Development of Advanced Simulation Methods for Solid Earth Simulations

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We performed high resolution simulations of geodynamo. The simulation code, that is based on our Yin-Yang grid method, is highly optimized and the production runs were performed with 512 nodes of the Earth Simulator. Another numerical algorithm that was originally invented by our group is ACuTE method for the mantle convection simulation. In this fiscal year, we developed a new spherical mantle convection code from scratch based on the ACuTE method implemented on the Yin-Yang grid. We also developed a new numerical method to solve the time development of visco-elastic fluid motion. The focus of this method is on the numerical accuracy and efficiency for the advection of rheological properties. A new approach to the earthquake cycle simulation was also explored.

Keywords: geodynamo, mantle convection, ACuTE method, Yin-Yang grid, visco-elastic fluid

1. High Resolution Geodynamo Simulation by Yin-Yang Grid

The Yin-Yang grid [*Kageyama and Sato*, 2004] is a kind of overset grid system applied to the spherical geometry through identical spherical dissection [*Kageyama*, 2005b]. As we reported in our previous Annual Reports [*Kageyama et al.*, 2004b, *Kageyama et al.*, 2005, *Kageyama et al.*, 2006a], the Yin-Yang grid is applied to geodynamo simulation [*Kageyama et al.*, 2004c, *Kageyama and Yoshida*, 2005, *Kageyama*, 2005a] and mantle convection simulation [*Yoshida and Kageyama*, 2004, *Yoshida and Kageyama*, 2006].

In this Fiscal Year, we performed large scale geodynamo simulations using the Yin-Yang geodynamo code. Fig. 1 shows a snapshot of high resolution simulation on 512 nodes of the Earth Simulator. The Rayleigh number in this calculation is $Ra = 2 \times 10^8$. The details of the code, especially on the optimization for the vector/parallel processing can be found in [*Kageyama et al.*, 2004c]. What is shown in Fig. 1 is two cross sections of vorticity distribution on the equatorial and meridian planes. The red and blue area in these planes are for positive and negative vorticity, respectively, or more strictly, the vorticity component parallel to the rotation axis. The stripe structure parallel to the rotation axis appears in the meridian plane as a consequence of Taylor-Praudman's theorem. As the straight structure of the stripes suggests, the flow of the core convection is strongly constrained by the rotation of the system; the Ekman number is in this calculation is $E = 2.3 \times 10^{-7}$. The grid size of the simulation is $N_r \times N_\theta \times N_\phi \times 2 = 511 \times 514 \times 1538 \times 2$, where N_r, N_θ, N_ϕ are grid size in radial, latitudinal, and longitudinal directions. The last factor × 2 is for *Yin* and *Yang*.

Magnetic field generation by the magnetohydrodynamic (MHD) dynamo action is already saturated by the time when the snapshot of Fig. 1 is taken. The total magnetic energy integrated over the spherical shell region, or the outer core,

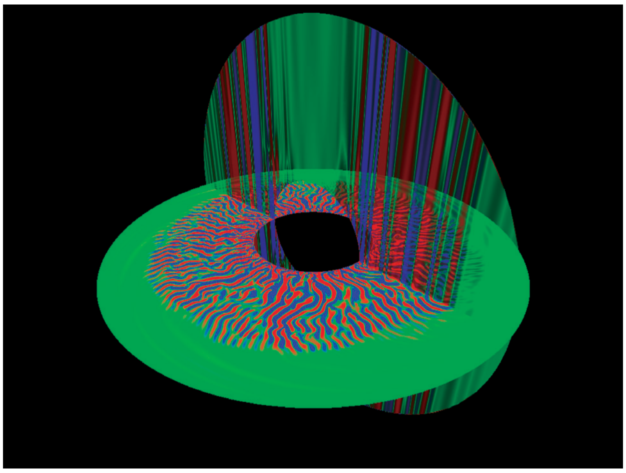

Fig. 1 A high resolution geodynamo simulation using Yin-Yang grid. Rayleigh number $Ra = 2 \times 10^8$ and Ekman number $E = 2.3 \times 10^{-7}$. The color distribution of blue-green-red shows the vorticity component parallel to the rotation axis. Cross sections in the equatorial plane and a meridian plane. The convection consists of many plume-like sheets.

is about ten times larger than the convection flow energy.

An interesting feature of the vorticity distribution in Fig. 1 is multiple sheet-like structure elongated in the perpendicular direction to the rotation axis: See the the equatorial plane. Since the velocity field (and therefore the vorticity field, too) is nearly two-dimensional due to the strong constraint of the rotation. The strong magnetic field is generated by these "plume sheets".

