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学位論文の概要及び要旨

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題　　目　Numerical methods for large-scale quantum material simulations
（大規模量子物質シミュレーションのための数値計算法）

学位論文の概要及び要旨

The present thesis is devoted to numerical methods for large-scale quantum material simulations that are applicable to large-scale systems, in particular, emerging from industrial application. We focused on fundamental numerical problems in quantum material simulations and these problems appear the Schrodinger equations in the time-independent or time-dependent forms.

The thesis consists of three main issues; hybrid parallel generalized eigenvalue problem solver, quantum wavepacket dynamics simulation solver, and extreme parallelism on the full system of the K computer for an order-N electronic structure calculation code (N is the number of atoms in a system). The three parts are relevant as follows; an order-N electronic structure calculation code ELSES(=Extra Large Scale Electronic Structure calculations) enables one-hundred-nm-scale quantum molecular dynamics (MD) simulations. Electronic structure can be calculated via generalized shifted linear equations or generalized eigenvalue equations. The order-N calculation is achieved when generalized shifted linear equations are solved. Generalized eigenvalue problem solver gives more reliable numerical result with larger (O(N^3)) computational costs. The order-N solver and the hybrid parallel generalized eigenvalue problem solver are complement to each other. They are massively parallel numerical solvers and show high scalability up to the full system of the K computer, one of the fastest supercomputers in the world. Based on the quantum MD results, quantum wavepacket dynamics simulations are executed to calculate transport properties.

At first the background of the thesis such as overview of parallel computing is explained. Organic materials play a crucial role among next-generation IoT (Internet of Things) products, such as display, battery and sensor, since they form flexible atomic structures and enable ultra-thin, light, flexible (wearable) devices with a low fabrication cost. Because disorder (or randomness) in atomic structures is important for properties of organ

ic materials, large-scale (100nanometer or 10^8 atom scale) quantum material simulation methods are required. Efficient parallel computation is a key technique for realization of such large-scale quantum material simulations. Algorithms and implementations must be carefully chosen depending on a required physical quantity and parallel architecture.

Hybrid parallel generalized eigenvalue problem solver Optimally hybrid numerical solvers are constructed for massively parallel generalized eigenvalue problem (GEP). The strong scaling benchmark was carried out on the K computer and other supercomputers for electronic structure calculation problems in the matrix sizes of M=10^4 - 10^6 with up to 10^5 processor cores. The procedure of GEP is decomposed into the two subprocedures of the reducer from the GEP to the standard eigenvalue problem (SEP) and the solver of SEP. A hybrid solver is constructed, when a routine is chosen for each subprocedure from the three parallel solver libraries of ScaLAPACK, ELPA and EigenExa. The hybrid solvers with the two newer libraries, ELPA and EigenExa, give better benchmark results than the conventional ScaLAPACK library. The detailed analysis on the results implies that the reducer can be a bottleneck in next-generation (exa-scale) supercomputers, which indicates the guidance for future research of parallel generalized eigenvalue problem solvers.

Quantum wavepacket dynamics simulation solver This part focuses on transport calculations for condensed organic polymers. One-hundred-nm-scale electronic structure calculations were carried out by ELSES on the K supercomputer. The transport calculations were carried out as a theoretical extension for the quantum (hole) wavepacket dynamics simulation. The calculation is based on a time-dependent Schrodinger type equation $i(d/dt)\psi = H_{WP}\psi$ for a hole wavefunction $\psi(r,t)$ with a modelled Hamiltonian H_{WP}. Analysis of time evolution of $\psi(r,t)$ gives mobility, which is an important parameter for electronic device performance. The method was applied to a single polymer chain and condensed polymers. The result of mobility calculation is consistent to the experimental trend.

Order-N electronic structure calculation code A novel parallel linear-algebraic algorithm was introduced to electronic state calculations. The benchmark shows an extreme strong scaling (75% in parallel efficiency) and a qualified time-to-solution (less than 10^2 sec in elapsed time) on the full system of the K computer. Their mathematical foundation is generalized shifted linear equations ((z S - H) x = b), instead of conventional generalized eigenvalue equations. The foundation has a highly parallelizable mathematical structure and applicable to many scientific areas. The simulation of organic polymer devices was carried out in academic-industrial collaboration. Using the electronic state calculations, a network analysis on connected polymer networks was carried out. Small networks of several polymers that electronically connected are extracted. The quantum wavepacket dynamics simulation was employed for transport calculations for the extracted networks. The simulation and data analysis reveal that electronic waves propagate on connected polymer networks and contribute the electrical current. The present simulation method will give the insights of next-generation electronic devices and their fabrication process.