Development of Macro-Micro Interlocked Simulation Algorithm

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The development of Macro-Micro Interlocked (MMI) simulation, which consists of the mutual connection algorithm between macroscopic and microscopic models, was advanced for several multiscale phenomena; combustion, plasma shock, auroral arc formation, solar flare, cloud and precipitation, and solid friction. In particular, the continuum-particle connection algorithm is demonstrated to be effective for combustion simulation as well as for multiscale plasma simulations. The MMI simulation of combustion, in which the kinetic Monte-Carlo molecular model and the finite volume (HLLC) fluid model are connected by the hand-shaking technique, can well capture the kinetic property of non-thermal component on the combustion front of detonation. The new technique to embed Particle-in-Cell micro-scale plasma model into magnetohydrodynamic (MHD) model has also been developed, and it was applied to the simulation of multiscale dynamics for the collision-less plasma shock. Moreover, the first principle cloud simulation based on "Super-Droplet method," which is the first-ever particle-based cloud model, was improved and applied to the study of aerosol-cloud relationship. A new type of MMI simulation using the parameterized connection method was also investigated, and the applicability of that was examined for the simulation of friction on solid surface, in which molecular dynamics model and elastic model based on SpH scheme are interlocked. All the results clearly indicate that MMI simulation is a powerful tool for the various types of multiscale simulations, and we can conclude that MMI simulation is a promising methodology for the multiscale study in the wide fields of sciences and engineering.

Keywords: Macro-Micro Interlocked Simulation, Multi-scale, Multi-physics, Super-droplet method, The Earth Simulator

1. Introduction

Multi-scale phenomena, in which the micro-scale elementary process and the macro-scale system evolution are tightly connected to each other, quickly comes up as a crucial issue in the wide range of research fields, such as material science, plasma physics, chemistry, astrophysics, geo-science, bioscience and so on. Computer simulation is usually constructed on basis of the theoretical description like the partial differential equation, and thus the applicability of simulation model has to be constrained by the limitation of basic theory.

Recently, in order to overcome this difficulty, several new techniques have been proposed. Macro-Micro Interlocked (MMI) Simulation is one of such a new methodology for multi-scale simulation (Sato 2005). The basic concept of the MMI simulation consists of the interconnection between macro- and micro-simulations. Micro-simulation can calculate elementary processes based on the first-principle, when the macroscopic approximation, such as the thermal equilibrium in fluid dynamics, was broken down as the result of

macroscopic dynamics, and send the accurate information to macro-simulation. On the other hand, macro-simulation can provide the environmental information for the micro-simulation, which is therefore able to be carried out only in a compact region embedded in the macroscopic domain. By optimizing the exchanging information between the micro and macro models, the MMI simulation would greatly reduce the computational demand for the multi-scale simulation.

The objective of this project is to develop the algorithms for MMI simulation as well as to demonstrate the applicability of that for typical multi-scale problems. In 2006 FY, we have developed the several applications of MMI simulation for combustion, cloud and atmospheric dynamics, plasmas, and solid friction.

2. MMI simulation of combustion

Combusting fluid dynamics is a typical multiscale phenomenon, in which the reaction in molecular scale and the macroscopic flow dynamics are mutually interacted. This

multiscale interaction is important especially in the rapid and violent combustion process called detonation, which is sustained by the interaction between combustion and shock waves. Besides its interest as a topic of fundamental chemistry, detonation phenomena have been interested in the field of engineering. Since thermal energy is efficiently extracted from a detonation, some type of propulsion device using pulsating detonation wave propagation, called a pulse detonation engine (PDE), is expected as a potential engine for next-generation aviation and power generation. The study of detonation is also important for safety engineering since detonation generated by a chemical accident may cause severe damage to the environment. Furthermore, the understanding of detonations in nuclear burning is important also for the study of supernova explosions.

In the dynamics of gas detonation, the spatially localized shock front plays a crucial role. High Knudsen number occurs on the shock front due to the strong steepness of state variables. Exothermic and endothermic chemical reactions may generate strong non-thermal equilibrium states on the shock front. Therefore, the local thermal equilibrium and continuum approximation, which are implicitly assumed in the conventional simulations of combusting fluid dynamics, is likely to be broken down, although the effect of non-thermal distribution function on the chemical reactions still remains to be clarified.