In order to analyze the generation mechanism of the magnetic field by these "plume sheets", we examined the distribution of $D \equiv -\mathbf{v} \cdot (\mathbf{j} \times \mathbf{B})$ in the spherical shell, where $\mathbf{v}$, $\mathbf{j}$, $\mathbf{B}$ are the flow velocity, electric current density, and magnetic field, respectively. The quantity D is the work rate done by the flow against the $\mathbf{j} \times \mathbf{B}$ force. In other words, D is positive where the flow energy is converted into the magnetic energy. By analyzing D distribution of the data at the same snapshot as Fig. 1, we found that strong positive D appears in the middle latitude both in the northern and southern hemispheres. Their distribution is approximately symmetric about the equatorial plane. The green regions in Fig. 2 correspond to the northern distribution of the strong positive D. The yellow-to-red color in the equatorial plane in Fig. 2 indicates the temperature distribution in the equatorial plane. The plume-sheet structure is also apparent in this visualization.

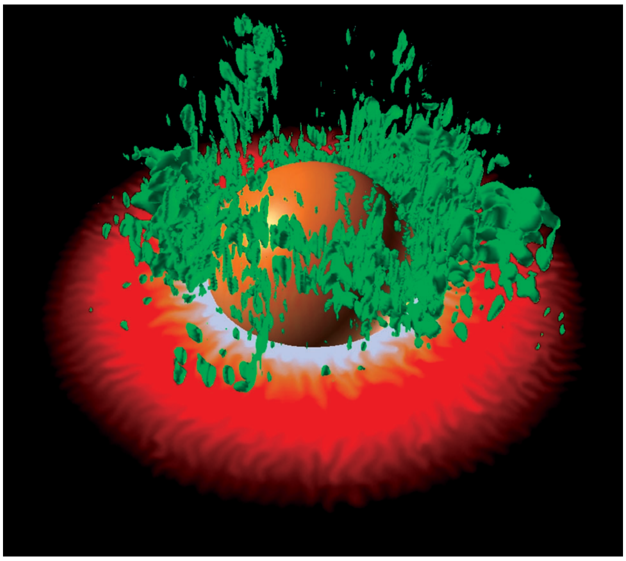

Fig. 2 The same data as Fig. 1. The yellow-to-red color shows the temperature distribution in the equatorial plane. The green regions stand for regions where magnetic field is generated by the energy conversion from convection kinetic energy into the magnetic energy. This dynamo distribution denoted by the green regions are symmetric about the equator.

2. Integration of ACuTE Method into Yin-Yang Grid: New and Advanced Simulation Code of Mantle Convection in Spherical Shell Geometry

One of the major difficulties in numerical simulations of mantle convection lies in the solution procedures of flow fields. Owing to the extreme rheological properties of mantle materials, one needs to solve ill-conditioned elliptic differential equations for velocity and pressure at every timestep. In order to promote the large-scale numerical studies on mantle convection, we had proposed a new algorithm, hereafter called "ACuTE", for solving the flow field of mantle convection problems [*Kameyama et al.*, 2005]. This algorithm iteratively solves the equations for conservation of mass and momentum for highly viscous and incompressible fluids, together with the multigrid method which is known to be optimal for solving boundary value problems. The parallel efficiency of multigrid calculation is enhanced by an agglomeration technique, where the computational meshes are "agglomerated" to new "process units" and redistributed to a subset of active processor elements (PEs) [*Kameyama*, 2005]. This optimization had successfully resulted in sufficient vector and parallel efficiency of multigrid calculations using up to 64 processor nodes (i.e. 512 PEs) of the Earth Simulator [*Kameyama*, 2005]. These techniques had been further incorporated in our simulation code named "ACuTEMan" for mantle convection problems in three-dimensional Cartesian geometry. The ACuTEMan had demonstrated the applicability of our algorithm to actual geodynamical problems, such as the influence of solid-state phase transitions on mantle dynamics [*Kameyama and Yuen*, 2006,*Kameyama*, 2007].

On the other hand, our invention of the Yin-Yang grid in FY2003 was immediately followed by an application to the simulation program of mantle convection problems [*Yoshida and Kageyama*, 2004]. This simulation code, developed separately from ACuTEMan, had been used to study the fundamental nature of mantle convection in spherical shell geometry [*Yoshida and Kageyama*, 2006]. Unfortunately, however, the simulation code has been suffering from the difficulty in conducting truly large-scale simulations on massively parallel environments. This is mainly because the solution algorithm for the flow field of mantle convection is unfit in essence for large-scale simulations: The SIMPLER method is used together with the classical SOR technique for solving the linear simultaneous equation for each unknown (velocity components and pressure). It is therefore very important to apply efficient solvers for the flow field of mantle convection in order to conduct large-scale simulations of mantle convection in spherical shell geometry on the Earth Simulator.

