From K computer to the post-K computer

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I'll describe the overview of the post-K computer project and how the scientific research using it will be organized, in particular in the field of planetary science.
K computer was completed in 2011 and its public use was started in 2012. It has the peak speed exceeding 10PF, being still the fastest supercomputer in Japan and the fourth fastest in the world. For the scientific research using K computer, five "strategic fields" were selected, and each field got the budget of around 500M JYE/year to develop application software for K computer and to do scientific research using K computer. For planetary and heliosphere sciences, in Field 5 "The origin of the matter and the univerce", large scale simulations of the convective zone of Sun and planetary formation have been performed. For these simulations, application programs which could achieve high efficiency on up to a few tens of thousands of computing nodes have been developed, and helped to obtain important results.
In 2014, the project to develop the successor of K computer ("post-K computer") was started. Its goal is the achieve the application performance 100 times that on K computer. It will be completed in 2019-2020 timeframe. The design and production will be done by Fujitsu, which developed K computer as well. The post-K will have the general-purpose many-core architecture and torus network, similar to those of K computer. For the post-K computer, nine "priority issues" and four embryotic issues have been selected. Planetary science is included to one of the four embryotic issues. For the priority issues, the organizations to perform the research and development have already been selected, but for embryotic issues they are yet to be selected (as of January 2016). At the time of the meeting, hopefully, the organization will be fixed, and I'll describe the status of the "embryotic issue" for planetary science.

Keywords: large-scale simulation, computational science

Complex organic molecules in star- and planet-forming regions

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Complex organic molecules (COMs) are intensively searched for around solar-mass protostars in recent years. For example, glycolaldehyde ($HCOCH_2OH$), the simplest sugar, was detected around IRAS16293 in the ALMA Science Verification program (Jorgensen et al. 2012). COMs are expected to be more abundant in ice mantles than in the gas phase, because their sublimation temperature is relatively high, and because grain-surface reactions would play significant roles in their formation. COMs in star-forming regions, especially in ice mantle, could be an important reservoir of organic compounds in the planetary-system formation and/or mother molecules of prebiotic molecules. It is, however, very difficult to directly observe COMs in ice mantle. Combination of line observations (of gaseous COMs) and theoretical modeling of gas-grain chemistry is thus needed to understand the formation and destruction of COMs in the gas phase and ice mantle. Computational modeling efforts include (i) radiation hydrodynamics of star formation, (ii) gas-grain chemical network calculations and (iii) physical/chemical calculations to determine the rates and efficiencies of various chemical reactions and micro processes. In this contribution, I will review recent progresses, especially in (ii) and (iii).

Keywords: astrochemistry, formation of star and planetary systems

Computational planetary science using FDPS (Framework for Developing Particle simulator)

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Particle-based simulations are widely used in the field of computational astronomy. Examples include the cosmological simulations or the planet-formation simulations with gravitational *N* body code, the simulations of star and galaxy formation with the Smoothed Particle Hydrodynamics (SPH) code or other particle-based codes, and the simulations of planetesimals formation with the Discrete Element Method (DEM) code. To develop an efficient program for particle-based simulation for large-scale parallel machines computer is not easy, and to some extent the efforts of many researchers have been spent on the programming and tuning. However, the algorithms of particle-based simulations are largely similar. Thus we have developed a framework which helps the researchers to develop efficient programs for particle-based simulation on large parallel machines, which we call Framework for Developing of Particle Simulators, or FDPS.
In this presentation, we introduce concept and implemantaion of FDPS. We also show some applications for planetary science using FDPS.

Keywords: Simulations, Planet formation

High-resolution N-body Simulations for Planet Formation: To 100 Million Particles, and Beyond

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In a collisional system, close encounters play an important role in dynamical evolution. Gravitational interactions between particles undergoing a close encounter are big bottlenecks in N-body simulations because of high computational costs. In fact, a direct N-body simulation in the context of planet formation faces a wall of ten thousand particles. Toward high-resolution N-body simulations with 100 million particles and beyond, we have developed three tips to overcome this sort of big wall, implementing them into our N-body code for planet formation: (i) a tree-based hybrid N-body scheme which reduces numerical integrations of gravitational interactions among particles, PPPT method (Oshino et al. 2011), (ii) GPU clusters which allow us to handle a large number of particles, (iii) parallelization and optimization for accelerating numerical integrations, specifically, a multi-purpose platform for a parallelized particle-particle simulation, the so-called “Framework for Developing Particle Simulator” (FDPS: Iwasawa et al. 2015). In this talk, we introduce what our brand-new N-body code is like and its performance and capability. We also show our preliminary results of N-body simulations of terrestrial planet formation, using ~ 0.1-1 million planetesimals.

