GPU-Based Parallelization of an Energy-Conserving 3D Electromagnetic Particle-in-Cell Simulation

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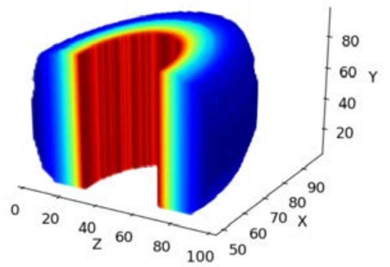
Nonlinear, transient, and kinetic effects are critical features of plasma dynamics. The particle-in-cell (PIC) simulation is superior to a fluid simulation for these aspects in a high-temperature magnetized plasma and a low-temperature partially-ionized plasma for the materials process. With the rapidly developed technology of graphics processing units (GPUs), the high-performance GPU-PIC simulation calculates the trajectories of billions of superparticles in a three-dimensional bounded plasma system.

The performance improvement of CPU-based parallelization of the energy-conserving semi-implicit PIC simulation [1,2] was reported for a three-dimensional (3D) rectangular geometry. With the increasing necessity of extreme high-performance computing, an improved parallelization of plasma simulation is essential. Furthermore, as the exascale performance of next-generation supercomputers must utilize the GPU architecture, parallelization of the particle-in-cell (PIC) simulation on GPUs is a critical issue.

In the particle-in-cell simulation, there are many kinds of numerical instabilities. At first, temporal instability occurs by the Courant-Friedrichs-Levy condition if the time step is not small enough to resolve the propagation of the speed of light. Also, spatial instability happens caused by aliasing. In addition, the resolution for the Debye length and the plasma frequency is also required. In order to avoid such restrictions, an implicit method is recommended. In addition, the conservation of energy is an important issue. The charge-conserving and the energy-conserving implicit scheme is adopted for arbitrary implicit time steps [3]. Therefore, a larger time step that is constrained only by the particle dynamics is possible to utilize without the loss in calculation accuracy. In this study, we explore a fully implicit 3D PIC method based on Newton-Krylov methods.

Conventional PIC simulations utilized a message passing interface (MPI) to treat a large number of superparticles under the concept of data parallelism. However, the heterogeneous computing in CPU + GPU mixed systems makes it challenging to improve the calculation speed only using MPI. Another essential feature of our new simulation code is the utilization of the just-in-time (JIT) compiler in the Python framework. This presentation proposes a new development of GPU-based PIC simulations for 3D electromagnetic fully-ionized plasmas to apply to the turbulence analysis of spherical tokamaks. We introduce a new software based on Python and JIT compiler and show the benchmarking results of the Tokamak simulation. The comparison of the numerical schemes for performance improvement is also analyzed.



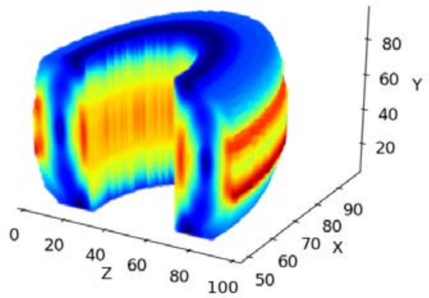


Figure 1. The considered profiles for the toroidal (top) and the poloidal (bottom) magnetic fields for the particle trajectories.

References

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