In our new algorithm, the simulation system is spatially divided into the two kinds of domains. One occupies most of the system in which the near-thermal equilibrium is satisfied. Another domain lies in the vicinity of shock front, where strong non-thermal equilibrium may take place. The dynamics of the near-equilibrium domains are treated by a macro-scale continuum model based on the Navier-Stokes equation.

The non-thermal equilibrium domains are treated by a micro-scale molecular model based on the Boltzmann equation. The former and latter models are solved by an approximate Riemann solver called HLLC method and a particle-based method called non-steady direct simulation Monte Carlo (DSMC) method, respectively.

As illustrated in Fig. 1a, the particle and continuum domains are interlocked via hand-shaking regions. The hand-shaking region consists of C→P and P→C connections, which pass information from the continuum domain to the particle domain and vice versa. The C→P connection generates simulation particles in the particle domain from thermal-equilibrium distribution corresponding to the macroscopic quantities. The P→C connection obtains macroscopic quantities such as density of each chemical species as the statistical average of the particles and passes them to the corresponding part of continuum domain.

Figure 1b shows a typical result of MMI simulation for detonation propagation. The narrow part enclosed by dotted lines corresponds to the particle domain. In this simulation, the particle domain can automatically track the propagating shock front. The result shows that the characteristic structure of detonation front with triple points is clearly reproduced by the particle mdel, and the flow field runs properly toward downwind through the hand-shaking region.

It is well-known that two-dimensional detonation propagates with successive collisions of triplet points, which form a scale-like cellular structure. Maximum pressure history shown in Fig. 2 reveals that the result of the MMI model is in good agreement with the particle-based simulation, in which all molecular kinetics is taken into account in the whole domain. This clearly indicates the advantage of MMI simulation from the point of view of computational efficiency.
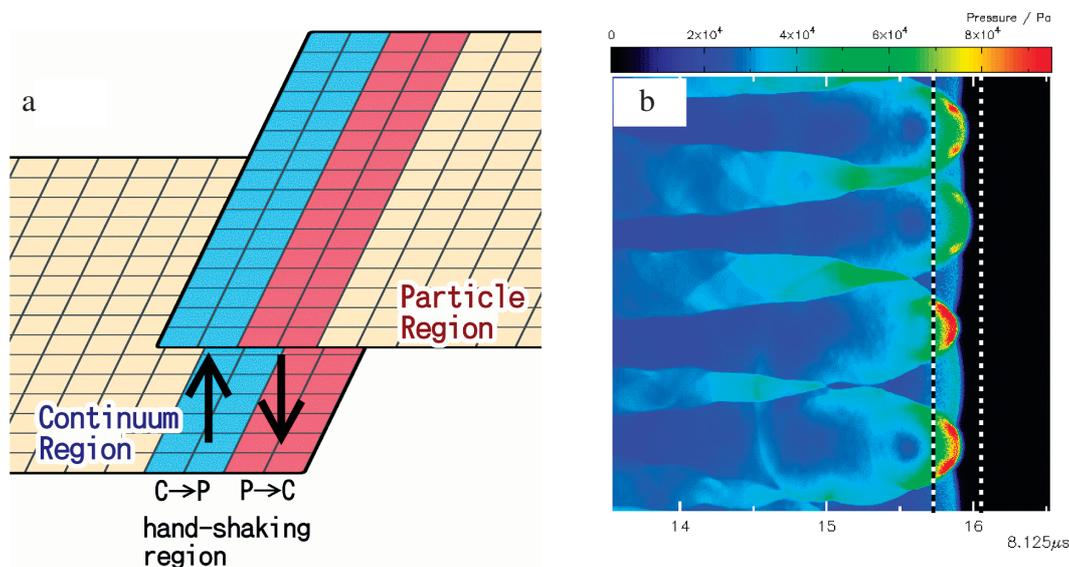

