Numerical Simulation of Mantle Convection and Material Properties of the Earth's Interior

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We have developed simulation codes to study dynamics and material properties of the Earth's mantle. We choose 3 codes for the mantle convection simulation to study prediction of the plate motion and flow structure of the mantle interior and 1 code for molecular dynamics calculation to examine diffusion process governing mantle rheology. Tuning codes for Earth Simulator has been performed. The first scientific result is that MD simulation of diffusion unable to be achieved by previous supercomputers is performed on Earth Simulator. The subgroup of the mantle convection study is starting to apply the developed code to basic 3-D convection computation and prediction of the plate motion.

Keywords: mantle convection, plate motion, rheology, stabilized finite element method, finite volume method, molecular dynamics

Introduction

Mantle convection is a principal driving mechanism of geological and geophysical phenomena we observe on the Earth. Many researchers of the mantle dynamics concentrate their effort on developing physical models using numerical simulation as a powerful tool to understand the dynamics of mantle convection. High performance computers bring us ability to construct models with realistic complex physical properties of mantle, which can be directly compared with observations such as seismic tomography. Earth Simulator can greatly improve resolution of the calculation so that we expect that 3-D mantle convection model with high resolu-

tion necessary to solve plate-mantle convection system is a realistic target.

On the other hand, high performance computing also enables us to perform numerical experiments to study physical properties of the Earth's interior under high pressure, which is difficult to be realized by the laboratory experiment. Especially, rheology of the mantle is quantitatively unclear although it significantly affects style of the mantle convection. MD simulation of diffusion process which determines pressure- and temperature-dependence of the viscosity is enabled by Earth Simulator.

We here carry out study on the dynamics and the rheology of the mantle because these issues have complementary relationship for better understanding the Earth's evolution. Our group consists two subdivision to study them. We here describe results by two subgroups in Section I and II.

I. Development of Mantle Convection Simulation Codes

1. Programs

To understand complex physical processes in the mantle, we have developed 3 codes:

(1) A stabilized finite element method for the convection in a 3-D spherical shell and a Cartesian box (by A. Suzuki). The unstructured mesh is employed in order to realize uniform resolution in the spherical shell and adaptive refinement according to the flow structure. An IC-CG method is employed as a linear solver for the momentum equation and an ILU-GCR method for the energy equation.

(2) A finite volume method with primitive variables for the convection in a spherical shell (by Y. Iwase and S. Honda). To couple velocities and pressure, SIMPLE scheme is used. A Jacobi-type linear iterative method is adopted to solve linear equations

(3) A finite volume method for the convection in a Cartesian box (by M. Kameyama) using SIMPLER scheme. SSOR-CG and localized ILU(0)-CG methods are employed to solve linear equations.

Codes (1) and (2) had been already developed on SMP-type computer and vector-type computer. A code (3) is newly developed in this project.

2. Status of tuning and achieved performances

We have performed tuning codes for ES. The status of the codes is described as follows.

(1) Vectorization has been finished. Because random access to the memory is required due to the unstructured mesh, conventional vectorization techniques are not efficient. A domain decomposition exploiting symmetry of the spherical shell is used for vectorization. A. Suzuki obtained 726 MFLOPS on a single processor. So called hybrid-type parallelization with OpenMP and MPI is now progressing.

(2) Vectorization and flat MPI parallelization have been implemented. Domain decomposition for the parallelization with the distributed nodes is adapted to r-direction. S. Honda and Y. Iwase obtained 2 GFLOPS on a single processor and 172 GFLOPS with 10 nodes (80 processors).

(3) This code is developed as a vectorized and parallelized program. For this code, we have developed and two linear solvers: SSOR-CG and checked its performance. Vectorization is adapted to do-loop for x-direction axis, inner node parallelization is for y-direction, and domain decomposition is for z-direction to parallelize with multi-node processors. M. Kameyama obtained 3.3 GFLOPS on a single processor and 76 GFLOPS with 8 nodes (64 processors). He is now changing the solver into localized ILU(0)-CG method and checking its performance.

3. Scientific results

S. Honda and M. Kido applied their code to 3-D spherical plate-mantle convection model to predict present-day plate motion and to infer internal flow structure in the mantle. Computation was performed with $100 \times 400 \times 800$ (r, θ, φ) meshes.