In this FY we developed a new simulation code of mantle convection in a spherical shell geometry which is suitable for large-scale numerical simulations. The new code came out from an integration of the ACuTE method [*Kameyama et al.*, 2005, *Kameyama*, 2005] into the Yin-Yang grid. The convergence of the ACuTE iterations is accelerated by a multigrid method. We adopt the full approximation storage

(FAS) algorithm and the standard V-cycle of the multigrid method. The benefit of the V-cycle is that it visits coarser grids at fewer times than other complicated multigrid cycles (such as W-, F-cycles) do. The internal boundary condition of each component grid (Yin and Yang) is set by mutual bilinear interpolations in a horizontal plane at each ACuTE iteration at every grid level. In particular, the interpolations at coarser grid levels are important for a sufficiently fast convergence, since the errors with the largest wavelength, whose convergence is typically the slowest, can not be well represented without connecting the suite of coarser component grids. As had been done in ACuTEMan, the parallel efficiency of multigrid calculations is enhanced by an agglomeration technique.

It is worthy to emphasize two key issues for the application of the ACuTE and the multigrid methods to spherical geometry by the Yin-Yang grid. First, the change in metric tensors is properly handled throughout the calculations in the curvilinear coordinate system. In particular, the fine-to-coarse transfer (restriction) operator is required to strictly fulfill the conservation of mass in the entire domain. Second, the ACuTE iteration should be adapted in order to eliminate the singular (or indeterminate) nature inherent in the Stokes problem of incompressible fluid. Since the pressure appears in terms of its spatial gradient, it is determined only up to a constant. In addition, the velocity field is determined only up to a rigid motion (translation and rotation), since it does not affect the strain rates at all. In order to obtain a unique solution for velocity and pressure, the ACuTE iteration must be performed together with the constraints on the flow field which remove the singularity in the problem. In the present code, we apply the constraints on the flow field such that (i) the global average of pressure is zero and (ii) the velocity field is free from a rigid motion. Our experience suggests that these constraints are particularly important in the calculations with an overset grid methodology, since such constraints help to remove the errors coming from the frequent interpolations between the component grids.

We show in Fig. 3 some examples of the convective flow patterns obtained by our new simulation code. Benchmark comparisons for the steady convection for low Rayleigh numbers (*Ra*) with previous calculations revealed that accurate results are successfully reproduced not only for isoviscous cases but also for the cases where the temperature-dependence of viscosity is included. The present numerical code will be further optimized and tested for large-scale simulations of mantle convection problems under more realistic conditions, such as introduction of high *Ra* and a strong variation of viscosity.

