Development and Parallelization of Gyrokinetic PIC Code for MHD Simulation

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(Received: 3 September 2008 / Accepted: 25 December 2008)

In order to simulate global magnetogydrodynamic phenomena in tokamaks, a new gyrokinetic PIC (particle-in-cell) code, Gpic-MHD, is developed. Gpic-MHD is written in cylindrical geometry and has single-helicity (two-dimensional) version and multi-helicity (three-dimensional) version. The kinetic internal kink mode is successfully simulated and compared with the results of gyro-reduced-MHD (GRM) code. The performance of the Gpic-MHD on the massive-parallel computer is studied. No saturation of the speed-up factor is observed as the number of cores (processors) increases.

Keywords: magnetohydrodynamics, particle-in-cell code, gyrokinetics, tokamak, internal kink mode, parallel computing.

1. Introduction

The simulation model, which can treat global magnetohydrodynamic (MHD) phenomena in the present-day and future high temperature large tokamaks like ITER (International Thermonuclear Experimental Reactor), is necessary to extend the operational parameter range of experiments. Such model must have an ability to simulate extended (or kinetic) MHD phenomena because a lot of phenomena observed in experiments seem beyond explanation by conventional MHD model. The fluid code based on the extended MHD model can treat such phenomena, however it is still very difficult to include effects of Landau damping, magnetic drifts, non-Maxwellian velocity distribution like alpha particles, etc into the fluid model. There is also a so-called 'closure' problem in the fluid model. Therefore physically more accurate model is needed to study mysterious and complex phenomena in tokamaks and to benchmark the results of extended MHD code. The gyrokinetic PIC (particle-in-cell) code [1,2], which is based on the fundamental gyrokinetic theory keeping important velocity space physics, is one of the candidates, although it requires huge computer resources. Assuming the availability of high performance massive-parallel computers of 10 peta-flops in the near future, we have developed a new gyrokineic PIC code for MHD simulation (Gpic-MHD). The experiences of the gyrokineitc PIC code in the rectangular coordinate system [3-7] and the gyro-reduced-MHD (GRM) code [8] gave us the basis developing a new code. The present version of Gpic-MHD is written for a cylindrical coordinate system. We have a single-helicity (two-dimensional) version and a multi-helicity (three-dimensional) version. The former is compact and fast enough because of the helical symmetry, while the latter can treat mode couplings between different helicities and is easy to make modification for the toroidal version. Gpic-MHD is optimized for the simulation of kinetic (or collisionless) internal kink mode and is expected to be one of powerful tools to treat global MHD phenomena including magnetic reconnection. The parallelization performance of Gpic-MHD on the massive-parallel computer was investigated with Altix3700Bx2 of JAEA computer center.

2. Simulation Model

Gpic-MHD is a gyrokinetic PIC code with delta-f method. A present version of Gpic-MHD assumes a lowest order tokamak model. Plasma fills a cylinder with a radius of a and a height of $2\pi R$. Top and bottom of the cylinder is connected with the periodic boundary condition. A magnetic field is represented by a sum of a constant toroidal magnetic field and a poloidal magnetic

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field, $B = B_0\hat{\mathbf{z}} + \nabla \times (A_z\hat{\mathbf{z}})$, where A_z is a z component of the vector potential and $\hat{\mathbf{z}}$ is a unit vector in the z direction. An electrostatic electric field is $\mathbf{E} = -\nabla\phi$, where ϕ is an electrostatic potential. On the wall at $r = a$, ϕ and A_z are set to be zero. Positions of r, θ, z and an angular momentum of p_z are followed for electrons and ions. Because p_z is used instead of v_z, an induced electric field does not appear in the equations of motion. Characteristics of the code are in the followings: (1) Normalization of the basic equations is the same as the gyro-reduced-MHD (GRM) code. (2) Non-uniform radial mesh is adopted. Mesh can be accumulated at the rational surface. (3) Mode expansion is used for poloidal and toroidal directions. Unimportant high frequency Alfven waves restricting the time step size can be eliminated in the Fourier space.