Fig. 1 a. Illustration of the handshaking between particle and continuum models.
b. The pressure distribution around the detonation front. The region bounded by dotted line corresponds to the domain for the particle-based model.
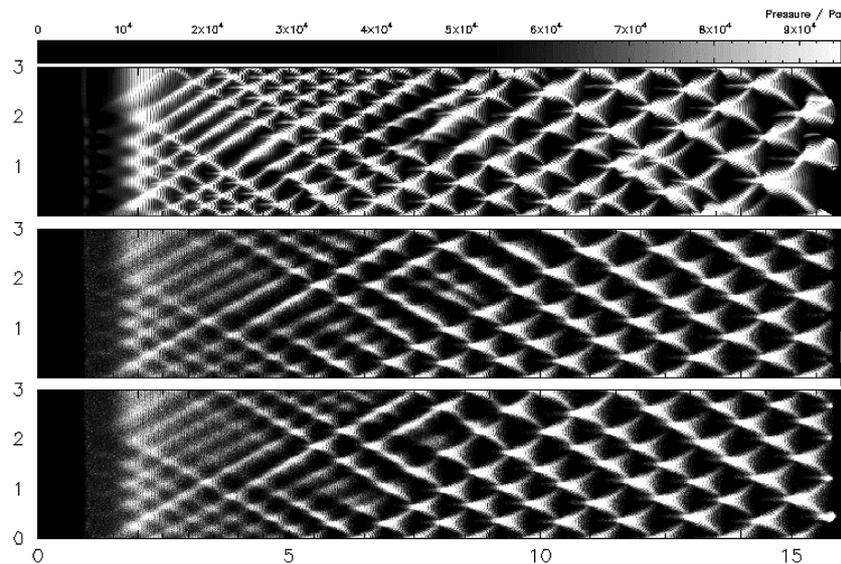
Fig. 2 The distribution of maximum pressure history. Top, middle, and bottom represent the results of continuum model, particle model and the interlocked model, respectively.

3. Super-Droplet Method: A New Algorithm for Cloud-Atmospheric Coupling

Although clouds play a crucial role in atmospheric phenomena, the numerical modeling of cloud is not yet well established. We are developing a novel particle-based simulation model of cloud microphysics, named Super-Droplet Method (SDM), which enables accurate numerical simulation of cloud microphysics with reasonable cost in computation (Shima et al. 2007). A simple SDM for warm rain, which incorporates sedimentation, condensation/evaporation, stochastic coalescence, was established. The methodology to couple SDM and a non-hydrostatic model was also developed.

In 2006 FY, we have more extended the study of SDM for examining the reliability and the feasibility of that. Figure 3 shows the result of SDM simulations, which was carried out to investigate the aerosol effect in cumulus formation and precipitation. The results clearly indicate that the amount of precipitation is sensitive to the number density of aerosols, which plays a role as cloud condensation nuclear (CCN). Though several extensions and validations are still necessary, SDM is a promising tool for the modeling of complicated cloud microphysics, and provide us a new approach to the multiscale processes of cloud-related open problems, such as the cloud and aerosol interactions.
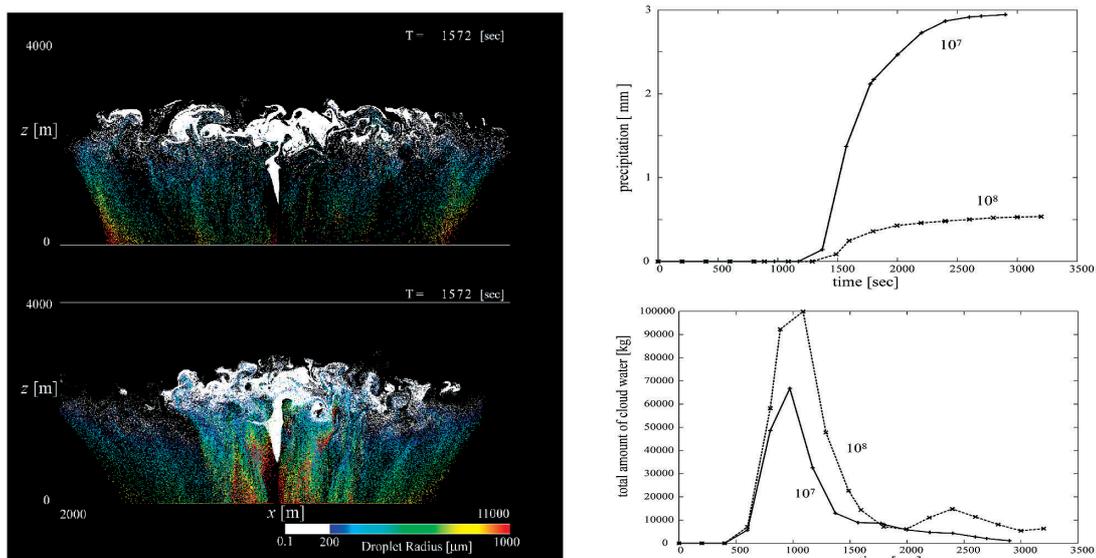

