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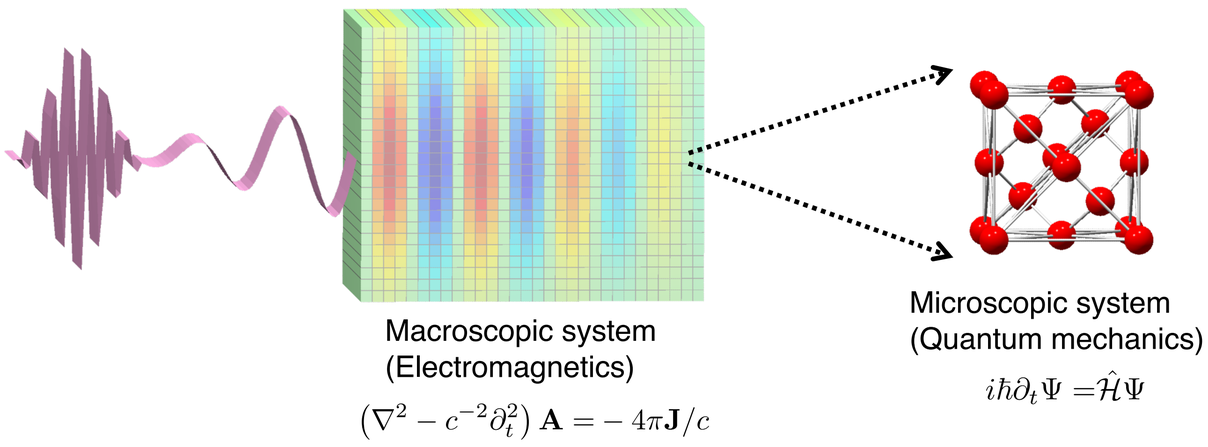
Applications with the Oakforest-PACS

ARTED: Ab-initio Real Time Electron Dynamics simulator



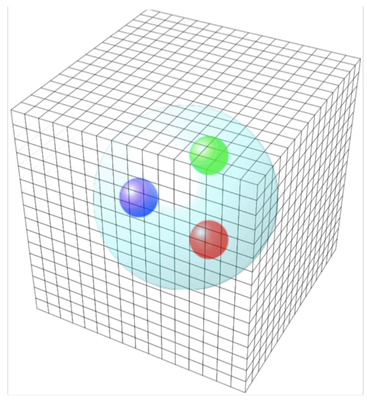
The computer code ARTED, Ab-initio Real Time Electron Dynamics simulator, is designed to describes interactions between light and materials based on first-principles quantum theory. It describes dynamics of the light electromagnetic fields and electrons in the material simultaneously in a multiscale modeling. Finite-difference time-domain method is used to solve Maxwell equations for light electromagnetic fields, while time-dependent Kohn-Sham equation is solved using real-time and real-space grid methods. ARTED has been successfully applied to simulate a number of experiments at the forefront of optical science such as attosecond science and intense and ultrashort laser science.

Y. Hirokawa, "Electron Dynamics Simulation with Time-Dependent Density Functional Theory on Large Scale Many-Core Systems", SC16 Poster Session, ACM SRC.

Quantum ChromoDynamics

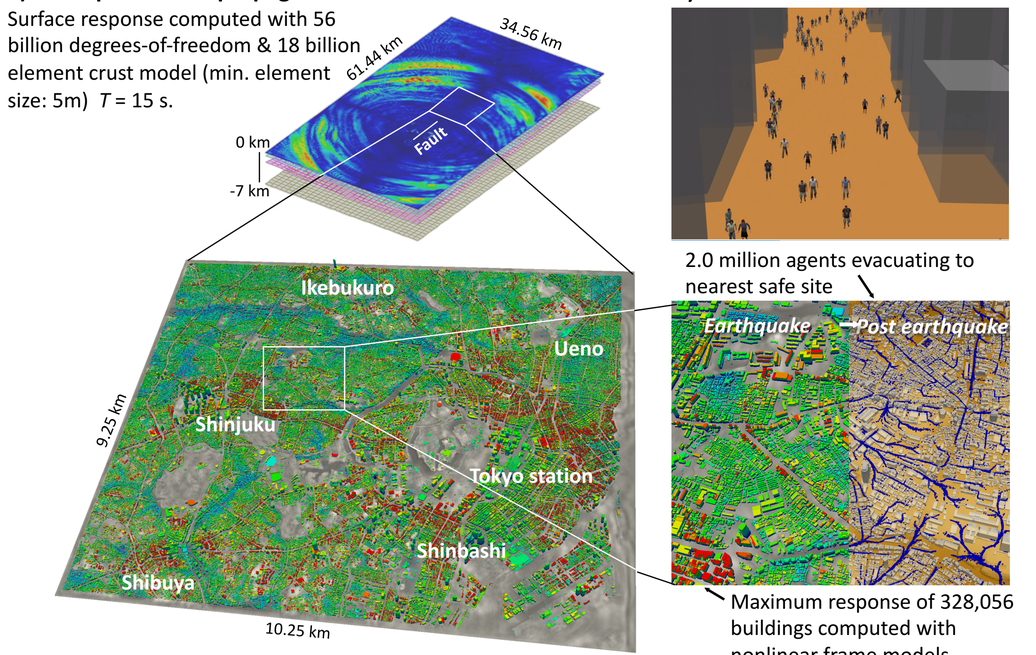
Lattice QCD is one of the most advanced case in quantum sciences: Interactions between quarks, which are elementary particles known to date, are described by QCD formulated with the quantum field theory.

With the use of Oakforest-PACS we plan to make a large scale simulation of lattice QCD with $(10\ \mathrm{fm})^3$ spatial volume at physical quark masses. The spatial size is large enough to accommodate light nuclei such as ^{4}He, and direct simulation at the physical quark masses provides us high precision measurement of physical quantities, which enables us to make a detailed comparison with the experimental results.



GAMERA - Fast and Scalable Implicit Finite-Element Solver for Comprehensive Earthquake Simulation System

We are developing a comprehensive earthquake simulation system designed to model all phases of an earthquake disaster. The key component of this simulation system is a fast and scalable implicit unstructured finite-element solver (GAMERA) for modeling nonlinear wave propagation in complex shaped domains, which was nominated as Gordon Bell Prize finalist of SC14 and SC15. As GAMERA was originally developed for multi-core CPU based K computer system, we are now modifying the algorithm such that it better suits many-core Xeon Phi (Knights Landing) processors. By using GAMERA on Oakforest-PACS, we expect to further improve time-to-solution and energy efficiency of comprehensive earthquake simulations.



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