Keywords: Planet formation, N-body simulation, GPU

Global High-resolution N-body Simulation of Planet Formation: Planetesimal Driven Migration with Type-I Migration

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By means of fully self-consistent N-body simulations, we investigated whether outward Planetesimal Driven Migration (PDM) takes place or not when the self gravity of planetesimals is included. We performed N-body simulations of planetesimal disks with large width (0.7 - 4AU) which ranges over the ice line. The simulations consisted of two stages. The first stage simulations were carried out to see the runaway growth phase using the planetesimals of initially the same mass. The runaway growth took place both at the inner edge of the disk and at the region just outside the ice line. This result was utilized for the initial setup of the second stage simulations in which the runaway bodies just outside the ice line were replaced by the protoplanets with about the isolation mass. In the second stage simulations, the outward migration of the protoplanet was followed by the stopping of the migration due to the increase of the random velocity of the planetesimals. Due to this increase of random velocities, one of the PDM criteria derived in Minton and Levison (2014) was broken. In the current simulations, the effect of the gas disk is not considered. It is likely that the gas disk plays an important role in planetesimal driven migration. Hence, we also carried out N-body simulations of PDM including the gas drag and type-I migration. Type-I migration and gas drag are known as the effects that drag the planeteismals and protoplanets toward the central star. We showed that the random velocity of the planetesimals are subdued by the gas drag and enhances the outward migration. We found that in Minimum Mass Solar Nebula (MMSN), there were a period that outward PDM overcomes the type-I mirgation.

New developments in planetary formation theory of solar system derived from ABEL model

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The Earth was formed as dry rocky planet without atmosphere nor ocean at 45.6Ga. Atmospheric and oceanic components were added at 4.4Ga by late heavy bombardment. This 2 step formation model of the Earth is named ABEL model (Advent of Bio-Elements Landing Model). The origin of solid Earth is enstatite chondrite which has been already clearly indicated by analysis of oxygen isotopic composition and other isotopic data. At the same time, the origin of water on the Earth is carbonaceous chondrites which is backed by hydrogen isotopic ratio. These 2 facts have been thought to be contradictory, but ABEL model is able to explain them perfectly. Also this model explains this two-step formation was the precursor of the reaction as metabolism.

Here, we give a comprehensive views for the research of planetary formation theory of solar system based on ABEL model for followings. (1) Moon formation theory (Giant Impact model), (2) Chemical zoning of asteroid belt with observational facts (they does not support the Grand Tack model that suggests random distribution of chemistry), (3) Chronology research based on meteorites, (4) H2 gas escaped during first 3 hundred million years after the formation of protoplanetary disk.

Based on above information, we give new developments in planetary formation theory of solar system.

Keywords: Planetary formation theory, ABEL model

Modeling the evolving interiors of planets

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There is a clear correlation between the size of a terrestrial planet and the style of tectonic activities that are caused by mantle convection in that planet: There is no clear indication of tectonic activities on the present Moon where the Rayleigh number of the mantle is below the critical Rayleigh number; plume magmatism has occurred almost throughout its 4.5 Gyr history on Mars where the Rayleigh number marginally exceeds the critical value; plume magmatism and tectonic activities are pervasive on the present Earth and Venus where the Rayleigh number is well above the critical value. To develop a comprehensive model of tectonic activities and evolution of these planets, it is necessary to systematically explore the elementary processes that exert control over mantle dynamics. Through my two-dimensional models of magmatism in convecting mantle, I have listed several crucial elementary processes: (1) the magmatism-mantle upwelling feedback that operates in Mars, Venus, and the Earth; (2) mantle bursts that occurs in the Earth and Venus owing to an interaction between magmatism and a high pressure induced solid-solid phase transition of mantle materials; (3) plate tectonics that occurs on the Earth probably because of the ocean that the planet hosts. Here, I argue that a three-dimensional modeling of these processes is necessary for ultimate understanding of mantle evolution in terrestrial planets.

