Current status of post-K Exploratory Challenge, computational planetary science

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In FY 2016, as one of research project for post-K supercomputer, "Exploratory Challenge 3 Elucidation of the Birth of Exoplanets and the Environmental Variations of Planets in the Solar System" has been started. In this talk, I'll overview this project (we call this project computational planetary science project for short).

The development of post-K supercomputer was started in 2014, and its planed completion year is 2020, with up to 100 times faster speed on real applications compared to K computer. As one of four "Exploratory Challenges", computational planetary science has been selected, and it is assigned to Kobe University, with other eight research institutes.

The computational planetary science project consists of four sub topics: planetary formation, dynamics and evolution of planets, solar activities and environmental change, and the origin of life. In this talk, I'll overview these topics, computational challenges, and expected scientific products.

Keywords: High Performance Computing, Computational Science

N-body Simulation of Planet Formation with the Effect of Fragmentation

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We carried out N-body simulations of planetesimal driven migration including the effects of gas drag, type-I migration and fragmentation. Kominami et al. (2016) showed that the planetesimal driven migration can still take place even if the self-gravity of the planetesimals are considered. They also showed that the random velocity increase of the planetesimals was crucial for the migration to continue or to halt. The random velocity of the planetesimals can be affected by the gas drisk and if the gas disk is considered, type-I migration of the protoplanet should be taken into account. Here we carried out N-body simulation that include the self-gravity of the planetesimals with the effect of gas drag, type-I migration and fragmentation. We show that the growth of the planetesimals in the perfect accretion cases prevents the outward planetesimal driven migration. If the fragmentation is considered, small planetesimals are produced, which enhance the outward planetesimal driven migration. We show some cases which outward planetesimal driven migration overcomes type-I migration.

Keywords: N-body simulation, fragmentation, type-I migration

GPU-accelerated High-resolution N-body Simulations for Planet Formation Toward 100 Million Particles

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We developed a fully-parallelized hybrid N-body code for planet formation (**PENTACLE**: Iwasawa et al., *submitted*), implementing the P^3T method (Oshino et al., 2011) and a multi-purpose platform for a parallelized particle-particle simulation (FDPS: Iwasawa et al., 2016) into it. PENTACLE enables us to handle up to ten million particles for N-body simulations in a collisional system, using a present-day supercomputer. Toward a high-resolution N-body simulation with 100 million particles and beyond, we are now developing a parallelized hybrid N-body code optimized for a NVIDIA-based GPU cluster. In this talk, we show the performance and capability of PENTACLE and results of terrestrial planet formation in a narrow ring containing one (and ten) million planetesimals. Then, we introduce the current status of our GPU-accelerated N-body code (**PENTAGLE**) and our future plans, for example, a global simulation of the delivery of water to the Earth in the protosolar nebula.

Keywords: Planet formation, N-body simulation, GPU

High-resolution *N*-body simulations using Pezy-SC processor

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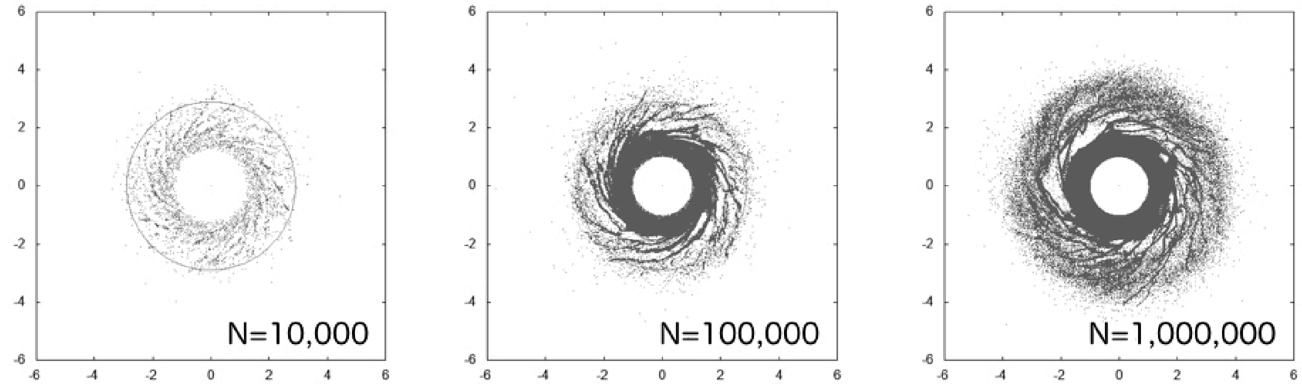
We developed an *N*-body simulation code on multiple Pezy-SC processors—Pezy-SC processor is a novel new architecture developed by Pezy Computing K. K. that has achieved large computational power with low electric power consumption. We adopt the rubble pile model for physical collisions, in which no mergers are allowed, and use FDPS (Framework for Developing Particle Simulator) to solve the self-gravity. We performed several sets of high- and extra-high-resolution *N* body simulations of the lunar accretion from a circumterrestrial disk of debris generated by a giant impact on Earth. The number of particles is up to 1 million, in which 1 particle corresponds to a 30 km-size satellitesimal. We show the performance and capability of our numerical code for high-resolution *N*-body simulations of planet/moon/ring formation.

