Development of Advanced Simulation Methods for Solid Earth Simulations

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Core formation: We have proposed new implicit time stepping method for a Stokes flow problem with a free surface. Our target is to simulate thermal convection in the long term planetary core formation process. In order to apply wider stability region for the oscillatory behavior of free surface deformation, we utilizes a Jacobian free Newton Krylov (JFNK) based Newton framework for an implicit solution of the Stokes flow system coupled to the marker in cell (MIC) method. In comparison with the general explicit Euler method, our methods reduce total computational cost successfully through the utilization of a large time step without sacrificing accuracy and stability. Magma: In order to numerically simulate a crystal settling of the magma dynamics, we have developed new simulation scheme for solving high-viscosity fluid and particle dynamics in a coupled computational fluid dynamics and discrete element method (CFD--DEM) framework. Our solution strategy is found to be robust and successfully captures the collective behavior of the particles. Mantle convection: We have studied mantle convection in super-Earths with ten times the Earth's mass. We systematically investigated properties of mantle convection for various Rayleigh number and temperature-dependent viscosity. From numerical simulation results, the regime diagram of mantle convection in super-Earths was clarified. Geodynamo: We performed test calculations with higher resolution than previous models' one for preparation of high resolution simulation with the new Earth Simulator from next fiscal year.

Keywords: Geodynamo simulation, Yin-Yang grid, Mantle convection, Super-Earths, Core formation, Stokes flow, Discrete Element Method, implicit time integration, Jacobian Free Newton Krylov

1. Core formation simulation: numerical planet (Furuichi)

We develop numerical schemes for solving global scale Stokes flow systems employing the "sticky air" (approximate free surface) boundary condition with marker in cell (MIC) technique [1]. Our target application considers the dynamics of planetary growth involving long time-scale global core formation process, for which the interaction between the surface geometry and interior dynamics play an important role [2, 3, 4]. The numerical problem becomes stiff when the dynamical balancing time scale for the increasing/decreasing load by surface deformation is very short compared with the time scale associated with thermal convection. Any explicit time integration scheme will require very small time steps; otherwise, serious numerical oscillation (spurious solutions) will occur. Due to this numerical difficulty form the deformable surface, the solution of Stokes flow problems including a free surface is one of the grand challenges of computational geodynamics.

For an efficient solution of the stiff system with the free surface, we proposed new the implicit time stepping method for MIC technique. The implicit time integration possesses a wider stability region than the explicit method; therefore, it is suitable for solving the stiff problems with large time step size. The non-linear equations defined by the implicit time integration of the marker advection are solved using a Jacobian free Newton Krylov (JFNK) framework. Following two key techniques are

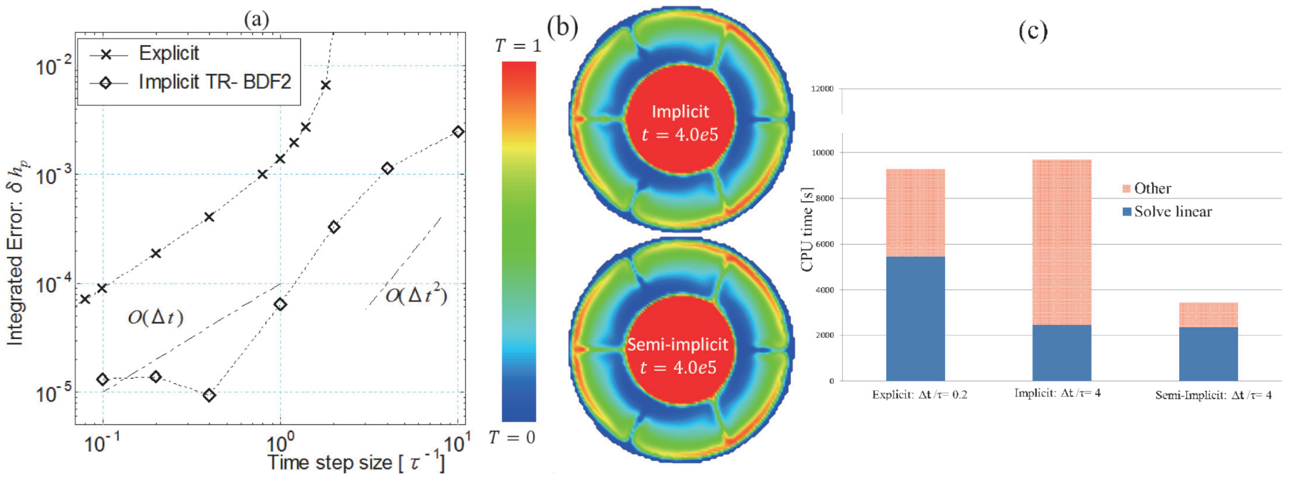

Fig. 1 Left:(a) Peak topography error of the viscous bump relaxation test. Center :(b) Temperature profile of free surface thermal evolution test. Right :(c) CPU time and load balance to solve free surface thermal convection.

combined for this nonlinear solver.

