JCAHPC

University of Tsukuba Center for Computational Sciences

INFORMATION TECHNOLOGY CENTER, THE UNIVERSITY OF TOKYO

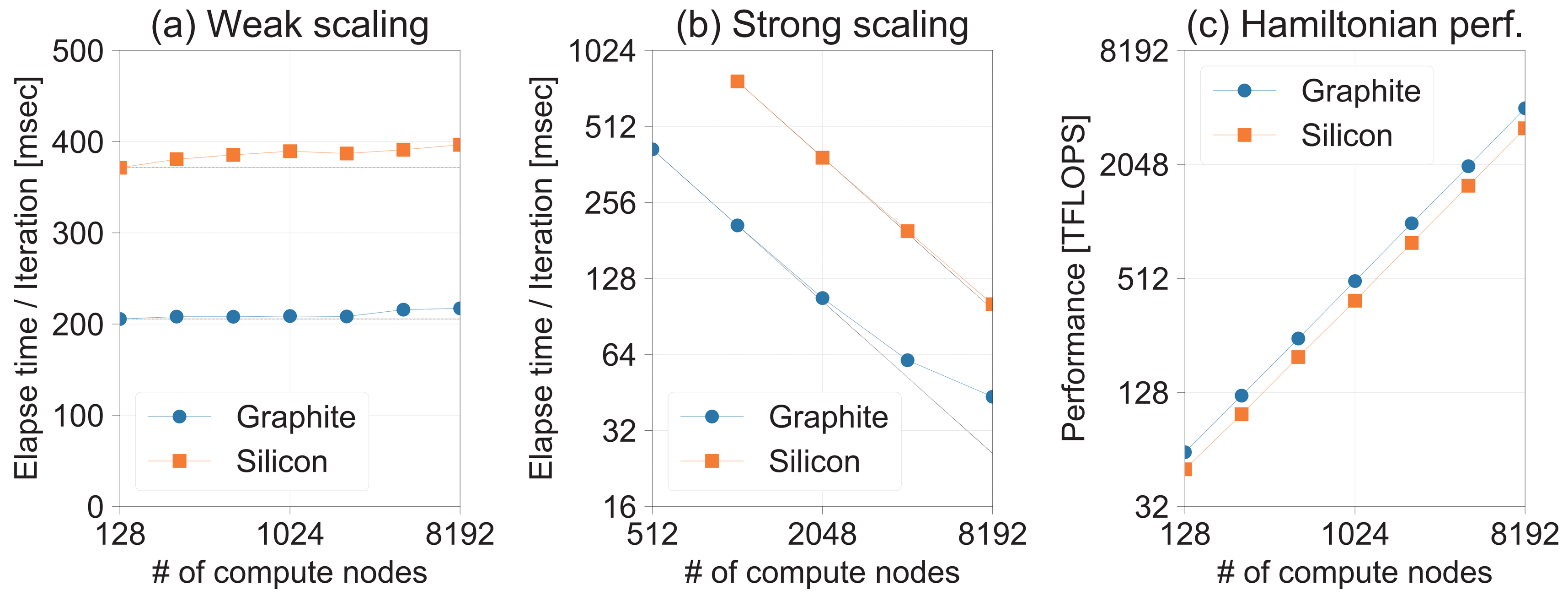
Oakforest PACS

Applications with the Oakforest-PACS