Keywords: N body simulation, moon formation, Pezy-SC



N-Body Simulation of Chariklo Rings

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Two dense narrow rings around Centaur Chariklo were discovered by occultation observation (Braga-Ribas et al. 2014). The inner and outer rings are located at 391 km and 405 km from the center of Chariklo, respectively. Chariklo's radius is about 125 km. The inner ring has the large optical depth, which is comparable to Saturn's A ring and Uranian delta ring. The width of the rings is about 6-7 km. A ring around Centaur Chiron was also reported (Ruprecht et al. 2015). These observations suggest that rings around large Centaurs may not be as rare as previously thought.

Several mechanisms for the formation of Chariklo's rings have been proposed: collisional ejection from the parent body, satellite disruption, the tidal disruption of the parent body (Pan and Wu 2016, Hyodo et al. 2016). However, the formation mechanisms of the rings is still not well understood. In order to understand the origin of the ring system, we need to investigate the stability and the structure of Chariklo's rings.

In the simulation of Saturn's rings, the global simulation is impossible because the necessary number of the particles is too large. Thus, the local N-body simulation has been used for reducing the computational cost. In this study, we performed the global N-body simulation of the rings for the first time.

We assume that all particles have the same mass and radius. We consider the mutual gravitational forces and the inelastic collisions between particles. We describe a collision as a damped oscillation (e.g., Salo 1995). We use the tree algorithm (Barnes and Hut 1986). Chariklo is located at the center, and its radius and density is 125 km and 1 g/cc, respectively. We use the N-body simulation library FDPS (Iwasawa et al. 2016).

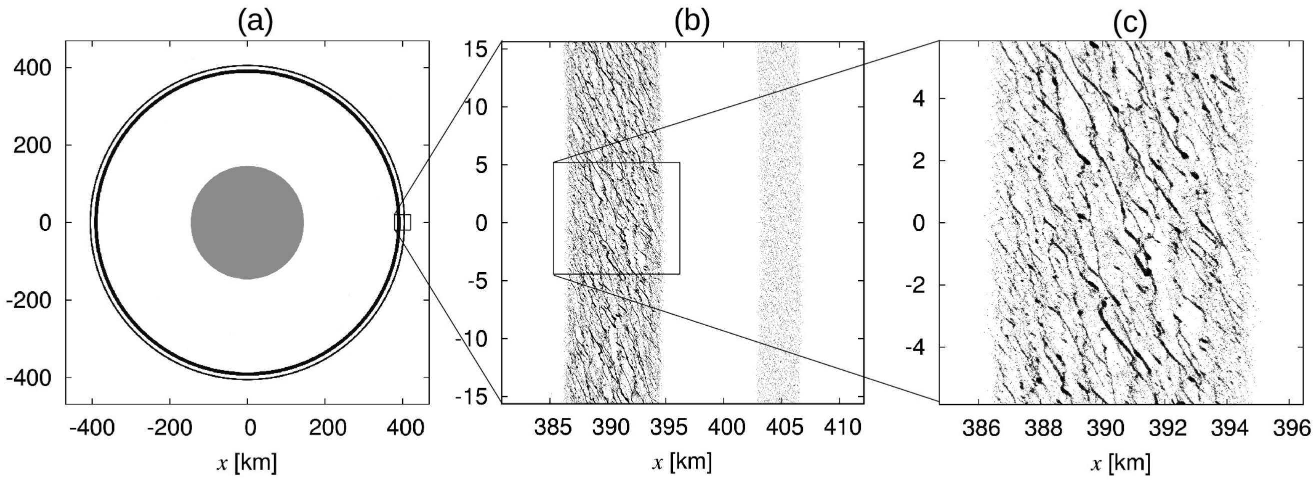
This simulation has two parameters: the particle size and the density. From the theoretical analysis of the apse alignment mechanism, the particle size was estimated as a few meters (Pan and Wu 2016). Thus, in the fiducial model, we assume that the particle size is 5m. We consider the ice particle and assume that the density is 0.5 g/cc in the fiducial model.

