Research on Structure Formation of Plasmas Dominated by Multiple Hierarchical Dynamics

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The present subject is to investigate the phenomena where the prominent structure formation dominated by hierarchical plasma dynamics plays an essential role. Specifically, we concentrate our attention on micro-scale turbulent driven structure formation, and macro-scale magneto-hydrodynamic (MHD) events in high temperature magnetically confined fusion plasmas, and also on that realized in natural or laser-produced plasmas. In order to tackle the subject, we transfer four key simulation codes to the Earth Simulator (ES). There are two tokamak turbulent transport codes based on the gyro-kinetic model, i.e. GT3D (toroidal Particle-In Cell (PIC) code) and G3DME (high resolution Fourier particle code), a nonlinear MHD code based on the finite beta single fluid model, i.e. JMH3D (3-dimensional finite difference code), and a particle code including various atomic and relaxation processes, EM3DEB (fully relativistic electromagnetic Particle-In Cell code).

By performing architectural modifications of the codes and appropriate tuning for the ES, we obtain vectorization efficiency and sustained performances of, 99.75% and 26% (64 node) for GT3D, 54% and 99.67% (512 node) for G3DME, 99.64% and 50% (8 node) for JMH3D, 97.7% and 12% (10 nodes) for EM3DEB, respectively. The Fourier-based particle code and fluid code exhibit high sustained performance with high parallelization scalability, so that it is ready for large scale physical simulations on the ES. However, the PIC based code reveals the essential problem in the recursive reference of a list vector that is inevitably used in the assignment of particle information on the grid.

Keywords: Earth Simulator (ES), multiple hierarchical phenomena, complex plasma, magnetic confinement fusion plasma, laser-produced plasma, gyro-kinetic model, Particle-In Cell (PIC) model, particle collision, relaxation, turbulent transport, magneto-hydrodynamic (MHD) code, lightening phenomena, discharge.

1. Introduction

Various phenomena associated with structure formation in high temperature magnetically confined fusion plasmas, space and astrophysical plasmas, and also industrial and laser-produced plasmas, are realized through the complicated nonlinear interaction among different scale fluctuations. One typical example in fusion plasma is the so-called "Internal transport barrier (ITB)", where a prominent thermal inhibition is revealed in a local thin layer inside the tokamak plasma column. The strong impact of the ITB's on fusion science is attributed to the idea that the feature of an efficient thermonuclear burning plasma should be sustained by such a prominent structure formation. Those phenomena are dominated by fluctuation dynamics with different time and spatial scales and are categorized as the characteristics of "Multiple-hierarchical Complex Plasma (MHCP)". Understanding these phenomena is crucial not only for academic purposes, but also for fusion energy strategy. In order to resolve the underlying physical mechanisms, an advanced numerical experiment that reproduces the phenomena in high accuracy has been highly desired.

Based on the above idea, we perform large scale simulations of the MHCP using the Earth Simulator (ES), concentrating our attention on micro-scale turbulent transport dynamics and macro-scale magneto-hydrodynamic (MHD) events in high temperature magnetically confined fusion plasmas, and also on the structure formation realized in natural and/or laser-driven plasmas where the complicated atomic and relaxation processes play an important role. We transfer four codes to the ES, which have been developed at JAERI and NIFS. These involve two tokamak turbulent transport codes based on the gyro-kinetic particle model, GT3D and G3DME, a tokamak nonlinear MHD code based on the fluid model, JMH3D, and a full particle code for the investigation of natural and/or laser-produced plasma, EM3DEB. We perform architectural modifications and proper tuning, so that we can achieve large scale simulations which extract the high potential of the ES. In the following section, we describe the numerical characteristics of each code and the guideline for the vectorization and parallelization, and the result of the performance tests on the ES.

2. Characteristics of the code, and vectroization and parallelization on ES

Here, we describe the characteristics and remarks for the vectorization and parallelization procedures of our code, GT3D (sec.2.1), G3DMT (sec. 2.2), JMH3D (sec.2.3) and EM3DEB (sec.2.4), respectively.

2.1. Gyro-kinetic PIC code for tokamak global turbulent simulation: GT3D

GT3D is a global gyrokinetic toroidal particle code, which was developed for studying tokamak anomalous turbulent transport arising from pressure driven micro-instabilities such as the toroidal ion temperature gradient driven (ITG) mode. The code was implemented basically using a finite element PIC method with an optimized particle loading technique and the quasi-ballooning mode expansion. In order to simulate the radial electric field or zonal flows in a toroidal plasma correctly, a newly developed δf method based on a Canonical Maxwellian equilibrium distribution was used [1].