Fig. 3 The result of testing simulations of cloud-aerosol interaction. The initial aerosol number density is changed as $10^8/m^3$ (upper left) and $10^7/m^3$ (lower left). We can see that the precipitation amount is crucially affected by the aerosol number density (upper right) though the cloud water content is not affected so much (lower right). Note that the precipitation is much amplified, when the number of aerosol is more reduced, in these calculations.

4. MMI Simulation of Plasmas

Plasma inherently forms a multi-scale system, because it consists of multi components (ions and electrons). Those components have their characteristic scales related to their mass and charge. There are several models to simulate the plasma system, which is related to various scales. PIC (particle-in-cell) model can incorporate full kinetic processes of ion and electron, while HYBRID model, which consists of electrons as mass-less fluid and ion particles, is useful for the study of ion kinetics. Several versions of continuum models, two-fluid-MHD (magnetohydrodynamics), Hall–MHD, single fluid MHD, have been respectively developed so far, for the studies of different plasma processes.

The interlocked model, which is formed by the connection of different models, is advantageous for plasma simulation, because it can directly calculate the mutual interaction between different scales, for instance between fluid-type dynamics and particle kinetics.

In this year, we have developed two kinds of the interlocked algorithm for plasma simulation (Sugiyama and Kusano 2007). They are MHD/PIC connection model, and Hall-MHD/PIC connection model, respectively. In both the cases, PIC model is embedded into the continuum (MHD or Hall-MHD) model. The physical variables are mutually exchanged between micro and macro models through the boundary using the sophisticated hand-shaking technique.

Figure 4 shows the results of the Hall-MHD/PIC connection model in one-dimensional system. The whole system is simulated by Hall-MHD model except for the shock region which is calculated by PIC model. Super-Alfvénic flows are injected from the both boundaries and form a pair of shock. The spontaneous excitation of whistler waves in shock region is well calculated by PIC model, and simultaneously the propagation of the wave into the Hall-MHD domain is smoothly simulated across the boundaries between PIC and Hall-MHD domains.

The formation of aurora was also investigated by MMI simulation. The large-scale structure of quiet auroral arc is believed to be created as a result of MHD process in magnetosphere. Ionospheric feedback instability was proposed as one of the candidate to explain that. However, high energy electrons, which lead to luminescence by the collision with air molecule, have to be accelerated by the double layer, which should be formed by kinetic process in micro-scale.

In order to realize the holistic simulation including both the MHD and the kinetic instabilities involved in the auroral arc formation, we had developed the MMI simulation code for the last two fiscal years (FY2004–2005). In this fiscal year, we improved this code in various technical points, and successfully studied the highly nonlinear process of this instability by carrying out the long time calculation of MHD model. The left panel of Fig. 5 shows the time development of ionospheric plasma density perturbation at a point on dusk side. This panel indicates that plasma density grows exponentially in the early stage. This growth rate is close to the value predicted by linear theory. Right panel represents the distribution of ionospheric plasma density perturbation. In this panel, there are some longitudinally striated structures mainly on dusk side. The striations in higher latitude area on dusk side move in the pole-equator direction, while those in lower latitude area propagate in the equator-pole direction. This fact is in good agreement with theoretical model. The role of accelerated particles in arc formation will be investigated in the next fiscal year.