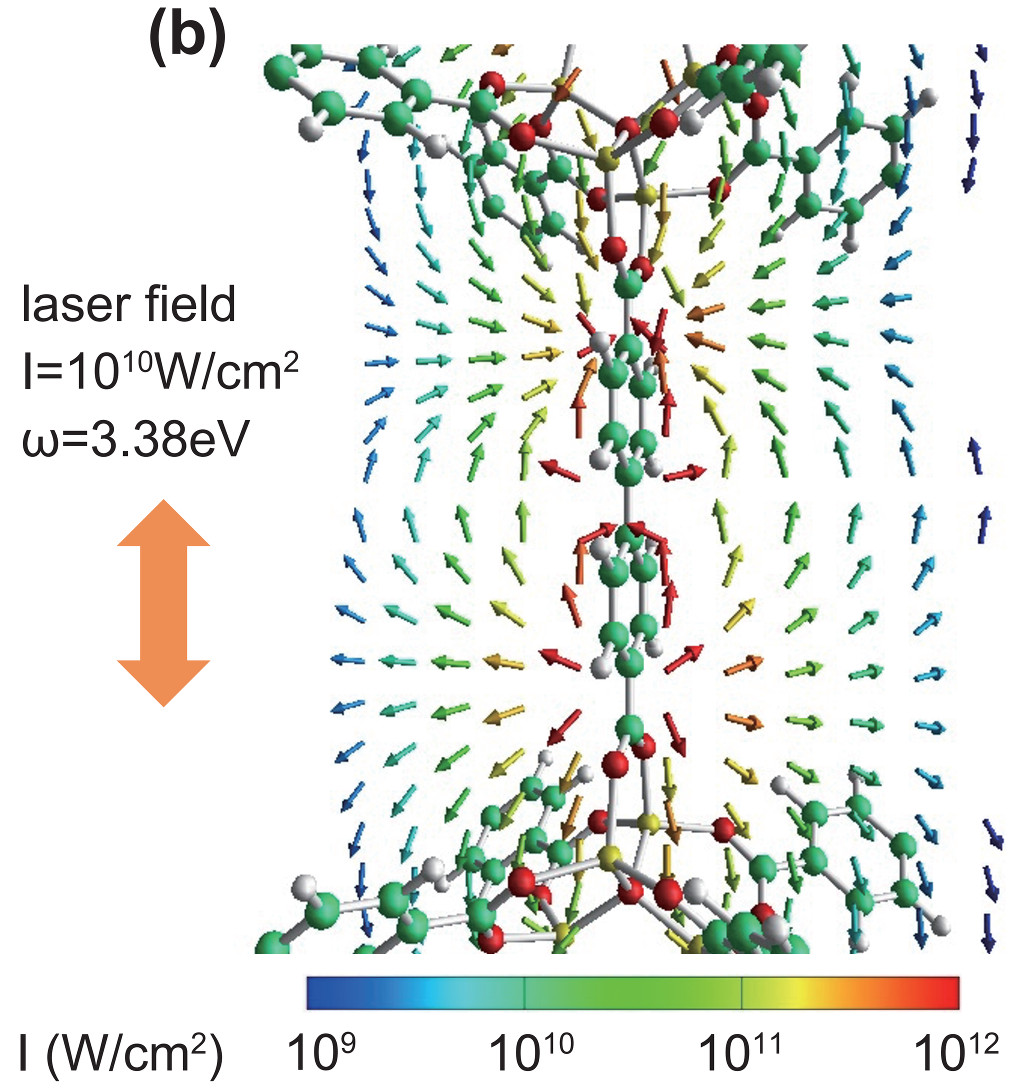
SALMON: Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience

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.

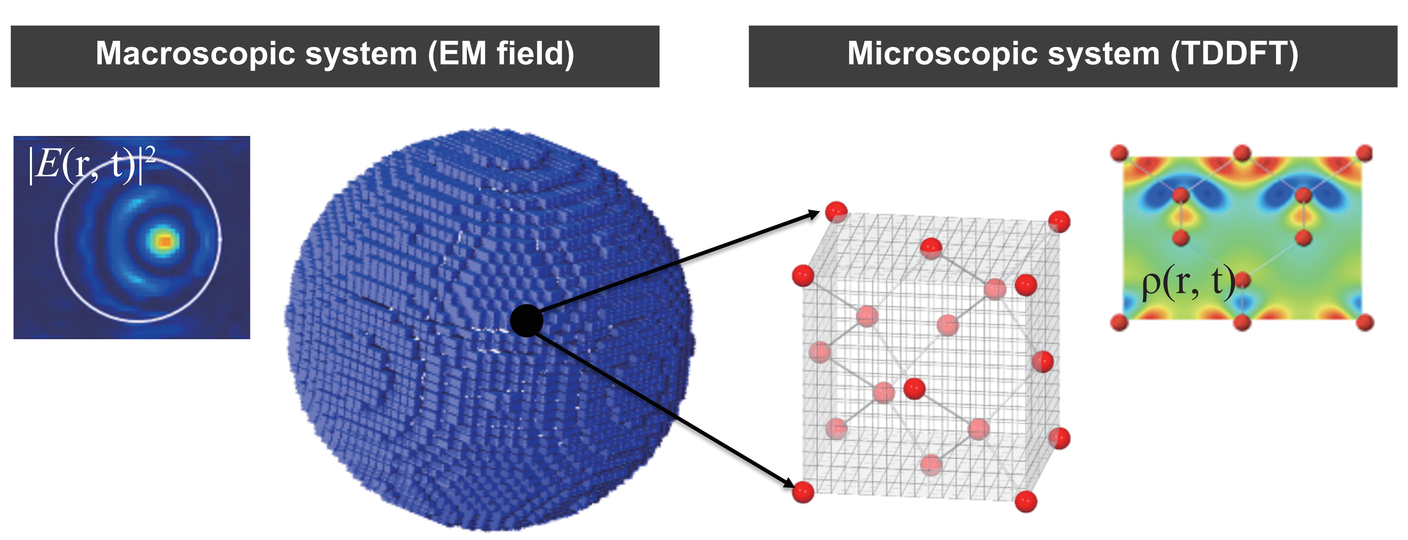
(a)



