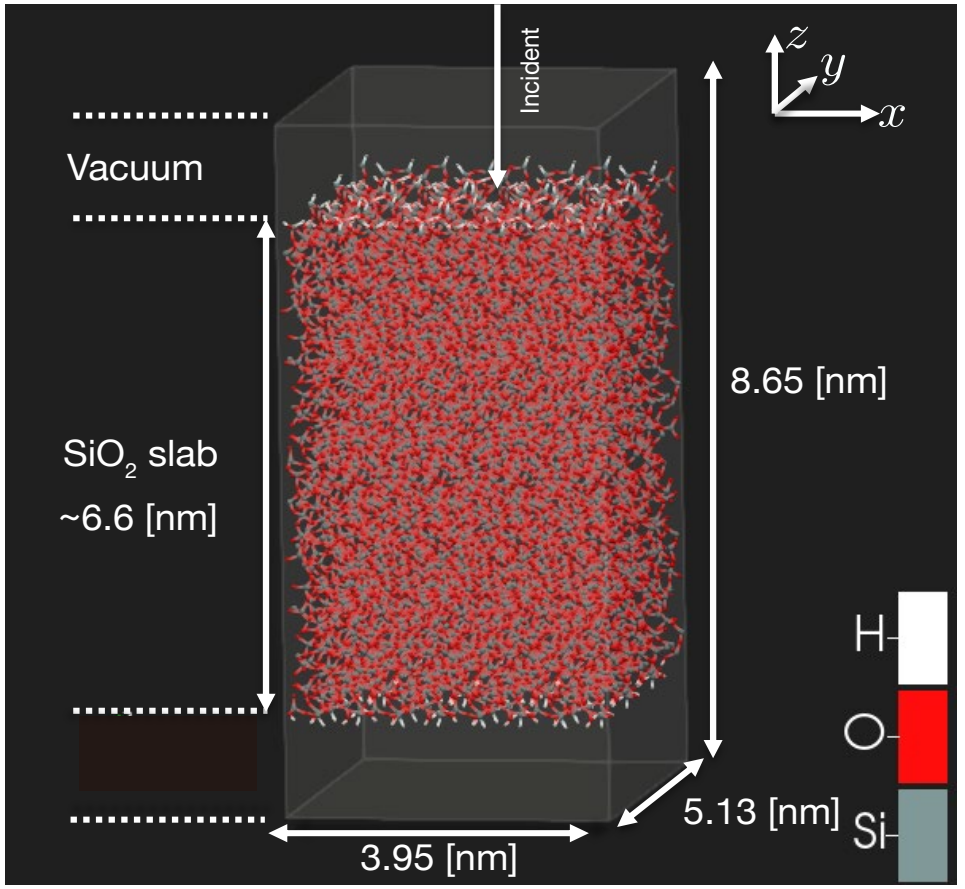
Large-scale computing using Fugaku

Microscopic (single-scale) Maxwell + TDDFT + MD

Dynamics of light EM fields, electrons, and ions of more than 10,000 atoms

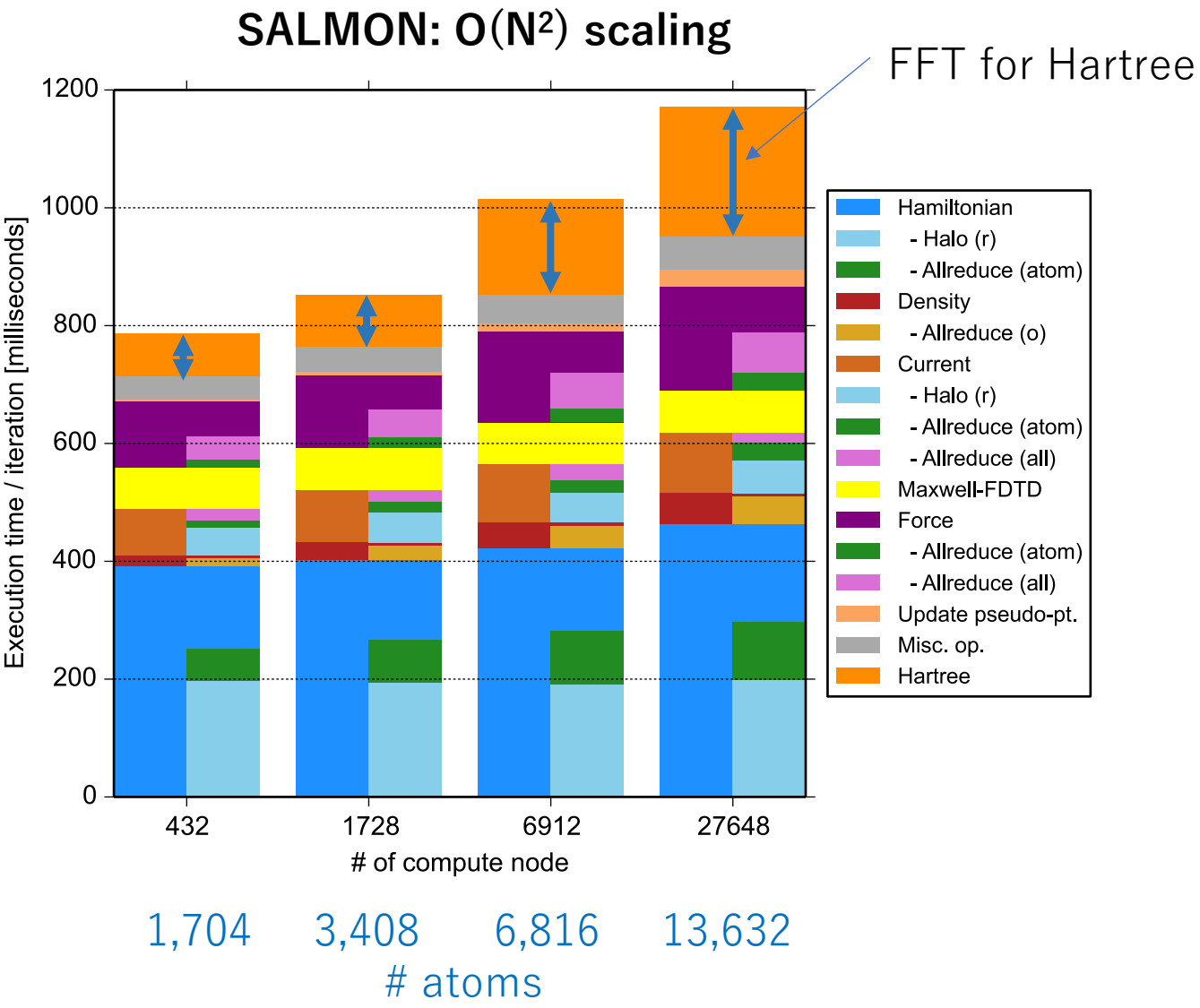
Fugaku Supercomputer

Top 500 1st (2020.6)
415 Pflops
158,976 A64FX (48 core)



27,648 nodes, about 1/6 of full system

Performance (Weak Scaling)



Achieved ~1s/iter up to 10,000 atoms.

Hamiltonian operation (Stencil, nonlocal PS) costs about half of total time.

60 – 70 % communications (halo, sum, etc).

FFT is bottleneck in view of weak scaling.

SALMON in GPU machine

- Code mostly written in fortran90
- To get performance, need to carry out all calculations in GPU
- Code frequently developed and modified by physics researchers

