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密度汎関数理論(DFT)計算のプラズマシミュレータに対する
コードチューニング

Code Tuning of DFT Calculation for the Plasma Simulator in NIFS

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National Institute for Fusion Science deployed the supercomputer system 'Plasma Simulator - Raijin' in July 2020.The new system adopts NEC SX-Aurora TSUBASA (SX) platform with vector processors and high band width memories. It consists of 540 vector hosts, each of which has 8 vector engines, and achieves 10.5 PFlops.

Our research group utilize OpenMX code [1], open-source package for material explorer, for atomic scale simulations of thermonuclear fusion reactor material [2-4]. OpenMX is based on density functional theories (DFT), norm-conserving pseudo-potentials and pseudo-atomic localized basis orbitals as electron basis functions [5,6]. Its methods and algorithms are designed for large-scale *ab initio* electronic structure calculations on parallel computers based on the MPI or MPI/OpenMP hybrid parallelism. It, however, was insufficient in terms of vectorization. Thus, we carried out vectorization and associated code tuning of OpenMX to extract computational performance of SX [7].

Benchmarking calculations were performed in order to evaluate the tuned code. In the benchmarking as a typical case of plasma-material interaction and fusion reactor material, 127 tungsten atoms which corresponds to 4x4x4 unit cells of body-centered cubic lattice structure with mono-vacancy are targeted. The calculation domain has three dimensionally periodic boundary condition, and the Brillouin zones are sampled with 4x4x4 *k*-points. Self-consistent field (SCF) iterations are stopped at 33 steps for avoiding variation of computational effort.

Benchmarking result in the table shows that tuned code achieves 3.1-3.3 times improvement than the original code and is comparable to the Intel Xeon Gold 5148 processor. It is noted that Xeon Gold 5148 is 2.816 TFlops per node while SX is 2.433 TFlops per node.

In this presentation, technical details and findings related to vectorization and associated code tuning of DFT-based simulation software package OpenMX are described, with showing benchmarking results for typical sample cases.

table: calculation time (in second) of benchmarking

Processor	Code	8 nodes	16 nodes
SX	original	1471	899
SX	tuned	476	271
Xeon	original	434	314

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