(b)



(c)

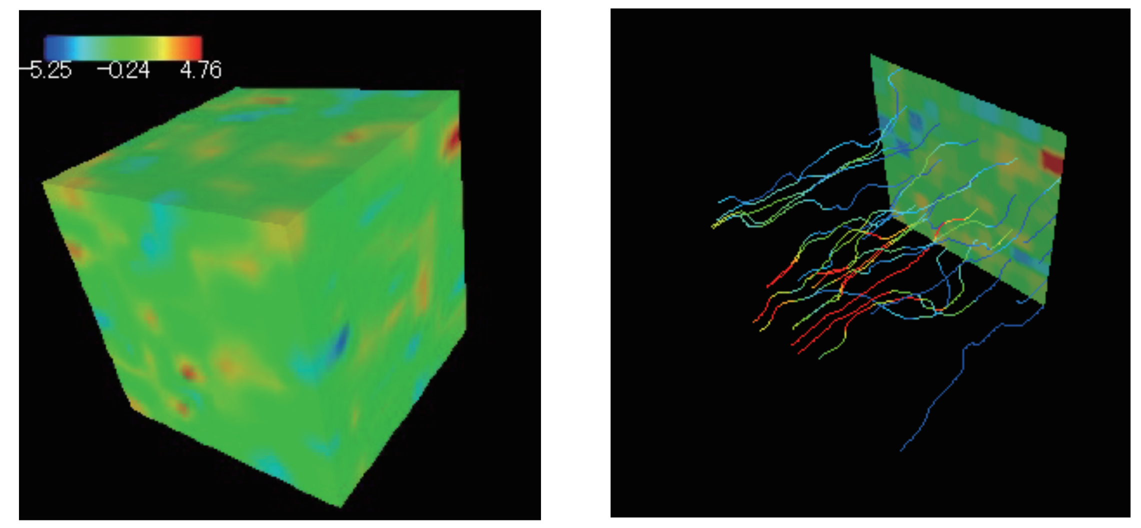


(a) Performance of SALMON using full nodes of Oakforest-PACS.
(b) Optical near-field generated in metal-organic framework, IRMOF10.
(c) Intense pulsed light irradiates on silicon nano-sphere of 250nm radius by coupled Maxwell-TDDFT calculation.

Parallel Multigrid Methods on the Oakforest-PACS System with IHK/McKernel

Parallel Multigrid Method

- Although the parallel multigrid method is expected to be one of the most powerful numerical algorithms in the exascale era due to its scalable features, there are many things to be done.
- Target Application: pGW3D-FVM for 3D Groundwater Flow through Heterogeneous Porous Media
  - MGCG Solver with IC(0) Smoother, V-Cycle
  - Sliced ELL Format for Storage of Sparse Matrices
- CGA (Coarse Grid Aggregation) [KN IEEE Cluster 2012]
  - Switching to coarse-grid solver earlier to avoid comm. Overhead
  - Significant overhead for coarse grid solver if number of MPI proc. is O(104)
- hCGA (Hierarchical CGA) [KN IEEE ICPADS 2014]
  - Hierarchical version of CGA (2-levels)
  - Number of MPI processes is reduced
  - Processes are repartitioned in an intermediate level before the final coarse grid solver on a single MPI process
  - Significant improvement of performance on Fujitsu PRIMEHPC FX10 with 4,096 nodes (65,536 cores) for a problem with 17+B DOF: Weak Scaling-1.61x, Strong Scaling 6.27x



Groundwater flow through heterogeneous porous media. (Left) Distribution of water conductivity; (Right) Streamlines

AM-hCGA: Adaptive Multilevel hCGA

- If the number of MPI proc. is O(106-107), number of proc. at the 2nd level of hCGA could be O(104).
  - 2-Levels might not be enough for more processes
  - More levels are needed ? -> AM-hCGA (Adaptive Multilevel hCGA)

IHK/McKernel

- Light Weight Multi Kernel OS for HPC by RIKEN [BG IPDPS 2016]
  - McKernel implements only a small set of performance sensitive system calls and the rest of the OS services are delegated to Linux.
  - Same binary on pure Linux can be used
  - Lower Noise, Lower Communication Overhead
  - to be available on K, Fugaku (Post K)

Summary of Preliminary Results

- IHK/McKernel provided more efficiency and stablility
  - Reduction of Noise, Communication Overhead
- Improvement is more significant, if the prob. size/proc. is smaller
  - 4%: Medium, 17%: Small, 22%: Tiny
- Improvement by AM-hCGA = 10% for Tiny Case at 2,048 nodes with IHK/McKernel
  - Effect of AM-hCGA was not clear without IHK/McKernel, because fluctuation of computation time was very large.