As for the parallelization, a particle division method was used for the particle solver, and a toroidal mode number division method was used for the finite element field solver. Since the code was originally developed for massively parallel scalar machines (the JAERI Origin3800 system / 768PE) using a full-flat MPI communication, the parallelization efficiency is enough to use 512 nodes on the ES. As for the vectorization, we have tuned the list vector recursive processing, which is used for a particle assignment on a finite element mesh, by means of a standard scheme using work arrays. However, the processing efficiency of this part was limited by that of the scalar processing of work arrays, and it was ~15%. Since this part occupies ~40% of the computational cost, the total processing efficiency was ~26% by using 64 nodes. According to the benchmark results in Table.1, the parallelization efficiency of GT3D is 99.976%, and the corresponding available node number (the rule of the ES), which is defined as the node number where a communication cost exceed 50%, is 520. Although the parallelization efficiency may be improved by implementing a shared memory inter PE parallelization such as microtask and OpenMP, the present performance is enough to perform the target problems, which are considered based on simulation results on the JAERI Origin3800 system. In the next FY, we will try the target problems.

2.2. Gyro-kinetic Fourier particle code for micro-scale tokamak turbulent simulation: G3DME

G3DME is a semi-local gyrokinetic slab particle code, which was developed for studying multiple hierarchical scale plasma turbulence where the ITG turbulence and the short wavelength electron temperature gradient driven (ETG) turbulence coexist and interact with each other [2]. In order to treat the orbit effects, in particular, the full finite Larmor radius (FLR) effct on short wavelength modes, a field solver was developed using Fourier representation in all directions, and particles are assigned to each Fourier mode. Since this scheme do not include the list vector recursive processing, the code is appropriate for vector processors.

The code was originally developed for vector parallel machines (the JAERI VPP5000 system / 64PE), and, therefore, the processing efficiency is very high ~54%. However, as for the parallelization, the original scheme with a full-flat MPI communication, which was designed for ~64PEs, is not enough to use 512 nodes (4096 PEs) on the ES. Thus, we have developed a new parallelization scheme, which consists of the inter PE shared memory microtask and the inter node MPI communication. As a result, a linear scalability up to 512 nodes was achieved, and the code tuning on the ES has been completed. According to the benchmark results in Table.1, the parallelization efficiency of G3DME is 99.998%, and the corresponding available node number is 781. In the next step, we

Table 1 Measured Performances for GT3D (339M particles, 162 × 64 mesh, 128 modes)

nodes	Time	parallelization (%)	vectorization (%)	GFLOPS	peak ratio (%)
32	3465.944		99.796	556.693	27.182
64	1834.814	99.976	99.757	1070.965	26.147

Table 2 Measured Performances for GT3D (33M particles, 256 × 1024 modes)

nodes	time	parallelization (%)	vectorization (%)	GFLOPS	peak ratio (%)
128	3531.548		99.675	4488.293	54.789
256	1802.737	99.998	99.673	8841.236	53.963
512	901.192	99.999	99.672	17649.307	53.861

will perform preparative simulations which are needed to determine the numerical resolution of the target problem.

2.3. Tokamak nonlinear MHD code based on fluid model : JMH3D

JMH3D is a MHD code based on a finite beta fluid model which is used to study nonlinear dynamical behavior of macro-scale electromagnetic fluctuations in a tokamak, such as the internal kink event, ballooning mode and relaxation event [3,4]. Basic equations are numerically solved in cylindrical coordinates with a second-order explicit finite difference scheme and a fourth-order Runge-Kutta-Gill time advancing scheme.

JMH3D deals with the dynamics in a three-dimensional Eulerian coordinate system. Therefore, it is easily parallelized using a flat MPI communication by the domain decomposition method which is adopted to the rectangular poloidal cross section. By carefully tuning the code, we successfully achieved a vectorization efficiency around 99.7%. We performed evaluation tests of the code, applying it to a tokamak disruption problem in consequence of the nonlinear evolution of the balloning mode. Here, we employed the large mesh number of $502 \times 66 \times 502$, where the 3rd dimension on the poloidal cross section is parallelized. We achieved parallelization efficiency of 99.873% with 8 nodes, so that the simulation employing 98 nodes (6.3Tflops) is now available according to the rule of the ES system. The sustained performance reaches 259.4 GFLOPS, i.e. 51% of the peak performance, resulting from a high vectorization ratio. From the above result, we may conclude that a large-scale simulation having more mesh number is now possible. In order to increase the number of nodes for a given mesh number, a 2-dimensional domain decomposition on the poloidal cross section may be necessary.

2.4. Relativistic particle code for the investigation of natural and laser-produced plasma: EM3DEB

EM3DEB is a fully relativistic electromagnetic 3-dimensional (3D) PIC code, which was developed for studying complex natural and laser-produced plasmas where various ionization and relaxation processes play an important role [5]. A 3-dimensional mesh with slab geometry for describing the electromagnetic field and an explicit finite difference scheme are used. A Monte-Carlo based relativistic pairing method is employed for the particle collision. Furthermore, by introducing the internal electronic state in each atom with the atomic number Z and by utilizing the electron-ion pairs already constructed in the collision routine, we included the process of the electron impact ionization and tunneling field ionization.

