Performance measurement of kinetic code on scalar processors

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Manycore scalar processors are one of recent trends of CPUs in high-performance computing, which run at low clock frequency to reduce the power consumption but have a large number of compute cores with processing units for operating multiple data, such as Advanced Vector Extension (AVX) and Single Instruction Multi Data (SIMD) units. It is not easy for users of scientific applications to achieve a high performance (e.g., a computational efficiency of more than 30% to the theoretical peak performance) on recent manycore scalar processors with the multiple data units.

As a high-performance application to scientific computing, the present study deals with a first-principle kinetic simulation based on the Eulerian grid. The first-principle kinetic simulation usually requires enormous computing resources since this solves time development of distribution functions defined in "hyper" dimensions (at most three spatial and three velocity dimensions). In Eulerian-grid-based simulations, such as fluid simulations and the present kinetic simulations, a bottleneck of the computational performance generally exists at the memory bandwidth.

Performance tuning of the Eulerian-grid-based codes on manycore scalar processors is an issue in high-performance computing. In the present study, performance evaluation of the Eulerian-grid-based kinetic code is made on a single compute node with two Xeon Broadwell processors, with a Xeon Phi Knights Landing processor, and with a SPARC64 XIfx processor.

The present kinetic code solves the first-principle equation called the Vlasov (collisionless Boltzmann) equation. The self-consistent electromagnetic and gravitational fields are obtained by coupling field equations such as the Maxwell equations and the gravitational field formula. The kinetic code solves the spatio-temporal development of distribution functions in position-velocity space. It is not easy to integrate such a "hyper-"dimensional equation numerically in time in terms of both computational accuracy and computational resources. In order to simplify the numerical operations, the Vlasov equation is separated into two advection and one rotation equations based on operator splitting [1, 2]. The three equations are solved with conservative schemes [3–5].

We adopt the "domain decomposition" with the standard message passing interface (MPI) library as the first-level process parallelism as standard Eulerian-grid-based methods do. However, we decompose the computational domain only in the position dimensions [6]. The velocity dimensions are not decomposed because there arise some additional communications overhead due to a reduction operation in the computation of the density and the momentum. It is well-known that the domain decomposition involves the exchange of halo layers for the distribution function and electromagnetic field data at boundaries of each computational subdomain. The present non-oscillatory and conservative scheme [3, 4] uses six grid cells for numerical interpolation. Thus, three halo grids are exchanged by using the "`MPI_Sendrecv`" subroutine in MPI for simplicity, portability and stability. As a second-level thread parallelism, we use the "`OMP (PARALLEL) DO`" directive together with the "`COLLAPSE`" clause to parallelize most outer multiple loops with less threading overhead [7].

A hyper-dimensional simulation requires a huge computer resource. For applications to practical scientific computing, however, massively parallel computation with multiple compute nodes is necessary, since more than 1 TB memory is usually used. Hyper-dimensional Boltzmann simulations are practically in use (but not so widely) in plasma sciences, especially for laser plasma [1], tokamak plasma in thermonuclear fusion devices [8], and collisionless space plasma [9, 10].

We use three systems for the performance evaluation, which have a single Xeon Phi 7250, a dual Xeon E5-2697, and a single SPARC64 XIfx processors. The size of job corresponds to ∼28 GB including temporary work arrays. The number of processes per compute node is fixed to two, but the number of threads per process is changed in the present strong scaling measurement. We measure the elapsed time for five time steps. Although the computational speed of the code on a single core of Xeon Phi KNL is much slower than the other two systems, the computational speed on one compute node is comparable to the other systems due to the large number of compute cores and HT. We has made a performance tuning of our code by the decomposition of most-inner loops and reduction of temporary work arrays. The code becomes faster by a factor of 1.2–2 on these scalar CPUs..

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