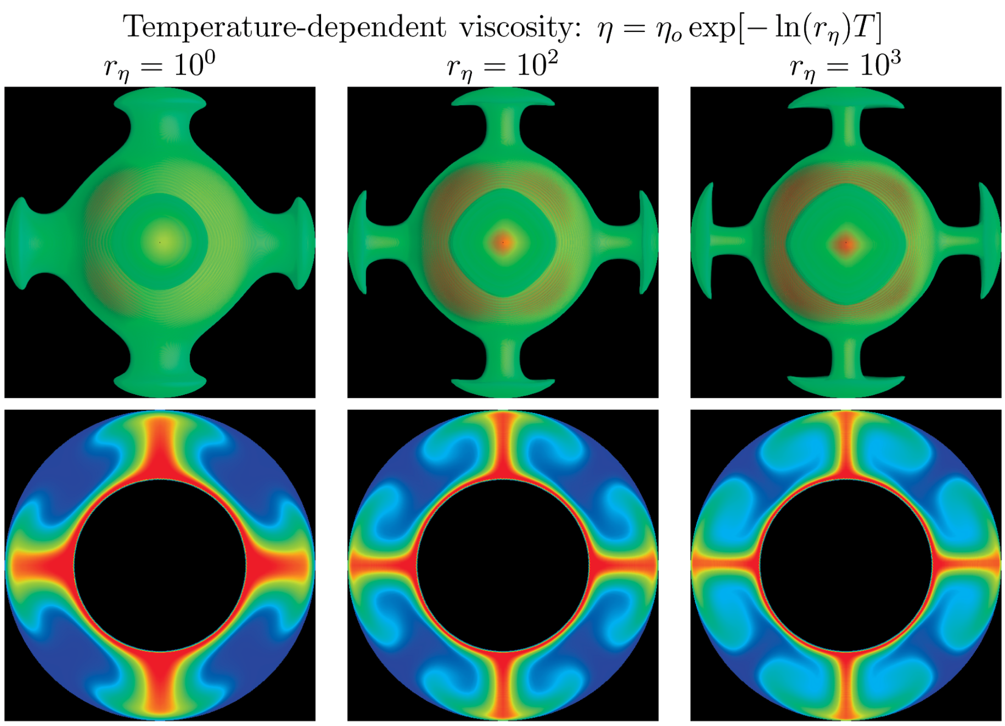

Fig. 3 Examples of the numerical results calculated using the newly-developed mantle convection code in combination with the ACuTE method and Yin-Yang grid. Shown are the snapshots of steady-state thermal convection with cubic symmetry of the fluid with temperature-dependent viscosity. The values viscosity contrast r_η are (left) 10^0, (middle) 10^2 and (right) 10^3, while the Rayleigh number defined with the viscosity η_o at the outer surface (where the non-dimensional temperature $T = 0$) is fixed to be 5×10^3. Shown in the top row are the volume-rendering images of the regions of $T > 0.4$, while in the bottom are the cross section of the temperature distribution in the meridian plane.

3. Development of Numerical Procedure for Visco-Elastic Fluid toward Plate-Mantle Simulation

It is well known that the tectonic plate shows strongly nonlinear behaviors in the mantle convection as the cool surface layer. For the purpose of simulating the realistic mantle convection including the plate tectonics, we have developed the method for solving the large deformation of a Maxwell visco-elastic material in the viscous fluid, in the Eulerian frame of reference.

In order to capture a sharp surface of material, we develop a numerical scheme based on the CIP-CSLR method. We suggest simple but effective flux correction scheme for an advection of slowly moving nonnegative profiles by the CIP-CSLR. Our correction scheme prevents an erroneous flow owing to an oscillation of a profile at sharp gradients around the zero, and guarantees a positiveness of cell integrated value. As for the Maxwell constitutive equation, we propose "Co-rotated Semi-Lagrangian method", in which not only the advection term but also the Jaumann-co-rotational term are solved separately by a time splitting method. In addition, we semi-analytically solve a residual time integration of the Maxwell viscoelasticity by an exponential time difference method. These techniques allow us to integrate the Maxwell constitutive equation without a numerical error of conventional discretization procedures, as long as a velocity does not change significantly over a time increment Δt.

We demonstrate an applicability of our method for large deformation problems of a viscoelastic fluid by a three-dimensional Rayleigh-Taylor instability test. A heavy (ρ_{upper} = 0.1) and rigid (η_{upper} = 1.0) material is initially confined in an upper half of a box and put a perturbation with small amplitude, as the colored region shown in Fig. 4 (a). A lower layer is filled with light (ρ_{lower} = 0) and soft (η_{lower} = 10^{-3}) viscous fluid (called "air"). Fig. 4 (b) and (c) show snapshots of a distribution of the viscoelastic fluid at t = 1000 and at t = 1500 respectively. The test calculation by our Semi-Lagrangian scheme successfully captures a sharp boundary of the material.

Fig. 5 shows an instability amplitude for the case where the fluid of upper layer has only a viscous character (i.e., Deborah number De = 0). We compare results calculated by three different numerical schemes for a viscosity advection; the RCIP, normal CIP-CSLR, and our CIP-CSLR. The advection with our flux correction method (red and green dots) is found to be very successful in spite of these simplicity.

On the other hand, Fig. 6 shows temporal evolutions of the amplitude with a viscoelastic property of upper layer. The solutions obtained by our method are in good agreement with the theoretical one in both cases of De = 0.05 and 2.5,