The initiation of solar flare eruption is also one of the typical multiscale plasma dynamics, because it should be triggered by mutual interaction between large scale MHD process and collision-less magnetic reconnection in high-temperature plasma. In this year, we have developed a new robust three-dimensional MHD code by applying HLLD approximate Riemann solver (Miyoshi & Kusano 2005) onto full spherical geometry. Figure 6 is the result of that, and shows the magnetic field evolution in flare eruption. The interlocking with kinetic model in reconnection process was undertaken.
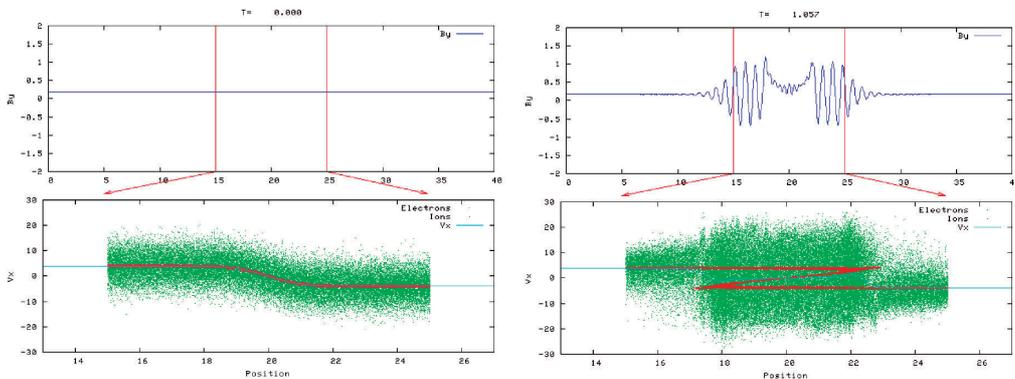

Fig. 4 Results from Hall-MHD/PIC interlocked simulation. PIC model is embedded into a region between two red lines in Hall-MHD system. Left panels show the initial condition, and right panels are the result at the time $1/\omega_{ci}$. Top panels indicate the distribution of tangential components of magnetic field, and bottom panels are the velocity-space (V_x-X) phase plot for ions (red dots) and electrons (green dots) in the PIC domain.
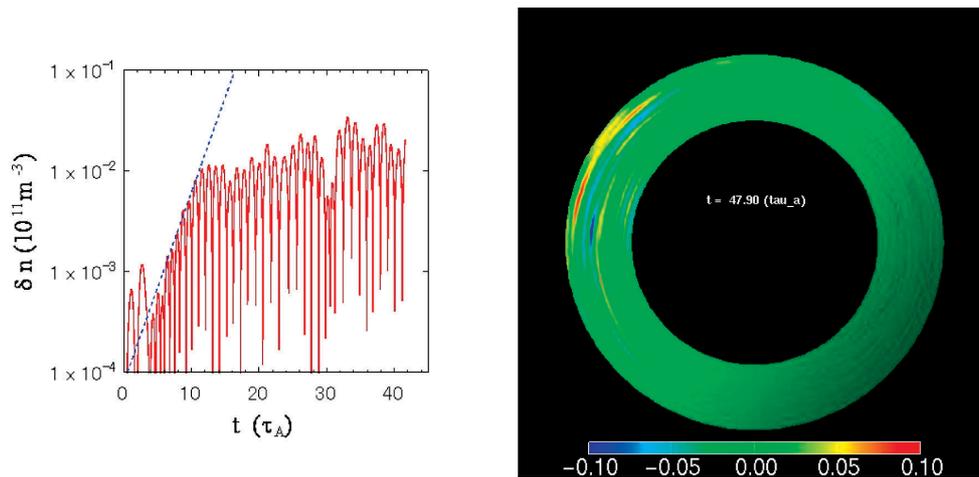
Fig. 5 The results of quiet auroral arc simulation using MHD (macro) model. Left: The time develop-
ment of ionospheric plasma density perturbation (absolute value) at a fixed point on dusk side.
Right: The distribution of ionospheric plasma density perturbation.
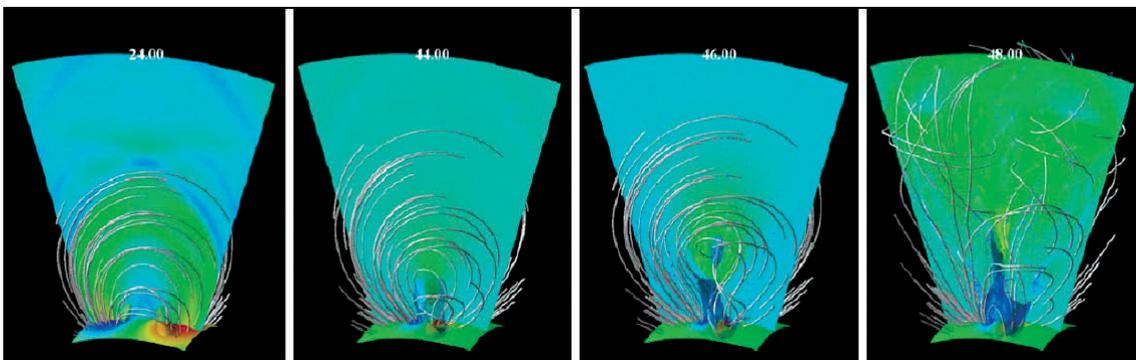

Fig. 6 Magnetic field evolution of solar flare simulation. Panels from left to right indicate the erupting process of
magnetic flux twisted by motion on solar surface (bottom plane). Color scale indicates radial velocity.

