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Large-Scale First-Principles Electronic Structure Calculations in Petascale and Exascale Supercomputers: A Real-Space Density Functional Theory code

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First-principles electronic structure calculation based on the Density Functional Theory (DFT) has been an indispensable tool for many fields of material science and engineering. With the development of supercomputers, the target size of a first-principles DFT calculation becomes larger and larger, and nowadays, a few hundreds to a thousand of atoms has been computable with standard plane-wave based DFT program codes. However, the computable sizes are still not satisfactory for clarifying or designing the material properties in realistic situations. The challenge for large scale calculations with state-of-the-art supercomputers is one of the ways to overcome the size difficulty in the first-principles electronic structure calculations.
In this talk, I'd like to introduce our program code RSDFT [1], which has been developed to perform large-scale first-principles calculations on massively-parallel computers including the Japanese flagship machine K computer [2].
RSDFT is based on the real-space finite-difference pseudopotential method. Contrary to the standard plane-wave methods, the real-space method needs not to use Fast Fourier Transformations, which requires heavy communication burden, and therefore the scalability of RSDFT is rather good even in the calculations with tens of thousands of compute nodes [3]. It has also been started to develop RSDFT for the next flagship computer called post-K computer, and we aim to make first-principles calculations on the system with a few thousand of atoms easy tasks. I would like to also talk about the development of RSDFT for the post-K computer.

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[2] http://www.nsc.riken.jp/index-eng.html
[3] Y. Hasegawa, J.-I. Iwata, M. Tsuji, D. Takahashi, A. Oshiyama, K. Minami, T. Boku, H. Inoue, Y. Kitazawa, I. Miyoshi, M. Yokokawa, The International Journal of High Performance Computing Applications 28, pp.335-355 (2014).

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