After 10 rotational periods, no large-scale structures are visible. However, we find small-scale structures. These structures are known as the self-gravity wakes in Saturn's ring (Salo 1992). Due to the inelastic collisions, the random velocity decreases and finally the gravitational instability takes place. The self-gravity tends to from aggregates. On the other hand the tidal force tends to tear them apart. These competing processes are the cause of these complex structures.

Next we perform the simulations with various particle size and density. The particles size is 2.5 m - 10 m, and the density is 0.05 g/cc - 1.0 g/cc. The number of ring particles is 21 to 345 million. We found that the particle density is important parameter to determine the ring structure. If the particle density is less than 0.1 g/cc, the ring remains uniform and the self-gravity wakes are not visible. This is because the energy dissipation is insufficient and the gravitational instability does not take place. If the particle density is between 0.1g/cc and 0.5 g/cc, the self-gravity wakes are visible as in the fiducial model. If the particle density is larger than 0.5 g/cc, the ring is disrupted to form the satellites. Therefore we conclude that the particle density should be less than 0.5 g/cc to avoid the disruption of the ring. Namely, the particle density should be less than half of Chariklo's density.

The self-gravity wakes enhance the ring diffusion. Taking into account of the the self-gravity wakes, we estimate the ring diffusion time, which is about 1 - 100 years. This diffusion is considerably shorter than the timescales suggested in previous studies. The diffusion time depends on the particle size. If the particle size sufficiently smaller than a few meter, the diffusion time can be long. If the putative moon exists, it can slow down the diffusion.

Keywords: N body simulation, ring, satellite



Development of an SPH code which works on the PEZY-SC devices and application to the giant impact

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Lately, heterogeneous HPC clusters which have CPUs and accelerators, such as GPUs, have been getting more common.
However, to develop such codes requires highly complex parallelization techniques and kernel codes for the accelerators.
Thus, it is quite difficult to develop high-performance codes which work on such a cluster.
In order to get rid of this complexity, recently, we develop a software named Framework for Developing Particle Simulator (FDPS), which automatically parallelise arbitrary particle-base schemes by using both OpenMP and MPI.
FDPS version 2.0 (or higher) also has the so-called ``Multi Walk mode'' to use accelerators.
We developed a smoothed particle hydrodynamics (SPH) code, which used FDPS and works on multiple PEZY-SC devices.
Among several versions of SPHs, we have implemented the standard SPH and the Density Independent SPH.
A PEZY-SC is an accelerator which has advantages to the other accelerators in terms of its performance per power.
We also compared the speed-up efficiency and found that our code is about 30 times faster in single precision than a code which works only on CPUs.
We will show the results of numerical simulations of the giant impact problem carried out by the code.

Numerical simulations of the coupled magmatism-mantle convection system in 2-D and 3-D geometries

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It is generally considered that a magmatism occurred very actively in the hot mantle in the early Earth. Ogawa (2014) proposed that a positive feedback can operate between the magmatism and the upwelling flows of solid-state mantle convection, by numerical experiments of a coupled magmatism-mantle convection system in two-dimensional Cartesian domains. In this study, we newly developed numerical models of the coupled magmatism-mantle convection in three-dimensional Cartesian box as well as in two-dimensional spherical annuli with various shapes, in order to investigate how the geometries of the convecting vessel affects the feedback between the magmatism and mantle upwelling (or "MMU feedback" in short).
We employed both three-dimensional rectangular box and two-dimensional spherical annuli with various ratios of their inner to outer radii. The solid-state convection of the mantle is assumed to be that of an isoviscous fluid with a very high viscosity. Mantle magmatism is modeled by the generation of liquid phase (magma) owing to the pressure-release melting induced by upwelling flows of solid-state convection and the motion of the generated magma as a permeable flow through the solid matrix. The permeable flow of magma was assumed to be driven by a buoyancy due to the density difference between the solid and the liquid phases.
We carried out preliminary experiments using two-dimensional spherical annuli by systematically varying the ratio of inner to outer radii and the Rayleigh number of solid-state convection of the mantle. Our results showed that the MMU feedback can operate in a qualitatively very similar manner when the Rayleigh number is sufficiently large. The threshold values of the Rayleigh number for the MMU feedback lie between $O(10^6)$ and $O(10^7)$, regardless of the shape of the spherical annuli. We also found that, despite the cooling due to solid-state convection and magmatism, the temperature in the mantle remains slightly higher for thinner spherical annuli with larger ratio of inner to outer radii. Our findings suggest that the curvature of the mantle can affect the operation of MMU feedback only in an indirect manner, by modulating the thermal state and the magma generation in the convecting mantle.