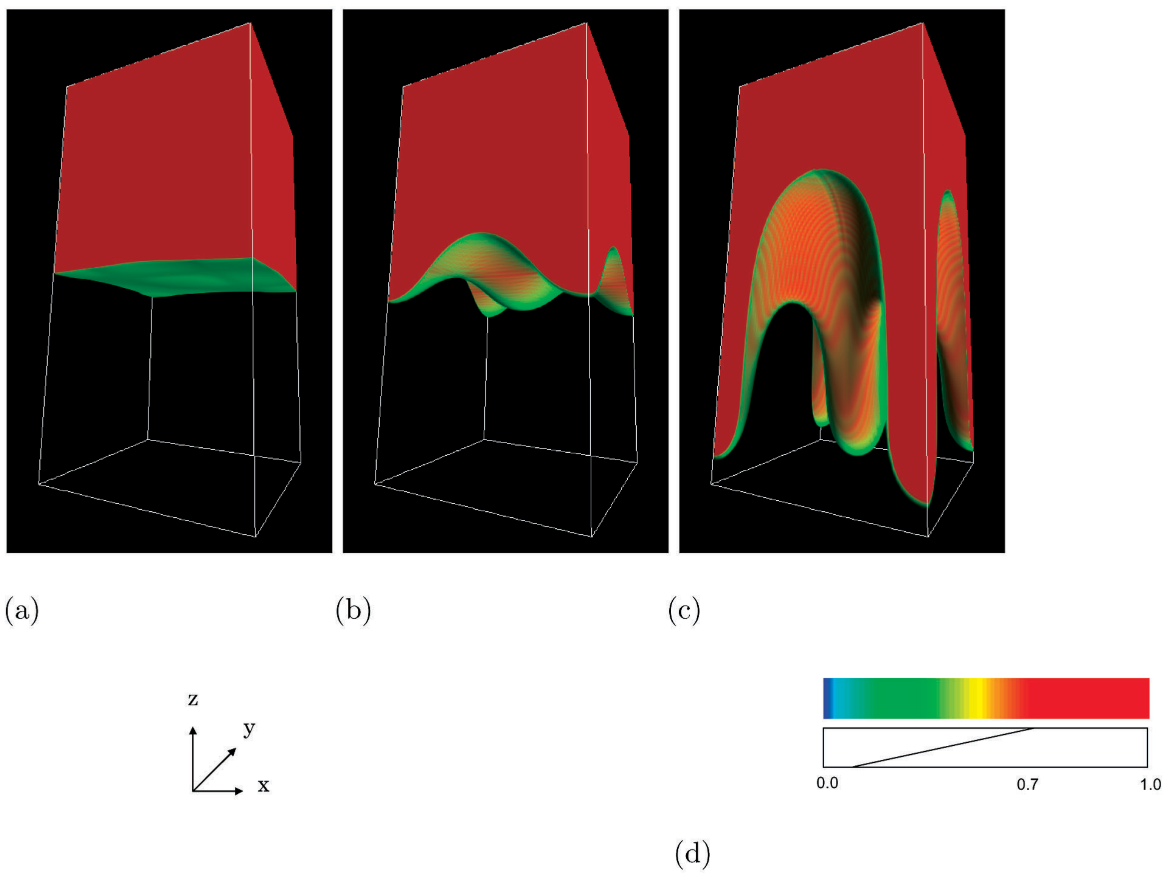

Fig. 4 Snapshots from Rayleigh-Taylor instability test in three-dimensional rectangular box of aspect ratio 0.5(x) × 0.5(y) × 1.0(z) and grid resolution of 64 × 64 × 128. Shown by volume rendering are the distributions of viscosity at time (a) t = 0, (b) t = 1000 and (c) t = 1500. Meaning of color and transparency are given in (d).

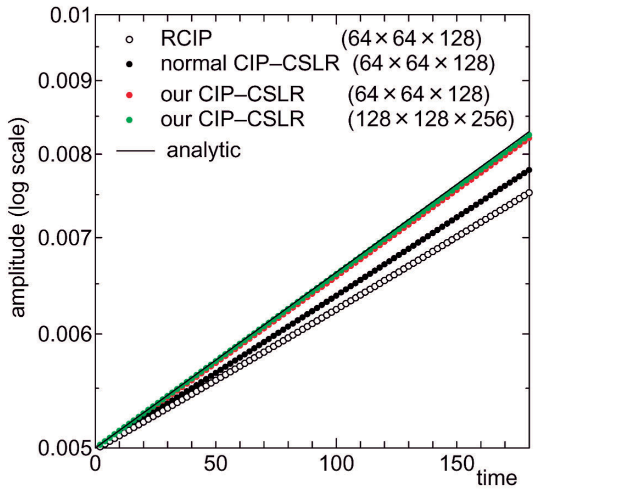

Fig. 5 Temporal evolutions of instability amplitude of three-dimensional Rayleigh-Taylor instability of viscous fluid calculated with different CIP schemes.