First, not to lose accuracy by using large time step, we apply second order (trapezoidal method (TR) and trapezoidal rule - backward difference formula (TR-BDF2)) accurate implicit methods for the MIC solution scheme. Fig. 1(a) shows the error analysis of viscous bump relaxation test. Compared with the solution with the explicit Euler time stepping method with $\Delta t/\tau$>1, Implicit TR-BDF2 method allows the use of larger time steps without compromising accuracy due to the oscillatory behavior. In addition, we can confirm numerically that the error curves for TR-BDF2 method are second order accurate. It clearly shows that the second order TR-BDF2 method have an advantage in that it can achieve a certain solution accuracy at a larger time step size than that required by the general first order Explicit methods.

Secondly, since the cost for evaluating a nonlinearity of MIC advection directly from the marker coordinate, we proposed the new method which evaluates update the nonlinear residual temporary by the Eulerian advection method. The accuracy and stability obtained by this method can differ from the full implicit method of MIC, because the profiles transported by the Eulerian method are inconsistent with those defined by the markers. Therefore we consider this method a semi-implicit time integration method. When using the semi-implicit method, we can expect reduced computational cost compared with implicit method because the Eulerian advection is cheaper than MIC operations. Fig. 1(b) shows the transit thermal profile of the core formation simulation surrounded by free surface from the same initial conditions with the implicit and semi-implicit time integration schemes. We can confirm that their solutions are visually consistent. This suggests that the temporal difference between the maker and Eulerian update does not play an important role in thermal evolution of global scale phenomena. Fig. 1(c) shows the breakdown of the execution time to obtain the solution of Fig. 1(b). Our proposed semi-implicit method shows the best performance because it reduces the cost not only from using large time step size but also from cheap nonlinear residual update [1].

2. Magma simulation including granular media (Furuichi & Nishiura)

The dynamics of a granular media has been suggested to play an important role in a reheated magma chamber by a hot intrusion(e.g. [5, 6]), but their contributions in the long geodynamical time scale are not clear yet. In order to solve high-viscosity fluid and particle dynamics, we have developed a coupled Stokes--DEM simulation code [5]. This simulation scheme is intended to be used for geodynamical magmatic studies such as crystal settling at the melting roof of a magma chamber.

The high-viscosity fluid is treated by the Stokes-flow approximation, where the fluid interacts with particles via the drag force in a cell-averaged manner. The particles are tracked with contact forces by DEM. Here conventional CFD--DEM solution procedures are not suitable for Stokes--DEM simulation because high viscosity of fluid causes the coupled system to be stiff, thus requiring a very small integration time step to obtain an explicit fluid and particle solution. Consequently, the associated computational cost is unreasonably high. To efficiently solve such Stokes--DEM coupled equations, we propose two key techniques. One is formulation of particle motion without the inertial term, allowing a larger time step at higher viscosities. The other is a semi-implicit treatment of the cell-averaged particle velocity in the fluid equation to stabilize the calculation.

Figure 2(a) shows the calculated average settling velocity of particles in hindered settling problem against the volume fraction of fluid. We can confirm that our Stokes--DEM scheme can quantitatively capture the collective behavior of settling particles predicted by theoretical and empirical models. We have also demonstrated the highly concentrated dense particles (fluid volume fraction is around 0.59) in the thermal convection

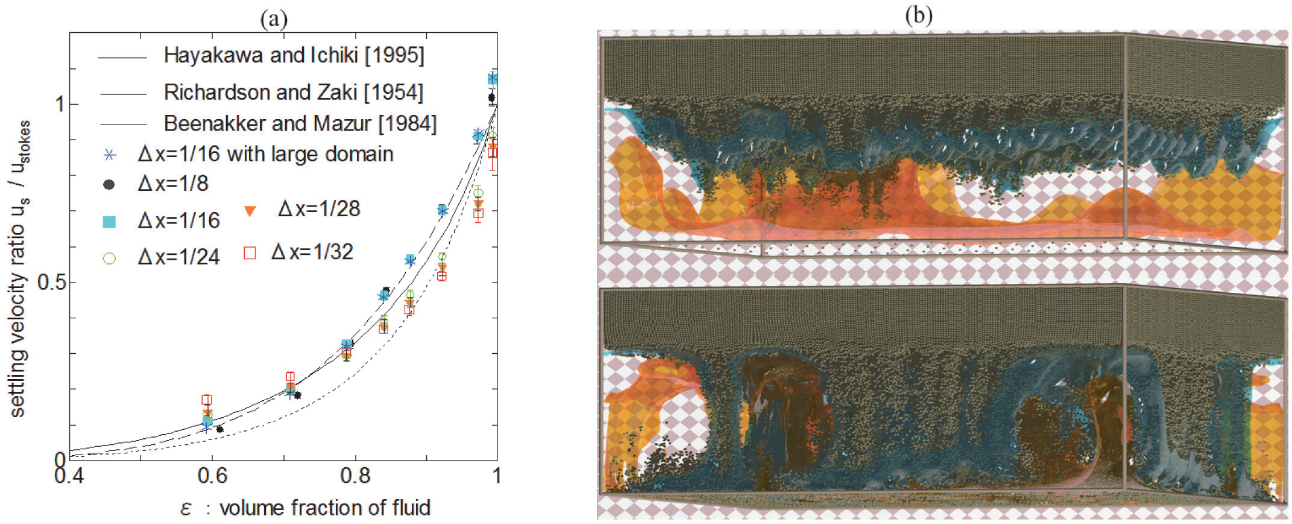

Fig. 2 Left:(a): Settling velocities of particles with various grid size and theoretical and empirical models (b) Settling particles in granular media with the thermal convection.

