Development of a Stokes flow simulation code for core formation

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1 Introduction

Development of the simulation code for the Stokes flow problems is an interesting challenge for the computational geoscience, because the Stokes system is relevant to the numerical study of long-time scale geodynamics of the planetary interior such as mantle convection [1-4]. Over thirty-five years, Stokes flow simulation code has been progressed to investigate the global scale geodynamical evolutions with realistic settings, for example, in the treatment of extremely viscosity variations, nonlinear rheology, transport of material, spherical shell geometry and adaptive grid resolutions.

We have developed a new simulation code for solving the Stokes flow motion named after "Nplat" to investigate the core formation process of the planetary interior [2]. The formation of a metallic core is widely accepted as the biggest differentiation event during the final stage of the planetary formation [5]. In our scenario, the dense metal-rich materials are formed by the impact-induced events and sink to the center in the long time-scales.

In order to deal the realistic mechanical setting of the core formation process, our simulation employs free surface condition under a self-gravitating field. We use the finite difference discretization on a staggered grid. Expressing the free surface motion, a stick air layer which is the low viscosity and zero density layer surrounding the planetary surface, is assumed. An ill conditioned Stokes problem arsing in a sharp viscosity contrast is solved by iterative Stokes flow solver, robust to large viscosity jumps, using a strong Schur complement preconditioner and mixed precision arithmetic utilizing the double-double method [3].

The core formation process could be triggered by impacts of planetesimals, but the impact induced process in the planetary interior had not been fully understood yet [5-7]. Here in order to investigate the various possible scenarios, our simulation can treat the several simplified models of impact event.

In this presentation, we introduce the overview of our simulation algorithms [1-4], and demonstrate the preliminary simulation results on massively parallel supercomputer Earth Simulator 2.

2 **Problem settings**

In this section, we introduce basic simulation settings of our core formation simulation. Our scenario starts with a Mars-sized protoplanet (PP) assumed as an undifferentiated planet for simplicity [6]. In the accretionary stage, the planet grows with many times impacts. As a consequence of each impact, molten regions such as magma ponds or oceans are formed on the planetary surface. During solidification of such regions, metal–silicate separation locally occurs over short time-scales. The target of our simulation is to reveal the essential global dynamics of the planetary interior after the solidification over long time-scales [7].

2.1 Stokes flow problem of Core formation simulation

We assume the Stokes flow problem in simple box domain $\Omega \equiv (0, 0, 1) \times (0, 1, 0) \times (1, 0, 0)$ of the three dimensional Cartesian geometry under the self-gravitational field. The free slip boundary condition is applied to every wall. Three material components which are form the protoplanet (PP) (s = 1), metal-rich (s = 2) and silicate-rich materials (s = 3), are assumed in our simulation. The surface of the material is tracked as the scalar color functions $0 < c_s < 1$, which is discretized at the center of the cell. The variables on the grid cells for example density ρ are obtained by,

$$\rho = \sum c_{i} \rho_{i} \,. \tag{1}$$

We define the color function of sticky air as $c_{air} = 1 - \sum_{s} c_{s}$ that has zero mass density and very small viscosity [4, 7].

The equation of the Stokes flow problem under an incompressible approximation is described as the balance of viscous stress, pressure gradient and gravitational force given as,

$$-\frac{\partial}{\partial x_{j}} \eta \left(\frac{\partial u_{j}}{\partial x_{i}} + \frac{\partial u_{i}}{\partial x_{j}} \right) + \frac{\partial p}{\partial x_{i}} = f_{i} . \qquad \nabla \cdot u = 0$$
(2)

where x_i is position (*i*=1,2,3 for three dimensions), and τ_{ii} , *p*,

and f_i are the deviatoric stress, pressure and gravity force respectively. Here we assume Newtonian rheology. The transport of color function is also solved.

The self-gravitating field is obtained by solving the gravity potential Φ which satisfies $\nabla^2 \Phi = \rho$. The gravity force is simply derived by $f_i = -\rho \nabla_i \Phi$.

2.2 Impact models

Our simulation code can deal with three types of impact events. First model is the three-layered model to investigate the overturn process which may occur when a dense metal-rich layer surround the central PP after the solidification of global magma ocean [5].

