Introduction

This issue is the proceedings of the RIKEN symposium, *Large-scale Calculation of Electronic States*, held on November 4–5, 1999 at the Wako campus of RIKEN. The meeting was organized by the Computational Science Division, Surface Chemistry Laboratory, Laser Technology Laboratory, and Semiconductor Engineering Laboratory. In this symposium, eminent scientists from the United Kingdom, Spain, Italy, Canada, Vietnam, China, France and Japan got together to discuss newly emerging methods for large-scale *ab initio* electronic state calculation and their application to various fields, such as surface reactions, spin devices, laser physics, geophysics and biology, where computational approaches based on electronic state calculations are expected to become as effective as experimental and theoretical approaches.

Many numerical methods, such as total energy calculation based on the density functional theory, the time-dependent calculation, Chebyshev polynomial expansion, and Suzuki-Trotter decomposition were proposed and discussed in the symposium: Several of the algorithms have computational cost of Order-N, or linear scaling to the system size, which is a promising feature in computing with very large systems. Electronic state calculations based on the density functional theory were challenged under extreme conditions such as at a surface of solid, under high pressures and/or high temperatures. Time-dependent methods have proven its effectiveness in studying the response functions of materials, and dynamics of atoms and molecules in an intense laser field, in a cluster or at the surface. Chebyshev polynomial expansions of quantum operators, such as time-evolution operator, the Green's function and the Fermi operator, become more and more popular in electronic state calculation because of its accuracy, stability, and efficiency in parallel computation. Suzuki-Trotter decomposition of exponential operators, which was first applied to the density operator in the quantum Monte Carlo method by Professor Suzuki, has also become one of the most popular method to compute the time-evolution operator in quantum dynamics. In the symposium, application of Suzuki-Trotter decomposition to other operators, such as the Gaussian operator, was also discussed. Path integral methods are expected to be one of the most powerful method for quantum systems.

The idea of organizing this meeting originated from Professor Tomo Munehisa after the Sectional Meeting of The Physical Society of Japan in October 1998 at Okinawa. Professor Munehisa proposed that now it is the time to have a small meeting to discuss newly emerging powerful algorithms for large-scale electronic calculations and their applications, and he donated some amount of money for this meeting, out of his pocket. Inspired by his enthusiastic proposal, Professor Hiroshi Tanaka, Professor Shintaro Nomura, and several researchers from inside and outside of RIKEN have soon established the organizing committee for the meeting, and decided to hold it at the Wako Campus of RIKEN as one of RIKEN symposia. Professor Masuo Suzuki, Professor Masaru Tsukada, Professor Shinji Tsuneyuki, and Professor Masaki Itoh have kindly accepted the request of the organizing committee for their joining the advisory committee, and made a lot of useful advice for the symposium. Especially, Professor Suzuki introduced us important candidates of invited speakers, and made an impressive opening address which emphasized the importance of computational methods in science, an inspiring lecture on the Separation of Procedures in Numerics, as well as many sharp questions and comments on the presentations, which made the symposium very active and enjoyable. We would like to thank all participants, including the above mentioned, who spared their time for the symposium and shared cheerful time for discussions and conversations during sessions, coffee breaks, and banquets. We hope that this symposium would contribute to the study of *ab initio* electronic state calculations. Finally, we are most grateful to our secretaries, Ms. Tomoko Ohata, Ms. Ryoko Akai, and Ms. Tokiko Suga, who took care of everything necessary for the symposium very efficiently.

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