in Fig. 2(b). This setting represents the first-stage toy model of the erosion process at the melting roof of the magma chamber. Figure 2 (b) shows drastic change of rheology of granular media near the surface to the bottom fluid with the thermal erosion by the upwelling plumes. Our solution strategy is found to be robust and successfully captures the collective behavior of the high-viscosity granular media [5].

3. Mantle convection simulation (Miyagoshi & Kameyama)

Super-Earths are extrasolar terrestrial planets with larger mass than that of the Earth. The most massive super-Earths' mass is about ten times the Earth's mass. It is an interesting question that whether super-Earths are habitable like the Earth or not. Mantle convection is one of the most important factors to clarify the habitability of super-Earths, because it affects the surface environment of the planet through the motion of the surface, and the generation and strength of the magnetic field of the planet through control of the vigor of thermal convection in the fluid metal core. To understand mantle convection in super-Earths, we performed numerical simulations with the Earth Simulator by the ACuTEMAN code [7, 8] which was developed by our ES project.

Super-Earths have a larger size than the Earth's one, so adiabatic compression effect is strong. This effect is important for thermal convection in the mantle. In numerical simulation models for mantle convection of the Earth, the Boussinesq approximation is often used. However, the approximation neglects the adiabatic compression effect so it is not relevant for mantle convection in super-Earths. We took into account the strong adiabatic compression effect which is relevant for massive super-Earths with ten times the Earth's mass, which has not been studied in earlier models.

We found that the hot plume activity in the mantle of massive super-Earths is considerably lowered while cold plume activity is not so lowered. These features are caused by the strong adiabatic compression effect. In addition, we found that the efficiency of heat transport by thermal convection is totally reduced compared with that expected from earlier Bousssinesq models. A part of these results were published in the last fiscal year [9].

We also have performed systematic research for various Rayleigh number and temperature-dependent viscosity contrast, and clarified the regime diagram of mantle convection in super-Earths. We found that the criteria for transition to the stagnant lid regime (in the regime plate is formed at the surface of the planet) is different from that of the Earth. In addition, we found that the thickness of plate is much larger than that of the Earth in the stagnant lid regime. The paper for detail is submitted.

4. Geodynamo simulation (Miyagoshi)

In this fiscal year we calculated higher resolution models than previous model's one to prepare for calculations on the new Earth Simulator from next fiscal year. Although calculations with target physical parameters could not be done, we got some information and hints to prepare new models for the calculation on the new Earth simulator.

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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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本課題では、線形・非線形ソルバ、格子・離散化手法等の先端的な数値シミュレーション技術を駆使したマントル・マグマ・コア等のダイナミクスのシミュレーションを開発することで、地球内部進化の未解決問題に取り組む。本年度の成果としては、まず熱対流を伴うコア形成シミュレーションの実現に向けて Newton Krylov 型の非線形ソルバを実装した移流陰解法を開発し、その計算精度と安定性領域の検証を行った。また、マグマ中の結晶とメルトの混相流シミュレーションの実現に向けて、粒子運動の一部を流体に陰的にカップリングさせて数値的安定性を改善した数値手法を提案し、高粘性流体と粒子との混合計算を可能にした。またマントル対流シミュレーションにおいては、本プロジェクトで開発されたマントル対流シミュレーションコード ACuTE 法を用いて、系外惑星スーパーアースのマントル対流シミュレーションを行った。これまでに見つかっている中で最も大きいクラスの、地球の 10 倍質量を持つスーパーアースについてのマントル対流シミュレーションを行った。マントル対流は表層環境にも、惑星磁場にも強く影響しており、スーパーアースにおけるマントル対流を理解する事はその惑星のハビタブル性を理解するための一つの鍵となると考えられる。本年度は特に、浮力の大きさの目安である無次元パラメータのレイリー数と、マントル物質の粘性率の温度依存性の強さを系統的に変化させた場合に、対流がどのようになるかを調べた。その結果、惑星表面にプレートが形成される条件が地球の場合とかなり異なる事が分かった。またいったんプレートが形成された場合、地球よりも非常に厚くなる事が分かった。ダイナモシミュレーションにおいては、試験的にこれまでよりも高解像度の計算を実施し、新 ES でさらに高解像度の計算を目指すための準備となるデータを得た。

キーワード : 地球ダイナモ , インヤン格子 , 地球回転変動 , マントル対流、コア形成 , ストークス流れ , 陰解法 ,
大規模非線形ソルバー