Development and dissemination of applications software for materials science simulation

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Thanks to advances in computers that are said to double the computing speed in one and a half years, and also due to researchers' efforts to master them, the world of materials science simulation has changed dramatically even in this decade only. Briefly, computation with a larger scale, longer time, and better approximation than before became possible, and applications of the simulation has been widely spread. Nonetheless, the development of high-performance, large-scale applications software is highly difficult since it requires a high degree of programming technology tailored to the latest machines. As a result, the number of developers has not necessarily increased, but the free publication and commercialization of applications software has progressed, and experimental or theoretical researchers as users are developing new material science research beyond the expectation of the developers. It is the recent trend of computational materials science. Researchers involved in the development of simulation methods also benefit from the software publication in that they can easily develop applications software with new functions using published ones.

In this talk, I will discuss the software development in nationwide organization and network, such as the recently completed K computer project and the currently undergoing post-K computer project. Subsequently, I will introduce MateriApps (see Figure), a portal site for materials science simulation, and related activities, which are being continuously operated mainly by the researchers in the Center of Computational Materials Science (CCMS), the Institute for Solid State Physics (ISSP). Also, I will describe the current status of the High Performance Computing Infrastructure (HPCI) in Japan including the K computer, and the recent movements of HPCI-based dissemination of applications software.

External links MateriApps http://ma.cms-initiative.jp

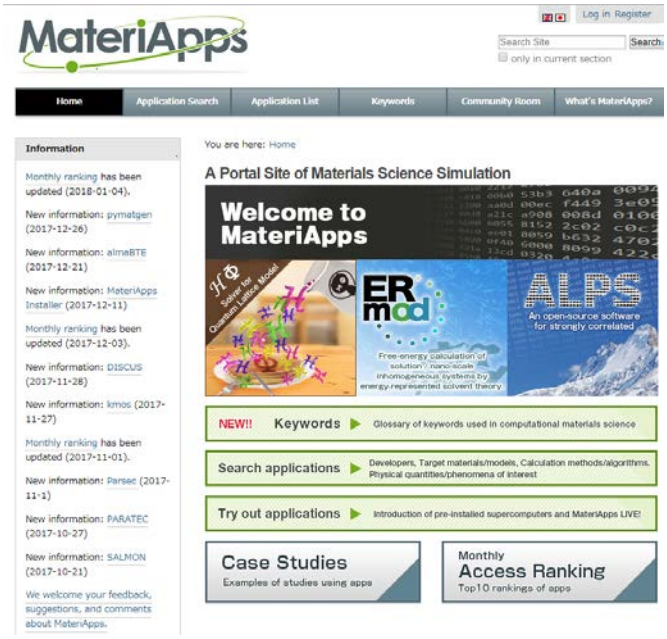

Figure: The top page of MateriApps, a portal site of materials science simulation.