Keywords: mantle convection, magmatism, numerical experiment

Separation styles of liquid phase in a convecting solid mantle

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In studying evolution of planetary interiors, separation of liquid phase in mantle is one of the essential processes. In rocky mantle of terrestrial planets, this process is related to magma migrations in crust and mantle, and water rising at subduction zones. It is important to know how the separation of liquid phase proceeds, and how the background solid convection is affected by the flow of liquid phase.
Here we treat a simple setting for liquid phase separation in a convecting solid mantle. We do not include melting and solidification of the liquid phase as a first step. In this model, migration of liquid phase is modeled as a permeable flow. Density of the liquid phase is set to be slightly lighter than the surrounding solid phase. When the relative motion between the liquid and solid phases occurs, the porosity changes and the permeability at that volume is reduced or increased. There are two parameters controlling the flow in this system, those are, Rayleigh number (Ra) for the convection of solid phase, and the initial non-dimensional permeability (M) for the permeable flow of the liquid phase. We compared the timescale of separation at wide ranges of Ra and M. The geometry is a 3D rectangular cell or a quasi-2D box.
We identified that the styles of separation can be categorized into four cases; (a) rapid separation, (b) gradual separation, (c) slight separation, and (d) no separation. When the M is very large, the liquid phase rises with a high velocity. Consequently separation proceeds within a very short time independent on the convective flow of the solid phase (a: rapid separation). When the M is very small, separation does not occur and the convection of the solid phase proceeds including liquid phase in it (d: no separation). Two styles are recognized between these two extremes. In (b: gradual separation), the liquid phase gradually separates at upwelling regions of the solid phase convection. If the background solid convection is time dependent, the liquid phase of the entire system is efficiently removed to the surface. In (c: slight separation), the distribution of liquid phase is slightly evolved from the initial uniform state, but a balance between separation and entrainment of liquid phase is achieved and no further separation proceeds. We established a regime diagram of the styles of separation on the space of Ra and M. Convection of solid phase delays separations of liquid phase. The differences among styles are understood well by a competition between two velocities, permeable flow velocity and convection velocity of solid phase.

Keywords: mantle convection, separation of liquid phase, porous flow

Three-dimensional numerical simulation of tectonic plates in thermal convection of a fluid with stress-history dependent rheology

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Rigid tectonic plates separated by sharp plate margins rather steadily move on the Earth. New plate margins develop, only when such tectonic processes as continental collision and vigorous magmatism known as Large Igneous Provinces induce unusually high stress in the lithosphere; once formed, plate margins remain there even after the stress level is reduced to the usual level in the lithosphere. Our earlier two-dimensional numerical studies of thermal convection of a Newtonian temperature-dependent viscosity fluid show that it is crucial to assume a stress-history dependent viscosity to reproduce these features of tectonic plates of the Earth: In our models, the viscosity takes a high value for plate interior, when the stress σ is sufficiently low; the viscosity drops to a low value typical for plate margins, when σ exceeds the rupture strength of plates σ_p; the viscosity remains low even after σ is reduced below σ_p, as long as it remains higher than another threshold σ_m, the coupling strength at plate margins. The viscosity is a two-valued function of stress in the range from σ_m to σ_p. We found that the basic features of tectonic plates arise, only when the typical stress in the lithosphere is within this range. We also found that the stress-history dependent viscosity is crucial for reproducing a thermo-chemical pile like the Large Low Shear Velocity Provinces, and to realize the asthenosphere that moves faster than the overlying plates around ridges. In this presentation, we extend this two-dimensional model of mantle convection to three-dimensional space by the use of the ACuTEMAN code we developed earlier. We calculated convection in a rectangular box with σ_p lower than the typical stress in the lithosphere to start a plate motion, and succeeded in reproducing sharp plate boundaries. We will raise σ_p and explore how the plates thus started behave, when the stress-history dependent viscosity plays a crucial role in their dynamics.

