Novel linear-algebraic algorithms and ten-million-atom electronic state calculations on the K computer

T. Hoshi\textsuperscript{ab}, T. Sogabe\textsuperscript{cb}, T. Miyata\textsuperscript{db}, S-L. Zhang\textsuperscript{db}

\textsuperscript{a} Tottori University, Japan; \textsuperscript{b} JST-CREST (PostPeta), Japan; \textsuperscript{c} Aichi Prefecture University, Japan; \textsuperscript{d} Nagoya University, Japan; e-mail: hoshi@damp.tottori-u.ac.jp

Novel linear-algebraic algorithms [1-4] were developed in an interdisciplinary research between physics and applied mathematics and applied to ten-million-atom electronic state calculations. The algorithms, ex. the multiple Arnoldi method [1,2], are Krylov-subspace (iterative) solvers for generalized shifted linear equations, in the form of $(zS-H)x = b$, in stead of conventional generalized eigen-value equation. The algorithms are purely mathematical and applicable to many physics areas with large matrices. [1] The method was implemented in our order-$N$ calculation code ELSES with tight-binding systems based on \textit{ab initio} calculations (http://www.elses.jp).

Figure (a) shows a high parallel efficiency on the K computer with nano materials in industrial application. In Figs. (b)(c), a post-simulation analysis is presented as a ‘big data’ problem with huge distributed electronic-state data; A novel analysis method, pi-COHP method [1], is used in an sp2-sp3 nano-composite carbon solid (NCCS), so as to distinguish sp2 (graphite-like) and sp3 (diamond-like) regions.

![Figure (a) Parallel efficiency on the K computer [1] for amourphous-like poly fluorene (aPF, a conjugated polymer) and NCCS (See text). (b)(c) Visualization analysis of NCCS for sp2 and sp3 regions (b) and only for sp2 region (c) [1].](image)