Materials Informatics using High Performance

Frontiers of Information Science has enabled the massive data handling with reasonable speed, and has made qualitative changes in materials science recently. The simulation handles vast amount of couplings from at most 100 kinds of realistic atoms on the earth with quantum mechanical calculations to predict materials properties those are useful for our life. Such activities are about to be promoted intensively by several countries as their scientific strategies. The world of quantum mechanics is out of our intuitive expectations and hence the power of computer simulation is essentially in demand.

Massive Parallel Simulations

We have worked on the statistical simulations involving random number samplings combined with quantum many-body theory (Diffusion Monte Carlo method). The framework provides the most reliable estimation of electronic properties of materials. Our simulations require massive computational resources, but inherently in harmony with parallel processing. JAIST super computing facilities enable us to carry out such simulations. Recently our group has also accomplished the acceleration using graphic card (GPGPU).

Interdisciplinary Challenge

There is a huge demand for researchers working on physics, chemistry, and materials science, who are good not only at mathematics but at 'computics' as another tool of analyzing phenomena. It is a great challenge for talented younger students to commit such a novel, exciting interdisciplinary field as a 'Simulation Scientist', experienced by rich computational facilities and fine course work provided by Jaist.

Publications


please visit our web page for more details: http://www.jaist.ac.jp/is/labs/maezono-lab/wiki/linkedPdf/newpub.pdf