3. Simulation Results

Simulation of the kinetic internal kink mode for the uniform density and uniform temperature is done by the single-hericity version of Gpic-MHD. The simulation shown in this section is done with 512 cores. The simulation parameters are: normalized collisionless electron skin depth of $d_e/a = 0.06$, normalized ion gyro-radius estimated by electron temperature of $\rho_s/a = 0.06$, $R/a = 18$, safety factor profile of $q(r) = q_0[1 - 4(1-q_0)(r/a)^2]^{-1}$ ($q_0 = 0.85$), radial and poloidal meshes of 129×128, number of particles of 512 millions, time step size of $\Delta t = 0.005$ and total time steps of 10000. Here, time is normalized by $2\pi R/v_A$ (v_A is a Alfven velocity). Fig.1 shows the temporal evolution of the magnetic field structure. The contours around the plasma wall are eliminated from the figure because those are so dense. The dashed circle in the figure shows the q = 1 rational surface for equilibrium. Full reconnection phase (t = 26.5, 31.5, 33.5) followed by the magnetic reconnection in the second phase (t = 38.5, 42.0 and 50.0) is simulated successfully. The time dependence of the growth rate, which is calculated from the amplitude of m/n=1/1 mode, is shown in Fig.2. The linear growth rate of γ = 0.27 is compared with γ = 0.32 obtained from the GRM code. Considering the difference in the simulation models, 20 percents difference in growth rates is reasonable. In the GRM model, a electron pressure term in the Ohm's law along the magnetic field, is approximated as $\langle v_z^2 \rangle = \langle (v_z - V_z)^2 \rangle + n_e V_z^2 \approx (T_e/m_e) n_e$ with constant temperature of T_e, where angular brackets designate the moment integration over v_z, m_e is the electron mass, n_e is the electron density, V_z is the fluid velocity along the magnetic field, and $n_e V_z^2$ is neglected. Gpic-MHD solves directly the velocity distribution. In Gpic-MHD, current along the magnetic field is generated by the shifted Maxwellian velocity distribution: equilibrium $V_z(r)$ exists. The linear angular frequency of ω_r = 0.024 is obtained for the Gpic-MHD code whereas ω_r = 0 for GRM code. The reason that the real angular frequency appears in Gpic-MHD can be explained by the gradient of $n_e V_z^2$, which also has the stabilizing effect as the diamagnetic stabilization when the density gradient exists. The nonlinear acceleration of the growth rate is also observed.

Mode profiles of the magnetic field structure, electrostatic potential and variation of the current density are shown in Fig.3. We can see a fine structure of a magnetic island (Fig.3(a)) and negative current layer (and positive current layer) at the opposite side (Fig.3(c)).

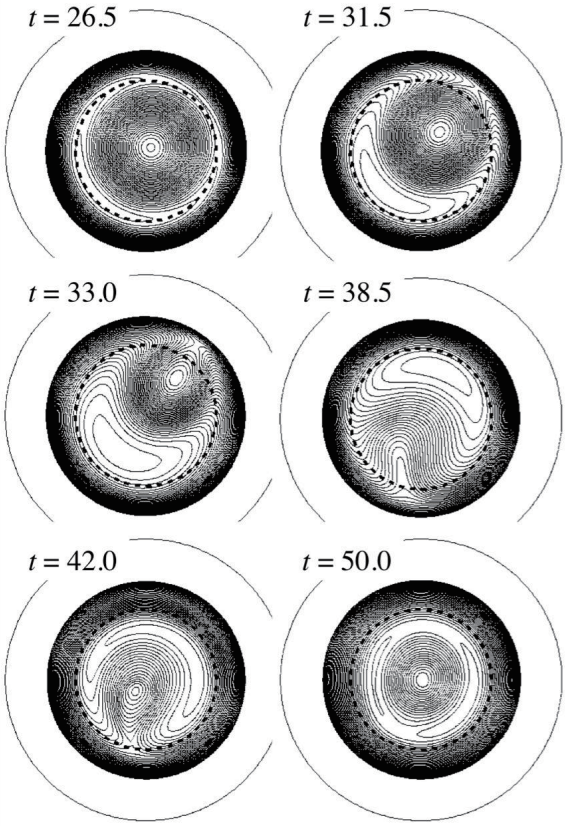

Fig.1 Temporal evolution of the magntetic field structure.

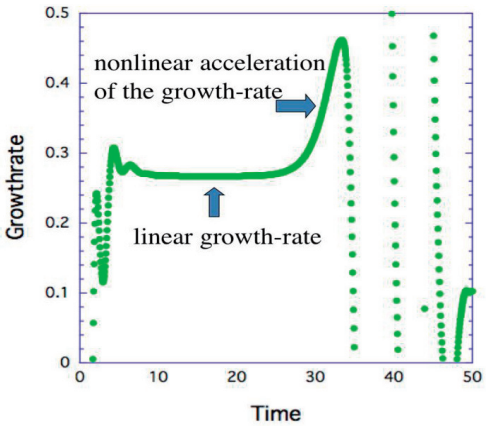

Fig.2 Time dependence of the growth rate.