The second model is the small iron diapers randomly distributed in the planetary body, which represents the solidification of the local magma ponds caused by the many impacts within a short time scale [7].

In the third model, we incorporate planetary growth as a result of impacts. During the simulation, the impactor comes from the random directions with a constant time interval and creates hemispheric magma pond on the surface. When a magma pond is solidified, the metal-rich material is segregated from silicate-rich material, which sinks at the base of the pond.

3 Method

3.1 Advection

In our simulation, the material transport including the color function of sticky air can be expressed as the advection equation.

Our code can use two types of advection method, particle-in-cell (PIC) and CIP-CSLR method [2, 8]. Although both methods provide low diffusive solutions, the CIP-CLSR is generally less expensive in a computational cost, but has more difficulty in the treatment of sub-grid scale profile and multiple components, than the PIC method.

3.2 Stokes flow solver

Since the viscosity contrast at the material boundary is sharp and large, an algebraic equation for (3) has strongly illconditioned structure. In order to solve such an ill-conditioned problem in 3-D, we have developed the robust iterative Stokes flow solver [3, 4]. We use fully coupled approach for the velocity-pressure saddle point system of (3) and (4) utilizing Schur complement preconditioner dependent on the local viscosity. Here the robust preconditioned Krylov subspace method can be a key for solving strongly ill-conditioned saddle point problems [9]. We therefore choose Arnoldi type GCR method as the Krylov subspace method combined owing to its robustness compared to the alternative Lanzos method. We also improve the robustness of the solution method by a mixed precision technique for the inner problem of velocity. In the mixed precision approach, the quad precision arithmetic is applied throughout the GCR algorithm except for during the application of the preconditioner. This is consistent with the idea that the preconditioner is used for a rough estimation of the real solution.

The quad precision arithmetic implements into the doubledouble precision algorithms (DD) [3], which operates a pair of double precision terms to express the quad precision. The loop calculation in DD precision can be vectorized, but not in the officially supported for the quad precision arithmetic. This is an advantage on the DD for running the code on the ES2. Details of this solver and numerical examples on the problems with locally and highly varying viscosity are presented in the references [3].

4 Results

In this section, we briefly introduce three examples of core formation simulation results. Fig. 1 shows the test calculation of three layer model in which the initial cubic layer (left figure) deforms to the steady state of self-gravitation (i.e. sphere of right figure). In this calculation we assume uniform viscosity and density for three layers. The global overturn scenario in the core formation can be simulated by switching the viscosity and density to the target material parameters.

The result of iron diapir model is shown in Fig. 2. The diapirs which are initially placed inside the planet at random sink to the center. This simulation setting is useful to investigate the behaviour of small diaper controlled by the rheological properties of planetary interior.

The simulation of the scenario of the growing planet with many impact events over long time scale is also presented in Fig. 3. This simulation can the change the mass balance of the planet with increasing the total volume by the impact events. This is the first 3-D core formation simulation code to incorporate planetary growth as a result of impacts.

Our simulation is found to successfully capture the large deformation of the materials following the three possible scenario of core formation with maintaining a sharp interface between them.



Fig. 1. Snapshots of the steady state calculation. Outer blue semitransparent iso-surface and half cropped white isovolume represent the silicate-rich and metal-rich materials respectively. Color on the slice shows the distribution of color functions.



Fig. 2. Example of small metal diaper model calculation. Outer semitransparent glass, brown, and metric objects represent silicate-rich, PP, and metal-rich material layer surfaces. The material properties are $\eta_1 = 10^{20}$ [Pa.s], $\rho_1 = 3,900$ [Kg/m3], $\eta_2 = 10^{20}$ [Pa.s], $\rho_2 = 3,500$ [Kg/m3] and $\eta_2 = 10^{19}$ [Pa.s], $\rho_2 = 7,000$ [Kg/m3]



Fig. 3 Snapshot of the core formation caused by a number of impacts. The semi-transparent blue surface represents the silicate-rich material. The white and orange object shows metal-rich and PP material respectively.

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