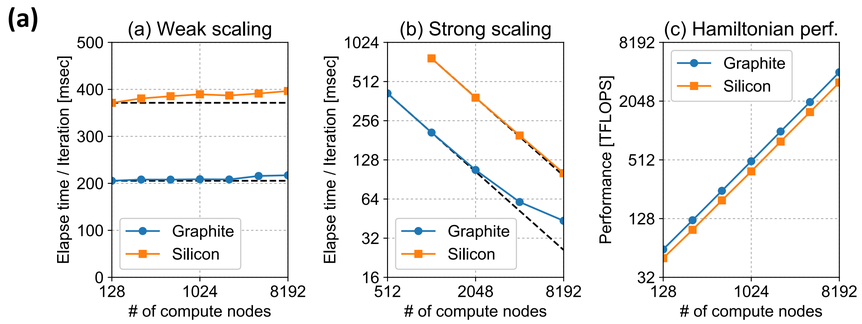
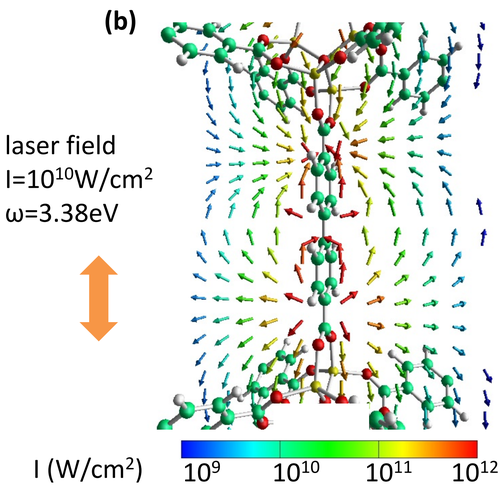
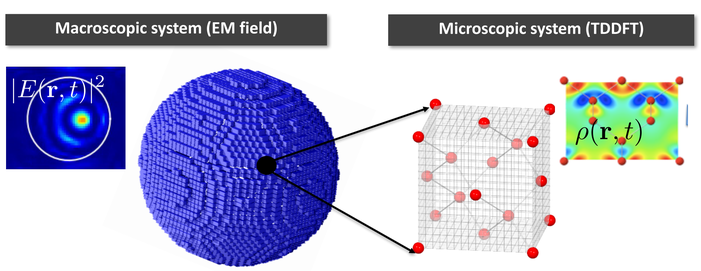
Applications with the Oakforest-PACS

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

We are developing a computer code SALMON, Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience (http://salmon-tddft.jp). It is based on first-principles time-dependent density functional theory and describes electron dynamics in molecules, nanostructures, and solids induced by optical electric fields by solving the time-dependent Kohn-Sham equation in real time and real space. Recently, we have successfully achieved large-scale simulations for nano-optics phenomena solving a coupled equation of 3D Maxwell for light electromagnetic fields and 3D time-dependent Kohn-Sham for light-induced electron dynamics. It provides an accurate and precise platform of numerical experiments that will be indispensable in forefront optical sciences.







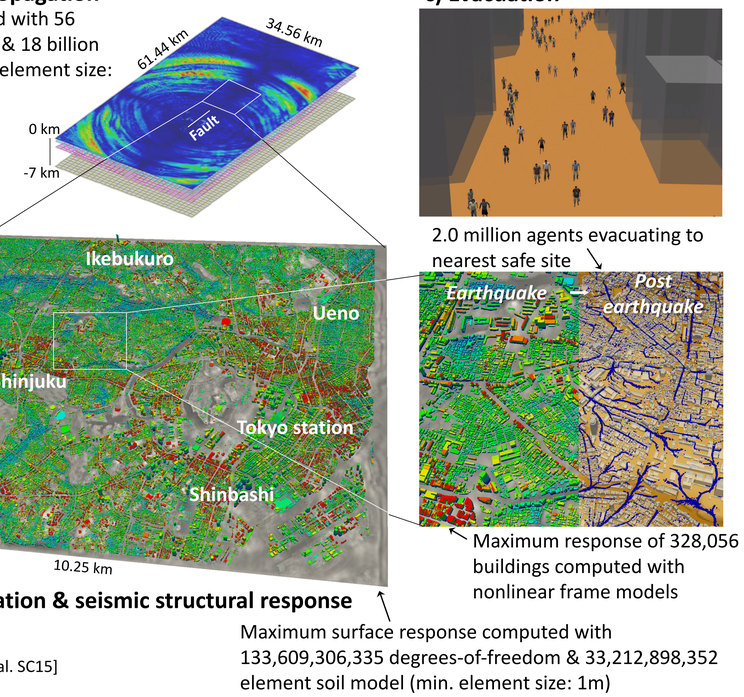
(a) Performance of SALMON using full nodes of Oakforest-PACS.
(b) Optical near-field generated in metal-organic framework, IRMOF10.
(c) Intense pulsed light irradiates on silicon nano-sphere of 250nm radius by coupled Maxwell-TDDFT calculation.

GAMERA/GHYDRA

Enhancement of earthquake simulation for disaster reduction requires fast analysis of very large scale low-order finite-element analyses. Group led by Earthquake Research Institute, the University of Tokyo has been developing high-performance low-order finite-element solvers by designing algorithms suitable for current computer architecture. The developed code was named GAMERA (multi-**G**rid method, **A**daptive conjugate gradient method, **M**ulti-precision arithmetic, **E**lement-by-element method, p**R**edictor with **A**dams-bashworth method). Achievements by GAMERA on the *K computer* have been recognized as SC14/SC15 Gordon Bell Prize finalist, and SC16 Best Poster Award.

GAMERA enabled 1.08 trillion degrees-of-freedom analysis using the full system of the K computer, and the solver attained 18.6% of the peak performance (=1.97 PFLOPS)
Research is continued to attain high-performance on Oakforest-PACS by developing time-parallel algorithms. The new code is called *GHYDRA* (Great-HYDRA, **HY**bird tempo-spatial-arithmetic multi-gri**D** solve**R** with concentrated comput**A**tion). Developed solvers are planned to be used for three-dimensional ground motion analysis for earthquake disaster estimation, as well as crust-deformation analysis for estimating earthquake generation cycles.

a) Earthquake wave propagation
Surface response computed with 56 billion degrees-of-freedom & 18 billion element crust model (min. element size: 5m) T = 15 s.



[Ichimura, Fujita et al. SC15]