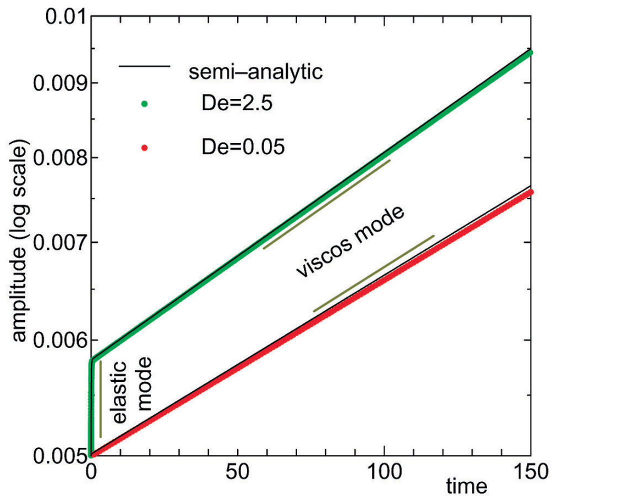

Fig. 6 Same as Fig. 5 but for viscoelastic fluid with Deborah number De = 0.05 and De = 2.5. Grid resolutions 64 × 64 × 128 are used.

indicating that our method including a stored stress tensor calculation reproduces viscoelastic properties very well.

Our results of three dimensional visco-elastic Rayleigh-Taylor instability test, which is sensitive to the advected mass profile, show not only the qualitative but also quantitative validity of our scheme.

4. Development of Earthquake Cycle Simulation Model

Simulation study of earthquake generation process is one of the most challenging problems in seismology. On the Earth Simulator, several groups have been conducting simulation studies of earthquake generations in and around the Japan Islands. In these studies, an earthquake is modeled as a frictional sliding between two elastic bodies. The goal of these simulations is to find physical conditions that reproduce the historical sequence of large earthquakes. Towards this goal, we should first know key parameters that control the qualitative pattern of earthquake generations in and around the Japan Islands. Previous studies show that small heterogeneities of frictional property on the plate interface determine the spatio-temporal patterns of large earthquakes. For the case of Nankai Trough, it has been shown by Hori et al. that the depth- (or temperature-)dependent frictional properties on the Philippine Sea plate interface and patch-like frictional heterogeneities off Kii peninsula and off Tokai region can successfully reproduce the occurrence pattern of large earthquakes that is similar to the historical one.

In addition to the frictional heterogeneities on the plate interface, another important factor that may control the earthquake generation is the the sub-surface heterogeneities of the elastic or visco-elastic property. However, the standard algorithms of the earthquake simulation are not designed to take the complex configuration of subsurface structures and, in particular, the nonlinearity of the material into account. Hence, in FY 2006, we began to develop a new numerical simulation model of earthquakes which is robust in the increased complexity of the configuration and the presense of the nonlinearity. In this model, we utilize a finite element library called GeoFEM which is developed for solid earth simulations. We have been using GeoFEM for earthquake cycle simulations for years [*Hyodo and Hirahara*, 2004]. Thanks to the flexibility of the grid design of the finite element method, we can easily handle complex fault geometry or heterogeneous distribution of subsurface structures. As a first step, we have developed a 2-dimensional code and performed preliminary simulations of quasi-static interplate earthquakes. We set up a model interplate fault with a rigid base and a 2-D elastic block placed on the base (Fig. 7). On the top surface of the elastic block, we apply a

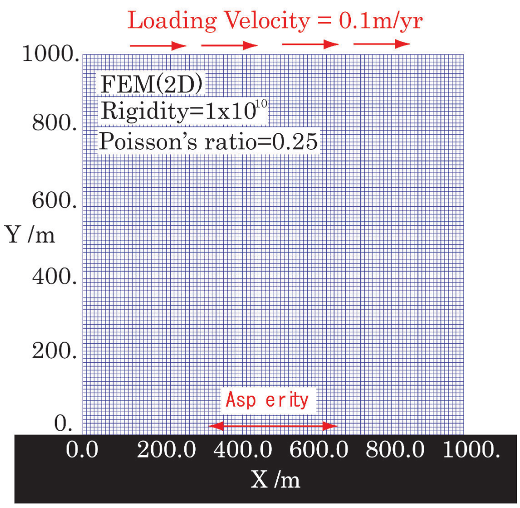

Fig. 7 A simplified two-dimensional model of interplate earthquake generation. Arrows at the top of the elastic block represent tectonic loading. On the asperity region of the bottom side of the elastic block, frictional stress given by a rate- and state-dependent friction law resists the movement of the upper block.

constant velocity as the tectonic loading. On the bottom surface of the elastic block, we assume an asperity region with prescribed friction law that depends on the slip velocity and the slip history (or state) of the surface. Assuming that the elastic block is in quasi-static state, we solve the force-balanced equation of the elastic block system at every time step. When the sliding speed on the interface exceeds a critical value, the effect of radiation damping is included to model the shear stress reduction by faulting. Figs. 8(a)–(d) are snapshots of velocity field during an earthquake cycle.