4. Future plan

In the next year, we will continue tuning of our code for ES. We plan to perform benchmark test between our different codes, to check stability for variable viscosity convection, and to run systematic numerical modeling to reveal basic properties of 3-D mantle convection. In the future, our code will be applied for the following geodynamical problems.

(1) Effect of the continental lithosphere on the self-consistent generation of plate boundary in 3-D plate-mantle convection system and the structure of the mantle.

(2) Geochemical evolution of the mantle.

(3) Backward tracing of plate motion and internal convective flow back to 200 to 600 m. y. ago.

II. Molecular dynamic simulation of self-diffusion in MgO in the lower mantle conditions

1. Code implementation for ES

"SUPER-MXDTRICL", a MD simulation program based on a "MXDTRICL" code by Kawamura (1996) is developed for ES. This code is vectorized, intra-node and inter-node parallelized by a cell-divide method. Obtained performance is as follows:

(1) Vectorization ratio: 99.2 %

(2) Efficiency of parallelization: 99.90 to 99.97 %

The efficiency of the parallelization is not deteriorated up to 128 nodes. When we use 512 nodes, it takes 1.8 seconds to calculate one time step with 10^6 particles. Earth Simulator permits MD simulation containing 10^6 particles with proper computation time.

2. Scientific results

In order to understand the deep mantle dynamics, we need rheological characteristics of lower mantle materials in the very high pressure and temperature conditions. The lower mantle materials are considered to be mainly composed of $MgSiO_3$ perovskite and MgO periclase containing a few amounts of iron, aluminum and calcium. The physical conditions ranging from 23 GPa to 140 GPa in the lower mantle are extremely high pressures in conducting rheological experiments. Therefore, we have to deduce theoretical flow of them in such extremely high pressure conditions by means of molecular dynamics method which is very improved to infer the physical characteristics of silicate minerals. Simulation experiments of self-diffusion of periclase and perovskite, however, require the vast amounts of calculations because of very large atom numbers within the basic cell of MD method. Here we have to make new software of MD having table-making subroutine of atomistic positions during main routine to avoid the n-square calculation.

We succeeded in coding and tuning the table-making super MXD programs for earth simulator of the center, in simulating the oxygen and silicon diffusivities in MgO extending 150 GPa and 6000 K. The step sizes reaching 10^7 are large enough to obtain the accurate diffusivities. Furthermore, we could conduct the 10^6 atoms in the basic cell to obtain the diffusion process similar to the natural vacancy density. This is really needed for molecular dynamics rheology construction in the earth sciences.

The results by MD simulations of oxygen diffusivities in the lower mantle conditions show that the activation energies of migration, formation and total are 202-215, 386 and 586-599 kJ/mol, respectively. Pressure effects of these diffusivities are exactly estimated. From these simulation experiments of MgO, we concluded that the Newtonian viscosity of the lower mantle changes from 10^{21} to 10^{22} Pa s to the 1500km but decreases to 10^{20} Pa s at the 2900km at the bottom of the lower mantle.

マントル対流と地球内部物性の数値シミュレーション

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マントルのダイナミクスおよび物性を明らかにするため必要なプログラムの開発、評価、およびそのプログラムを用いた数値シミュレーションを行った。我々のグループでは、マントル対流と地球内部物性の2つのグループに分かれて研究を行った。主な結果は、以下の通りである。

(1)3次元箱モデルマントル対流計算コードを開発し、地球シミュレータ用にポアソン型方程式ソルバーのコードを開発した。(2)3次元球殻対流安定化FEMコードのベクトルチューニングを行った。(3)3次元球殻対流FVMコードのチューニングを行い、10ノードで172 GFLOPSのパフォーマンスを得た。そのコードを利用して、プレート運動の予測の高分解能計算を行った。(4)MDコードを地球シミュレータ向けにチューニングし、初めて拡散の計算を行うことが可能になった。その結果を用いてマントル深部の粘性率を推定した。

キーワード：マントル対流、プレート運動、レオロジー、安定化有限要素法、有限体積法、分子動力学法