The code is parallelized using a one-dimensional domain decomposition using a flat MPI communication. As a characteristic of the mesh based PIC code, a significant amount of the CPU time is required for the renewal of the particle index in each processing element (for example, about 52% of total CPU time). By carefully tuning the indexing method, we successfully reduced the CPU time down to 39% without deteriorating the vectorization efficiency. The Monte-Carlo based collision and ionization routines are also one of key factors that deteriorates the vectorization efficiency, so that the interval to call the Monte-Carlo routine has to be carefully optimized. We performed the performance evaluation of the code, applying it to a lightning simulation, where the number of electrons and also the ion charge state vary with time. A large mesh size of 256x1280x2 is chosen, where the 2nd-dimension is parallelized. The Monte-Carlo calculation was done every 5 time steps. We achieved the parallelization efficiency of 99.75%, so that the simulation employing 50 nodes (3.2TFlops) is available according to the rule of the ES. However, the sustained efficiency stayed at a low level around 13%, resulting from the vectorization efficiency around 97.8%. Further implementation of the indexing routine, where most of the CPU time is exhausted, is necessary. Furthermore, in order to remove the limitation arising from the mesh number for a large scale simulation, an extension to multi-dimensional domain decomposition is also desired.

Table 3 Measured Performances for JMH3D ($502 \times 66 \times 502$ mesh)

nodes	time	parallelization (%)	vectorization (%)	GFLOPS	peak ratio (%)
2	1458.558		99.702	68.649	53.632
4	745.419	99.859	99.680	134.494	52.537
8	386.452	99.873	99.642	259.353	50.655

Table 4 Measured Performances for EM3DEB (144M Particle, $256 \times 1280 \times 2$ mesh)

nodes	Time	parallelization (%)	vectorization (%)	GFLOPS	peak ratio (%)
5	1835.882		97.96	42.284	13.214
10	1002.736	99.746	97.76	76.728	11.989

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多階層ダイナミックスが支配するプラズマの構造形成に関する研究

利用責任者

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本研究課題は、多階層的プラズマのダイナミックスによって支配される構造形成現象を解明することを目的とする。特に、高温の磁場閉じ込め方式による核融合プラズマにおいて、ミクロスケールの乱流輸送やマクロスケールの電磁流体力学（MHD）的事象によって引き起こされる構造形成や、自然プラズマやレーザー生成プラズマによって創出される非定常プラズマの構造形成現象を対象とする。これら構造形成の典型例として、磁場閉じ込め核融合プラズマでは、プラズマ内部の狭い領域において熱輸送係数が急激に低減するITBと呼ばれる内部輸送障壁形成現象や、自然プラズマでは、大気圏や電離層において普遍的の観測される雷・放電現象等が挙げられる。これらの現象は、様々な時間・空間スケールの揺らぎ間の相互作用によってもたらされる多階層・複合系プラズマ（MHCP：Multiple-Hierarchical Complex Plasma）としての特性を強く有している。

ここでは、これらの現象の数値実験を行うことが可能なコードを地球シミュレータ（ES）に移植し、ESの最大性能を引き出すことを目標にベクトル化・並列化の作業を進展させた。これらは、ジャイロ運動論モデルに基づくトカマクプラズマを対象とした乱流輸送コード：GT3D [1]（トロイダル配位におけるPIC手法に基づくグローバル粒子コード）及びG3DME [2]（高精度フーリエ粒子手法に基づく準グローバル粒子コード）、同様にトカマクプラズマを対象とした圧縮性の一流体モデルに基づく非線形MHDコード：JMH3D[3]（トロイダル配位3次元有限差分コード）、および、自然プラズマ・レーザープラズマを対象とした様々な原子過程や緩和過程を考慮した粒子コード：EM3DEB [4]（相対論的電磁モデルに基づくPIC手法によるスラブ配位粒子コード）である。ES上において適切なチューニングを施すことにより、それぞれのコードに対して以下のベクトル化効率と実行性能、GT3Dにおいて99.75％と25％（64ノード）、G3DMEに対して99.67％と54％（512ノード）、JMH3Dに対して99.64％と50％（8ノード）、MH3DEBに対して97.7％と12％（10ノード）をそれぞれ達成することができた。

フーリエ粒子コード（G3DME）および流体コード（JMH3D）は高い並列化の線形性を失うことなく高い実行性能が達成され、ES上での大規模計算が可能となっている。一方、PIC手法をベースにした粒子コードでは、粒子情報を空間グリッド上に割り当てる際に必要なリストベクトルの回帰参照に本質的問題があることから、コードのアーキテクチャーを含めた更なるチューニングが必要である。

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キーワード：多階層・複合系プラズマ、磁場閉じ込め核融合プラズマ、レーザー生成プラズマ、ジャイロ運動論モデル、Particle-In Cell（PIC）モデル、粒子衝突、乱流輸送、MHDコード