5. Other topics and publications

Along with major research topics described in the previous sections, we also study other themes published in the following papers and articles: [*Kageyama et al*., 2006b, *Kageyama and Hyodo*, 2006, *Tagawa et al*., 2007, *Yuen et al*., 2007, *Sakaguchi et al*., 2007].

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Technical supports from Dr. Nobuaki Ohno of Advanced Perception Research Group at Earth Simulator Center are

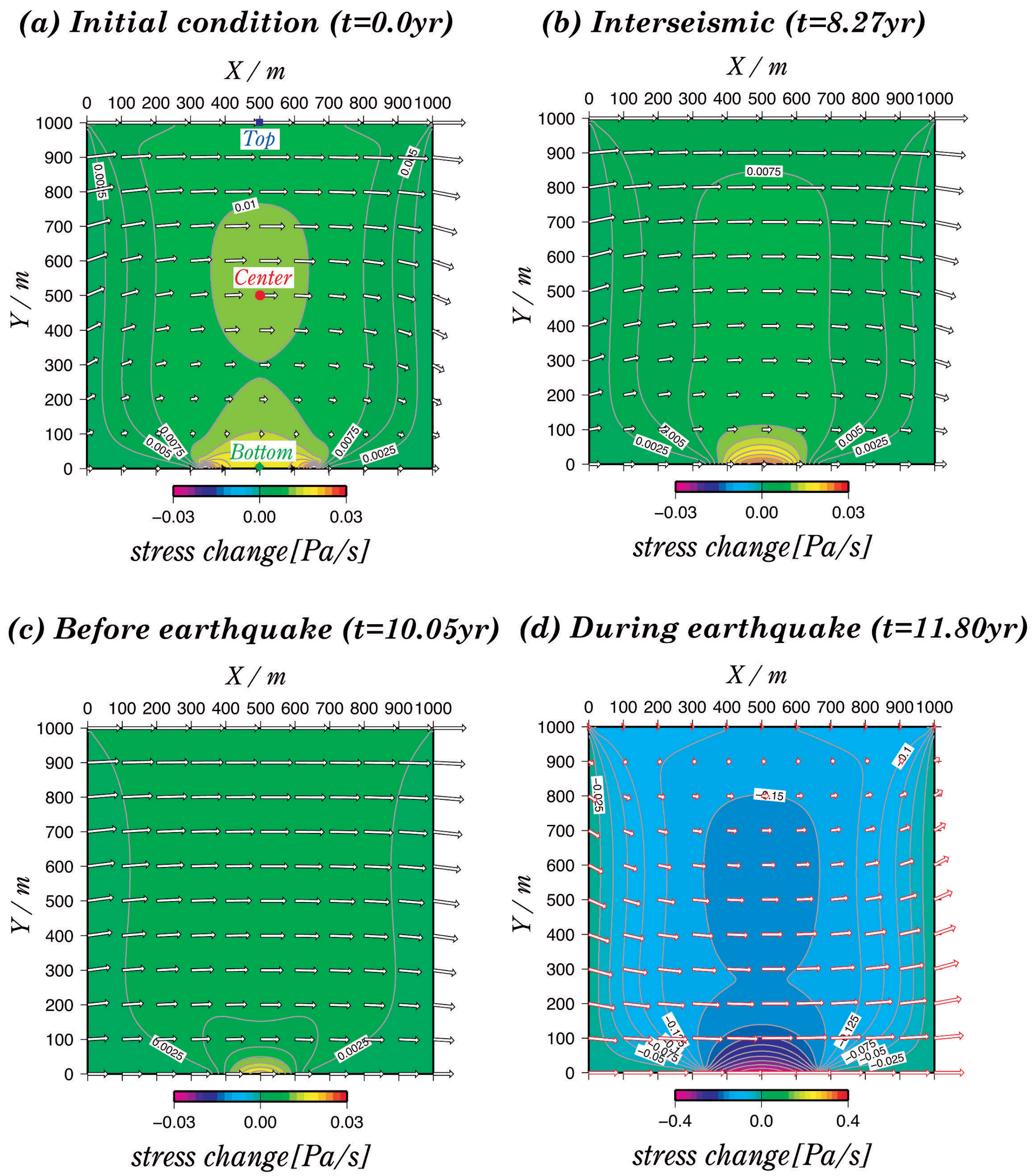

Fig. 8 Snapshots of velocity field at instances of (a) Initial condition of calculation, (b) Interseismic period, (c) Just before an earthquake, and (d) Intra-earthquake period. In all 4 figures, contours and arrays indicate shear stress rates and slip velocities, respectively.

greatly appreciated in the visualization of numerical results.