5. MMI Simulation of Friction Dynamics

A famous law called "Coulomb – Amonton's law" says that the frictional force is proportional to the pressure acting on the interface. This law is commonly used to compute frictional force in macroscopic elastic dynamics since the frictional force cannot be determined in the framework of elastic dynamics. On the other hand, it is also well known that the "Coulomb – Amonton's law" doesn't hold in many cases where there is lubricant or active grain at the interface. Therefore, to perform precise simulation of macroscopic friction problems, one needs ab initio computation of frictional force using molecular dynamics (MD) that describes the microscopic (atomistic) contact.

We have newly developed a MMI simulation scheme for friction dynamics using the "patch dynamics" model. This scheme invokes MD simulations only for patches in the macroscopic space-time to improve computational efficiecy. The specific algorithm is as follows: (1) The smoothed particle hydrodynamics (SPH) method is employed for macroscopic simulation of elastic dynamics. (2) When friction occurs at a contact surface between two bodies, the pressure P and sliding velocity V are measured at all contact points.

(3) Invoked for every contact point to get the frictional coefficient is an MD simulation, where two atomistic clusters are pushed together with the pressure P and sheared with the sliding velocity V. (4) The frictional coefficients measured in the MD simulations are given to the SPH simulation to compute macroscopic frictional forces at the contact surface.

6. Summary

The MMI simulation algorithms for the different multi-scale problems have been developed (Kusano et al. 2007). One key technique is the hand-shaking connection between continuum and particle models. It may work well in the case that microscopic model is needed only in some localized region. On the other hand, patch dynamics, which was adopted in the MMI friction simulation, is a new method to connect between micro- and macro-scales.

Several basic algorithms were already developed for the MMI simulation of various problems. The new techniques established in this project is planed to be applied onto more practical problems to demonstrate the feasibility of MMI simulation in the next FY.

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連結階層シミュレーションアルゴリズムの開発

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　ミクロスケールとマクロスケールの階層間相互作用が本質的役割を果たすマルチスケール現象は自然科学と技術開発のあらゆる分野に普遍的に現れるため、数多くの先端分野における最重要課題として急速に注目されている。しかし、単一の方程式や計算ルールに基づく従来のシミュレーション手法では、異なる階層の相互連関効果を第一原理に基づいて扱うことはできなかった。本プロジェクトの目的は、単にシミュレーションの規模を巨大化するだけでなく、各階層に適合した複数のシミュレーションモデルを効果的に連結することで統一的にマルチスケール現象を計算することができる連結階層シミュレーションのアルゴリズムを新たに開発することにより、マルチスケール問題に対する強力な計算方法論を確立することにある。

　本年度は、粒子流体連結アルゴリズムを利用したデトネーションの連結階層シミュレーションを開発すると共に、超水滴法による雲微物理モデルを使った応用計算を実施した。また、プラズマにおける粒子流体連結アルゴリズムを無衝突衝撃波の研究に応用した。また、オーロラ発生とフレア爆発に関する大規模モデルの開発もそれぞれ実施した。さらに、パッチダイナミクス手法を利用して分子動力学モデルとSPH法による弾性モデルを連結した、新しい摩擦シミュレーションの開発を開始した。

　これらの研究結果は、マルチスケール研究における連結階層シミュレーションの有効性を示すものである。ハンドシェーキング法によるミクロモデルとマクロモデルの境界連結は、局所性のあるマルチスケール問題に有効であることが示された。また、非局所的問題に関してはパッチダイナミクスを利用した新たな階層連結手法の有効性が試されている。今後は、これらのアルゴリズムをより現実的な問題へ応用することにより、本プロジェクトを連結階層シミュレーションの実用可能性を実証する研究へ発展させる予定である。

キーワード：連結階層シミュレーション, マルチスケール, マルチフィジックス, 超水滴法, 地球シミュレータ