OpenACC + Unified Memory

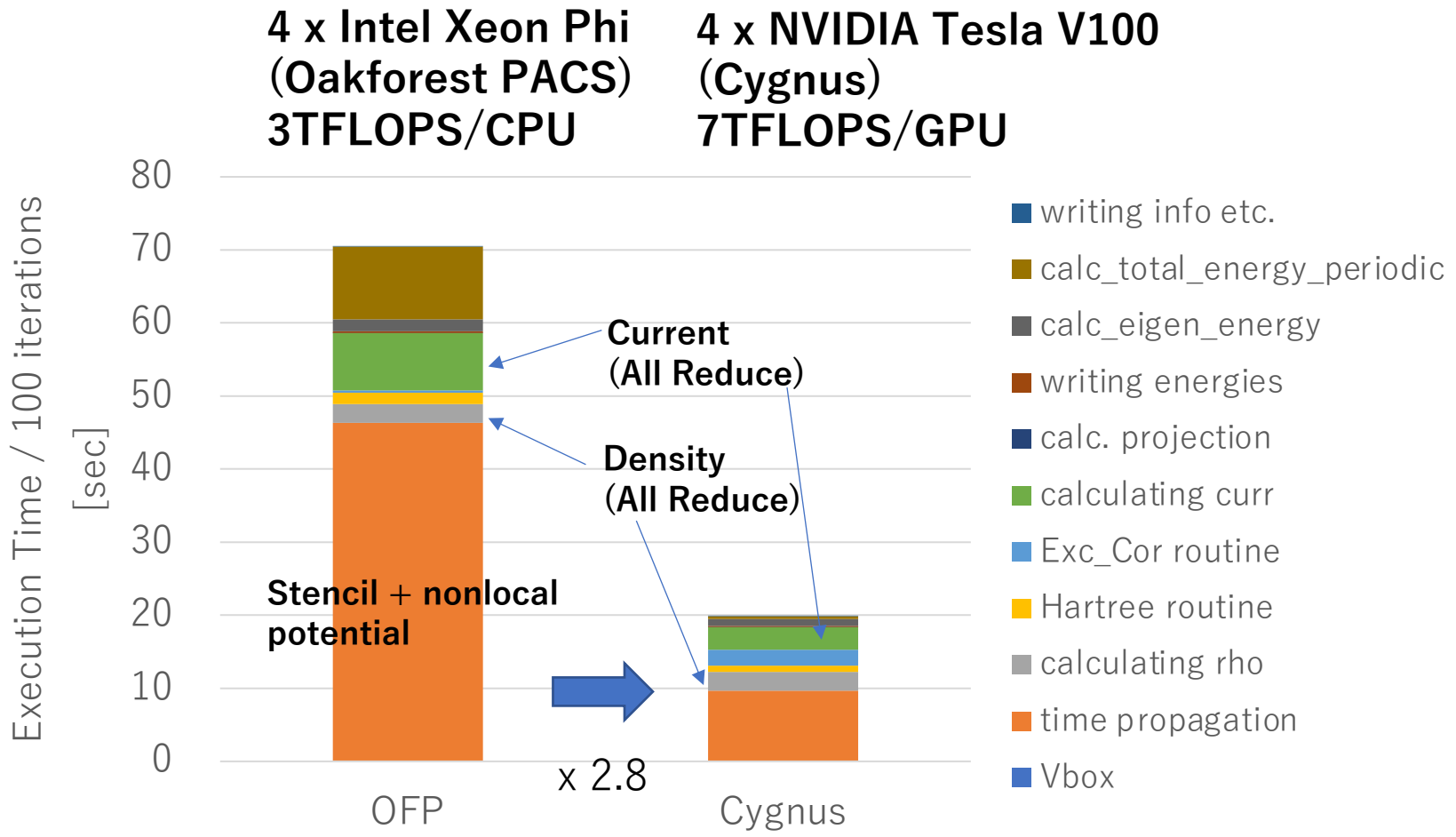
Performance comparison: CPU vs GPU

Electron dynamics calculation in 512 atom unit cell of silicon

Spatial grid 64^3

K-point. 1^3

Orbitals 1024



GPU > CPU using OpenACC+Unified Memory

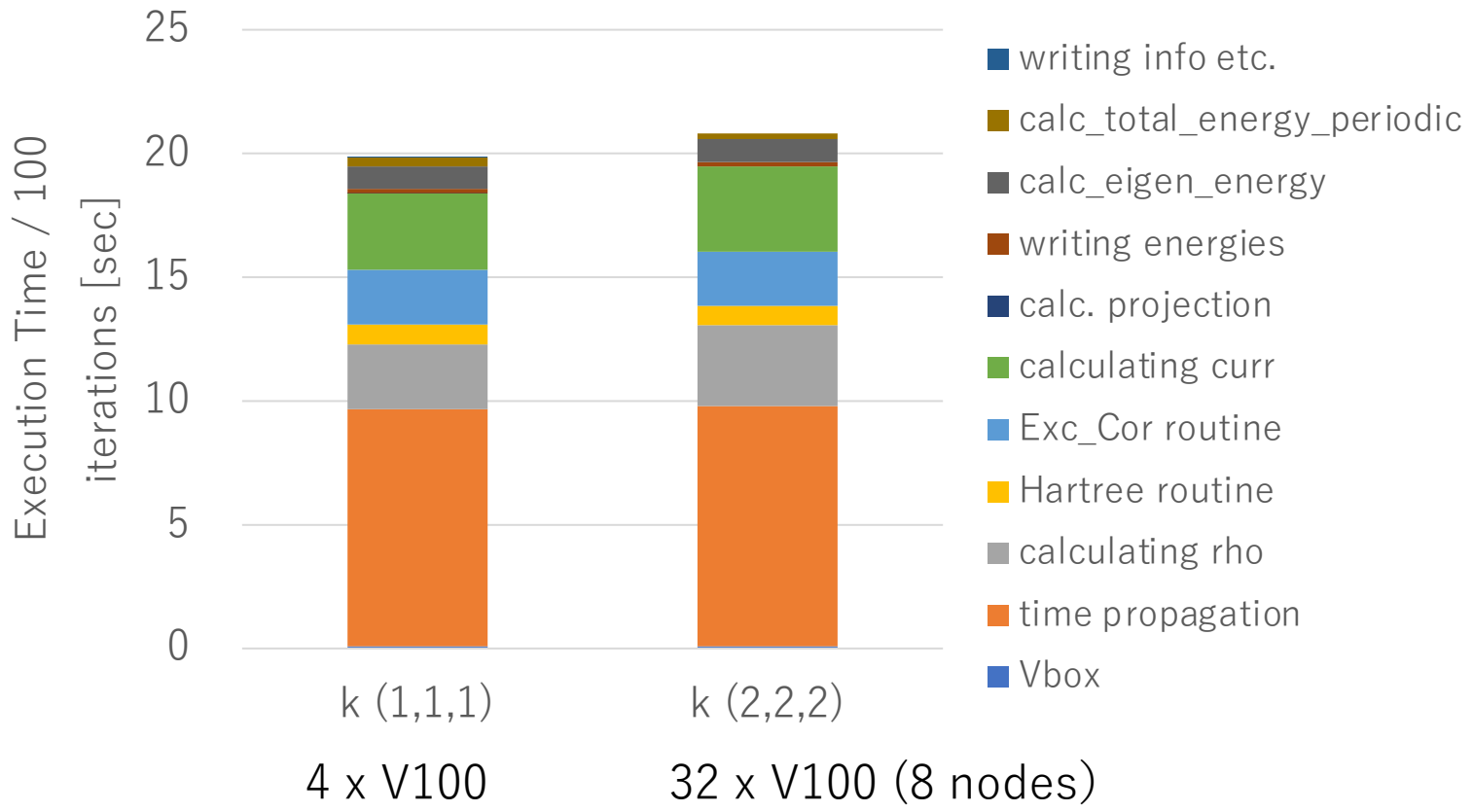
Weak scaling performance

Electron dynamics calculation in 512 atom unit cell of silicon

Spatial grid 64^3

K-point. 1^3 vs 2^3

Orbitals. 1024



Almost perfect scaling performance

Summary

https://salmon-tddft.jp

We develop SALMON, first-principles calculation for optics and nano-sciences.

It describes electronic dynamics induced by light.
Unique feature: light-propagation calculation from first-principles.

In the development,
- (self-) interdisciplinary computational physics (nuclear method meets first-principles calculation).
- In-house co-design was successful.
- Large-scale computing, efficient use of GPU.

Acknowledgement

Young collaborators (SALMON project)

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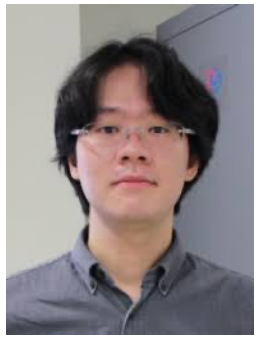

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