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先端的固体地球科学シミュレーションコードの開発

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我々の最終的な目標は、地球シミュレータ(ES)を駆使した大規模計算機シミュレーションを通じて、地球ダイナモとマントル対流をはじめとする地球内部全体の構造とダイナミクスを理解することである。そのために必要となる大規模並列計算手法や基本数値アルゴリズムの独自開発にも積極的に取り組んでいる。

地球ダイナモシミュレーション：インヤン格子を用いたダイナモコードは17年度までにほぼ完成した。18年度前半は、本格的なプロダクトランに必須となるデータ処理プログラムと可視化ツールの開発に注力した。そして後半、512ノード(4096プロセッサ)を中心とした大規模計算により、高いレイリー数Ra、低いエクマン数Eでの地球ダイナモシミュレーションを行った。低いエクマン数(=低い粘性率)のシミュレーションには高解像度が要求されるために実行が困難であったが、インヤン格子を用いた我々のダイナモコードは、その高い並列計算性能により、これまでだれも到達できなかったほど低いエクマン数領域におけるダイナモを計算することに成功した。

インヤン格子とACuTE法による3次元球殻マントル対流の高速シミュレーションプログラムの開発：我々はこれまで3次元球殻マントル対流シミュレーションコードとして、インヤン格子に基づいたプログラムを構築し、既に昨年度までにいくつかの成果を挙げてきた。しかしながら、このコードは大規模なモデルに適用すると計算速度が極端に遅くなるという課題があった。これはマントル対流の流れ場の求解に用いているアルゴリズムに起因する。この点を解決するために今年度我々は3次元球殻マントル対流シミュレーションコードを新たに作り直した。このコードでは流れ場の求解に我々が開発したACuTE法を採用している。そのため計算の大規模並列化が可能となった。このコードは、インヤン格子とACuTE法という我々が独自に開発した二つの計算手法の融合であるという点を強調しておきたい。

プレート・マントル統合計算を目指した粘弾性流体の新解法の開発：粘弾塑性流体として見たときにマントルとプレートは物性が大きく異なる。この二つを統一的に取り扱うシミュレーションを行なうための第一ステップとして、本年度は大きな粘性コントラストを持つ粘弾性流体の数値解法を新しく開発し、その手法の有効性を検証した。我々はまず新しい移流計算スキームを開発した。これはセミラグランジュ法の一種であるCIP-CSLRを改良したものである。プレートの複雑なレオロジーを解くためには、応力テンソルの移流も考慮する必要がある。我々は構成方程式としてマクスウェルモデルを採用し、応力テンソルの時間変化に関してはヤウマン共回転微分による形式を採用した。そして、応力テンソル場が物質と共に回転する効果を、セミラグランジュ的な手続きの中で移流項と共に取り扱う新しい手法(共回転セミラグランジュ法)を開発した。構成方程式の中で移流と回転以外の項、つまり応力の弾性的な蓄積や、粘性による緩和の効果は、いわゆる指数関数法で積分する。こうして今年度我々は、高精度でありながら時間ステップを大きくとることができる粘弾性流体の新しい数値解法を完成させた。そしてこの手法をACuTE法に組込み、3次元での粘弾性問題を高速に解く事を可能にした。我々の手法の有効性と精度を検証するため、3次元の粘弾性レイリーテイラー不安定性の計算を行い、粘弾性的な性質が再現されていることを実証した。また、粘性差のある流体に特徴的なliquid rope coilingと呼ばれる現象を再現することにも成功した。

地震サイクルシミュレーションの新手法開発：現在主流となっている地震サイクルシミュレーションの計算手法は計算の簡単化のために半無限遠まで広がる媒質や粘弾性分布一様性、線形性などを仮定した半解析的な手法である。そのため、媒質が不均質であったりあるいは非線形性を持つと計算時間が膨大になったり、あるいは原理的に適用できなくなるという問題が従来の手法にはある。そこで我々は不均質・非線形媒質に対しても適用可能な新しい地震サイクルシミュレーションの手法の開発を今年度から始めた。このコードの開発にあたっては日本で開発された有限要素法コードGeoFEMを基礎とした。テストとして、床に置かれた弾性ブロックの上面を水平方向に定常的に駆動する数値実験を行い、ブロックの間欠的なすべり挙動を再現できた。

キーワード：地球ダイナモ, マントル対流, ACuTE法, インヤン格子, 粘弾性流体, 地震サイクルシミュレーション