Keywords: mantle evolution, mantle convection, magmatism

Thermal convection in the mantle of massive super-Earths

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Understanding thermal convection in the mantle of super-Earths is one of the most important key to clarifying their thermal history, surface environment, and habitability. The reason is that the plate motion, material circulation, the vigor of core convection and planetary dynamos are controlled by the thermal convection.
In contrast to the Earth’s interior, the strong adiabatic compression effect is important in massive super-Earths. We have studied the thermal convection in massive super-Earths (about ten times the Earth’s mass) with this effect by the ACuTEMAN method [Kameyama M., 2005]. We also take account for high Rayleigh number which is relevant for super-Earths, and temperature-dependent viscosity contrast and depth-dependent thermal expansion coefficient.
The summary of results is as follows. (a) The activity of ascending hot plumes is considerably lowered compared with that of descending cold plumes. (b) The efficiency of heat transport by thermal convection is lowered compared with the results of Boussinesq (no adiabatic compression) models. The thickness of plate at the surface is considerably thicker than that of the Earth. (c) From the convective regime diagram, the threshold value of viscosity contrast for transition to the stagnant-lid regime convection increases as Rayleigh number increases in contrast to the result of Boussinesq models (in which the threshold value is constant). The details of a-c are given in Miyagoshi et al. [2014, 2015].
We also found that the convection remains in the initial transient stage for a substantial portion of the thermal history of massive super-Earths. In the transient stage, the convection is layered. Cold plumes descend from the surface very slowly, and the convection remains inactive in the upper layer, until the cold plume heads descend to the layering boundary. The layering boundary is located at the depth where the actual temperature gradient coincide with the adiabatic temperature gradient. After the initial transient stage, cold plumes penetrate through the boundary, and the convective structure changes to the whole layer one.

Keywords: super-Earths, mantle convection

Development of cumulus parameterization based on cloud-resolving model

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A cumulus parameterization was developed using cloud-resolving model. Cloud-resolving model was used to estimate macrophysical cloud properties which were considered in the cumulus parameterization through modeling of entrainment and detrainment rates. Analysis on composite structure of updraft convective clouds simulated by cloud-resolving model indicated that there was similarity in the both structures of deep and shallow convection. The similar structures were possible to be modeled using updraft velocity of cloud mass flux in conjunction with in-cloud buoyancy and detrainment. Based on the composite analysis on data obtained from the cloud-resolving model, (organized) entrainment could be parameterized using in-cloud buoyancy and a recently proposed (organized) detrainment model. The developed cumulus parameterization diagnoses the updraft velocity when the model determines updraft convective cloud structure, considering lateral mass exchanges performed by entrainment and detrainment. The downdraft cloud structure was analogously parameterized by height-dependent entrainment using negative in-cloud buoyancy which was produced by evaporation (and sublimation) of precipitation. The diagnosed cloud structure was generalized in which shallow and deep convection was treated in a unified manner.
An atmospheric general circulation model (AGCM) was developed employing a composite grid system and recently presented parameterizations (land surface, non-orographic gravity wave and boundary layer schemes), and the developed cumulus parameterization was implemented into the AGCM, in order to examine sensitivity to the selected parameters and physical performance of the scheme. Evaluations of the scheme were performed using the AMIP-type low-resolution experiments against climatological reanalysis data. In the evaluations, difference of detrainment model was especially examined, and it was found that (organized) detrainment model had significant impact on the model’s physical performance. This was because the present entrainment rate was modeled using detrainment rate, and thus these parameters were strictly connected each other. Although all employed detrainment models were based on the fact that detrainment was proportional to buoyancy loss in convective clouds, a detrainment model originally developed for shallow convection showed worse physical performance, and detrainment model which was based on cloud-resolving model and did not separate modeling procedure for different convection depths worked better.

Keywords: cumulus parameterization, cloud-resolving model, atmospheric general circulation model

Toward simulations of weather and climate of planetaries in general

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The aim of this presentation is to visit quickly the present status of numerical simulations for possible weather and/or climate on a planet or a satellite with an atmosphere other than the Earth, and to place some foresight of development of simulation in the near future.
Until almost the end of 20th century, it had not been recognized as a fruitful research but as a hobby work to consider generality and particularity of a surface environment of a planet by demonstrating weather and climate, which may be realized on a given planet, by constructing its virtual atmosphere in a computer. There have been vigorous research activities on the evolution of planetary surface environment from the viewpoint of energy budget analyses by solving the radiation transfer equation for a given set of atmospheric chemical species, but little from the viewpoint of atmospheric circulation with an explicit representation of material transport by the atmospheric motion.
Unfortunately, the present understandings of the weather and climate on the planets in our solar system, for which we can utilize observational data by the use of exploration devices and/or telescopes to a certain extent is not enough for us to predict confidently the environments of exoplanets or the planets of our solar system in the early stages of its evolution. The a-periodic appearance of the Martian global dust storms still remains to be understood. The four day circulation (the rapid zonal wind) which characterize the looks of Venus remains to be understood in a dynamically consistent fashion where atmospheric disturbances and their roles are revealed. The banded structure observed in the atmospheres of the giant planets still remains in a stage with many controversial arguments. This is because the development of observations for the Earth's environment which enables the development of weather and/or climate prediction can not be expected for the planets in our solar system and for
exoplanets. The issue to proceed the research activities in these fields is to establish reliable ways of verification for numerical
methods with the lack of such observational backups. As an effort to respond this issue, our group is now constructing a series of
hierarchical models and a group of software libraries to support them.

Keywords: numerical simulation, planetary environment in general, weather and climate