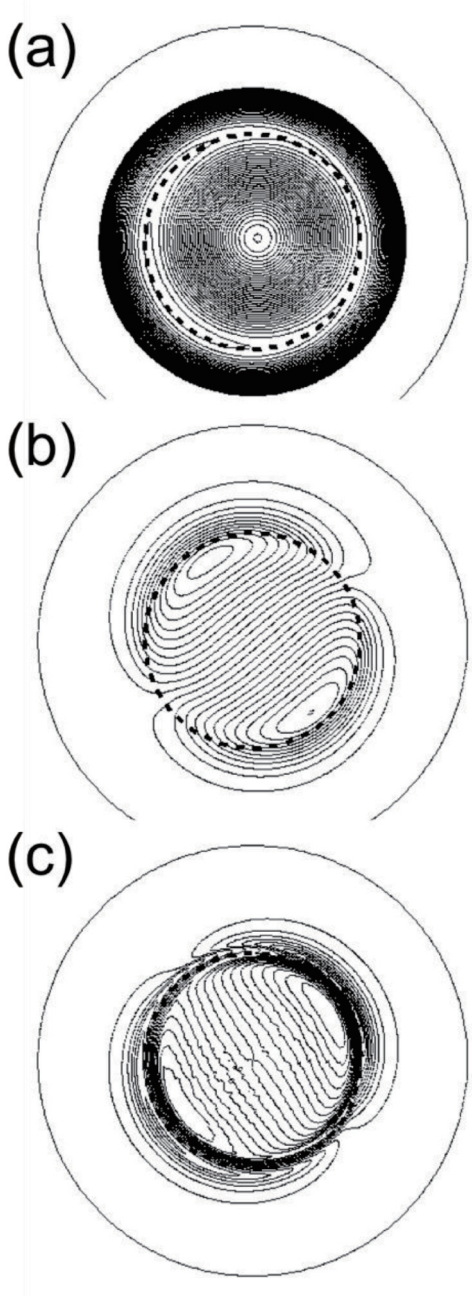

Fig.3 (a) The magnetic field structure, (b) electrostatic potential profile and (c) current density profile at a poloidal cross-section for the weakly nonlinear phase of $t = 25$.

4. Parallelization Performance

For the parallelization of Gpic-MHD, we used a Message-passing-interface (MPI) model. The single-helicity version utilizes copies of the field quantities. Figs.4 and 5 show examples of parallelization performance on Altix3700Bx2 of JAEA computer center. Each core contains 0.5 millions ions and 0.5 million electrons. Hence, the total number of particle is (number of particles / core) × (number of cores: n_{core}). Time steps are 10000, however if the computing time is over 3 hours with cores less than 64, time steps are reduced and computing times for the full steps are estimated by the linear interpolation. The computing time for n-cores calculation is designated by τ_n. The communication time between cores, mainly comes from the summations and distributions of charge and current densities over cores, is estimated by $\tau_n - \tau_1$. Calculations of field quantities are redundant and utilize the summed charge and current densities. The speed-up factor defined by $\tau_1 \times n_{\mathrm{core}} / \tau_n$ versus number of cores is depicted in Fig. 5, which shows so-called weak scaling because the program size per core is fixed. No saturation is observed as the number of cores is increased. However, the communication time is not negligible and the scaling will saturate for cores more than 2048. In order to extend the scaling to more than several thousands cores, domain decomposition in the radial direction will be needed.

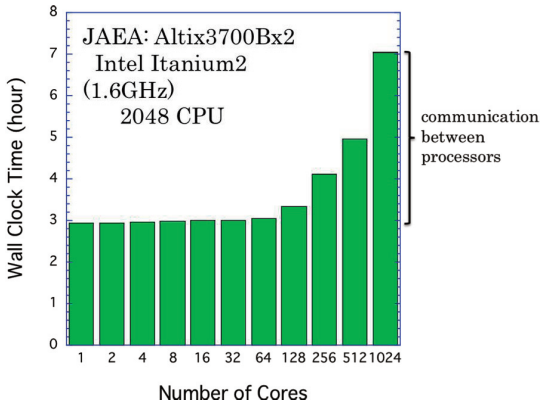

Fig.4 Wall clock time versus number of cores for the single-helicity version of Gpic-MHD. The jobs are for one million particles/core, 129×128 spatial meshes and 10000 time steps.

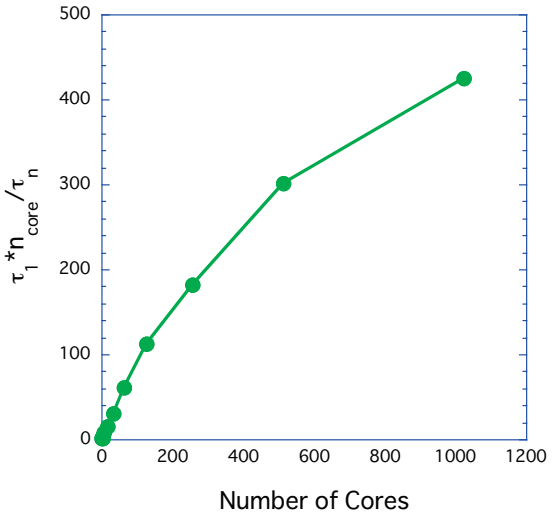

Fig.5 Speed-up factor versus number of cores for the single-helicity version of Gpic-MHD.