Toward high-resolution simulation of planetary atmospheres—Model dependencies of a QBO-like oscillation.

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Scales of atmospheric motions in Earth range from a few meter to the planetary scale, and multi-scale phenomena interact with each others. This is a reason for promoting an atmospheric simulation with higher resolution. The situation must be same in other planets such as Mars and Venus. Higher resolution is required for better understanding of the planetary atmosphere. However, especially for the planetary atmospheres, we should advance carefully on a higher resolution simulation, because there is almost no observations for small scales.

On the way to higher resolution, there are some gaps both in governing equations and in calculation methods.

For large-scale motions, the atmosphere keeps the hydrostatic balance, and it is assumed in the governing equations. On the other hand, for small-scale (a few tens of kilometers) motions, the assumption of the hydrostatic balance is not valid, and we need to calculate a prognostic equation of vertical momentum. Hence, the making the resolution higher requires change in the governing equations.

To achieve a high performance in massive parallel computers, calculation methods also must be revised. A spectral method has been widely used for numerical simulation of the atmosphere in a spherical geometry. This is because the spectral method has an advantage of a high precision and avoiding inequality in the resolution on a sphere. However, it is not suitable for the parallel computing due to spectral transformation. To benefit the power of the massive parallel computers, an icosahedral grid systems has been constructed (Tomita et al. 2001, 2002). Difference in calculation methods may influence numerical solutions in a significant scale, though it is undesirable.

To overcome the above gaps—to understand the dependency of numerical solutions on governing equations and calculation methods and to obtain robust results and knowledge, which are independent on them—comparative studies are important. In this study, we use two numerical models: DCPAM and SCALE-GM. DCPAM assumes the hydrostatic balance and uses the spectral methods. SCALE-GM is a non-hydrostatic model using a finite volume method in the icosahedral grid systems. Optionally, SCALE-GM can be used with the hydrostatic assumption.

We have performed an idealized experiment of the Earth-like atmospheric circulation (Held and Suarez 1994) with an extension of the model top to around 50 km, by using both models. In the lower atmosphere (< 15 km), similar atmospheric circulation was obtained in both models; whereas the behavior of zonal wind in the upper atmosphere differs significantly. SCALE-GM showed QBO-like oscillation, that is, the direction of the mean zonal wind above the equator changes with a period of about two years. However, DCPAM did not show such oscillation. Such QBO-like oscillation and its model dependency were reported by Yao and Jablonowski (2013, 2015), but is not well investigated.

To explore the model dependency of the QBO-like oscillation, we have performed numerical experiments

with a variety of horizontal eddy diffusion and model resolution. Numerical results show that a QBO-like oscillation also occurs in DCPAM when the horizontal diffusion is weak. For both models, the weaker horizontal diffusion results in shorter period of the QBO-like oscillation. In addition, the finer resolution makes the period shorter. An analysis of the momentum transport shows that the vertical transport of zonal momentum by disturbances from the zonal mean is stronger in the shorter oscillation cases. Such vertical transport would be caused by vertical propagation of atmospheric gravity waves. Hence, the horizontal eddy diffusion and model resolution influence the occurrence of QBO-like oscillation and its period via the excitation, propagation, and/or breaking of the gravity waves.

Keywords: atmospheric general circulation model, Held and Suarez (1994) experiment, quasi-biennial oscillation

Computational science of dust coagulation process in protoplanetary disk turbulence

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By using recent supercomputers, it is becoming possible to use larger-scale direct numerical simulation (DNS) of high-Reynolds-number (Re) turbulence for understanding complex turbulent flow phenomena. Coagulation process of silicate dusts in protoplanetary disk is one of the most challenging problems in planetary science. By tracking huge number (more than one billion) of inertial particles in high Re turbulence, we could simulate turbulent clustering of particles directly and quantitatively. Our DNS of turbulence showed that dust coagulation is expedited by turbulence clustering of particles. The next step is to realize dust growth simulations to quantitatively estimate the growth rate of dust particles and the size-distribution in high Re turbulence. In the presentation, what we have obtained so far and what we are trying will be discussed.

