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京における局所的ジャイロ運動論的シミュレーションコードGKVの並列化
Parallelization of the local gyrokinetic simulation code GKV on the K computer

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One of the most important issues in magnetically confined plasma researches is turbulent transport. Numerical simulations based on the gyrokinetic theory have strongly promoted the understanding of micro-instabilities and associated plasma turbulence. Most of gyrokinetic simulations have assumed scale separations between ions and electrons to reduce computational costs. Ion-scale and electron-scale turbulence, however, are able to nonlinearly interact via mesoscale structures. Therefore, plasma turbulence is intrinsically multi-scale physics, which includes temporal and spatial scales of electrons and ions simultaneously. Since multi-scale turbulence simulations require high temporal and perpendicular spatial resolutions, their computational costs are estimated to be $(m_i/m_e)^{3/2}$ times higher than that of ion-scale turbulence. To deal with this numerically challenging problem, highly-scalable simulations on peta-scale super-computers, such as the K computer, are necessary. Our proposal for the general use of the K computer has been accepted, and we have been developing numerical schemes and parallelization methods for multi-scale turbulence simulations.

We have extended the gyrokinetic Vlasov simulation code GKV [Watanabe,NF2006] to run efficiently on the K computer, where a key numerical technique is the speed up of the parallel two-dimensional (2D) Fast Fourier Transform (FFT) algorithms. MPI/OpenMP hybrid parallelization with 4D domain decomposition is newly implemented to use a large number of cores. Perpendicular dynamics is solved by using the spectral method with 2D FFTs, where the data transpose often degrades scalability. The MPI process mapping is optimized for the 3D torus inter-node network on the K computer, so that the transpose communications are performed among the neighboring nodes located in a 3D box shape. This maximizes a bi-section bandwidth available on the torus network, and reduces communication costs of data transpose. Additionally, overlaps of computations and communications are implemented by using OpenMP directives. Applying the developed overlap method to parallel 2D FFTs, we mask communication costs of data transpose with FFTs and computations in the spectral method. The Figure demonstrates that the overlaps of transpose and FFTs significantly improve strong scaling. The case with the overlaps achieves 168 TFlops (8.03% of the theoretical peak performance) at 131,072 cores, which is 29% higher performance than that in the case without overlaps. Thanks to the developed methods, GKV achieves almost linear speed-up beyond 100k cores with high parallel efficiency ~99.9998%.

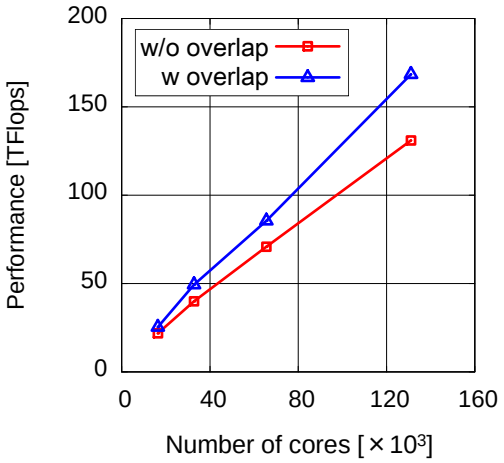

Fig. Strong scaling test of GKV on the K computer [where 1024 × 1024 × 64 × 64 × 32 grid points are employed in five-dimensional phase space (x, y, z, $v_{\parallel}$, μ) and parallelized into 8 (and 16, 32, 64) × 8 × 8 × 4 subdomains and 8 threads]. Square and triangle dots plot the cases without/with overlaps on parallel spectral calculations, respectively.

We note that the newly developed overlap methods of FFTs and transpose communications are applicable not only for the kinetic simulations but also for fluid simulations, if one finds independent multi-dimensional FFTs.