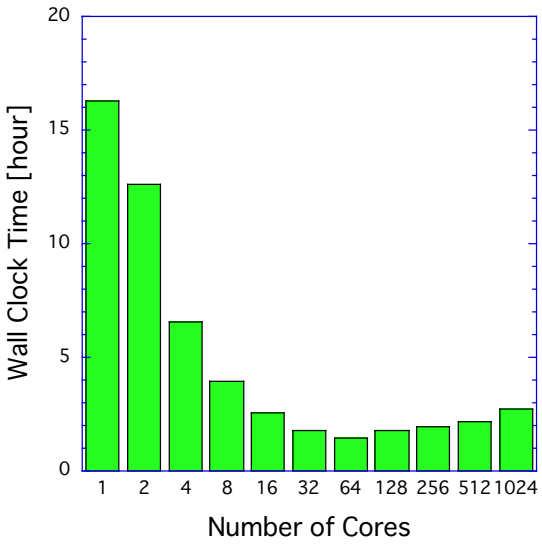

Fig.6 Wall clock time versus number of cores for the multi-helicity version of Gpic-MHD. Domain decomposition technique is used together with the copies of the field quantities. The jobs are for one million particles/core, $129 \times 128 \times 128$ spatial meshes and 2000 time steps.

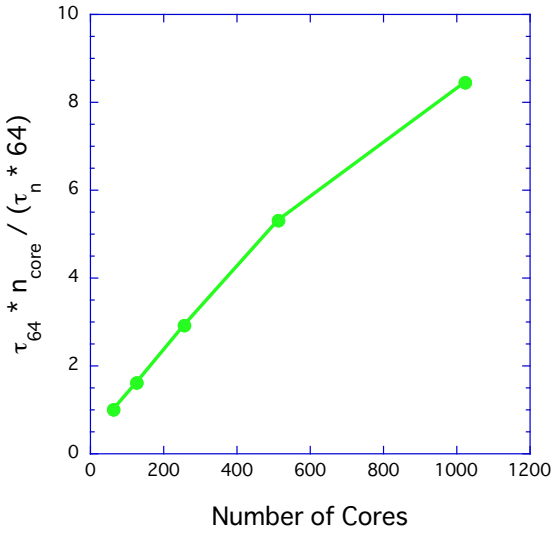

Fig.7 Speed-up factor versus number of cores for the multi-helicity versiotn of Gpic-MHD.

The parallelization performance of the multi-helicity (three-dimensional) version on Altix3700Bx2 is depicted in Fig.6. The computing time for the field quantities largely increases compared with the two-dimensional code. The domain decomposition is done in the z-direction. When the number of domain decomposition is increased, the calculation of the field quantities reduces because its load is distributed over cores; hence, the computing time decreases. In Gpic-MHD, the maximal number of domain decomposition is a half of the number of meshes in the z-direction. When the number of cores becomes larger than maximal number of decomposition, we use copies. The speed-up factor is depicted in Fig.7 for $n_{\mathrm{core}} > 64$, which shows weak scaling. No saturation is observed as the number of cores increases up to 1024.

5. Discussion and Conclusions

Gpic-MHD is a gyrokinetic PIC code for global MHD simulation, which utilizes rather conventional techniques. In order to simulate with more realistic parameters, advanced algorithms such as split-weight-scheme [9,10], the total characteristic method [11] or some new algorithm must be incorporated. Present version of Gpic-MHD code is intended to be the basis to test the various advanced scheme. The parallelization of Gpic-MHD code is done both for single- and multi-helicity versions. The single-helicity version is parallelized only by using copies for the field quantities, while the multi-helicity version is parallelized by using both one-dimensional domain decomposition and copies; when the number of cores is larger than the number of domain decomposition, copies of field quantities are used. The performance of Gpic-MHD code on Altix 3700Bx2 of JAEA is studied. When the number of cores is increased up to 1024 no saturation of the speed-up factor is observed in spite of the degradation of the scaling for the large number of cores. For the productive run in the future, the test of the code over more than 10000 cores will be done. For this purpose the domain decomposition also in the additional direction is inevitable and will be done in the near future.

6. Acknowledgement

This work is partly supported by the Grant-in-Aid for Scientific Research of Ministry of Education, Culture, Sports, Science and Technology of Japan and by the collaboration programme of JAEA. The authors are grateful to Mr. Y. Tauchi of Yamaguchi University for the computational support.

7. References

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