Development of Macro-Micro Interlocked Simulation Algorithm

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The Macro-Micro Interlocked (MMI) simulation, which is performed by the mutual connection between the different numerical models for macroscopic and microscopic process, is believed to be a prospective methodology for the numerical simulation of multiscale phenomena in different fields. We have advanced the development of the MMI simulation algorithm for the applications of cloud/atmospheric coupling, plasmas, combustion, friction, fracture, and reaction-diffusion processes. In particular, the applicability and the feasibility of particle/continuum connection models were investigated for the particle acceleration on collision-less shock, and the detonation dynamics. Also the particle-based could simulation was extended to the large-scale three-dimensional model, and the molecular dynamics simulation for friction and fracture was improved to simulate the complex structure on a friction boundary. All the results demonstrate the effectiveness and the flexible expansibility of the MMI simulation. The collaboration for the MMI simulations is also extended for the interaction between macro and micro economics, and the numerical modeling of space weather forecast.

Keywords: Macro-Micro Interlocked Simulation, Multi-scale, Multi-physics, plasma, cloud, combustion, friction, fracture,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, bio-science and so on. Computer simulation is usually constructed on basis of the theoretical description usually using the partial differential equation, and thus the applicability of each simulation model has to be constrained by the basic theory and is limited only to some range of scale, although vastly different scales are mutually interacted in multi-scale phenomena.

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 [1, 2]. 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 for relevant phenomena when and where the macroscopic approximation, such as the thermal equilibrium in fluid dynamics, was broken down, and it gives the accurate information to macro-simulation. On the other hand, macro-simulation can provide the environmental information for the micro-simulation, which is carried out only in a compact region embedded in the macroscopic domain. By optimizing the information exchanged between the micro and macro models, the MMI simulation could greatly reduce the computational demand for the multi-scale simulation.

The primary objective of this project is to develop the MMI algorithm for different physical processes, aiming to demonstrate the applicability and the feasibility of the MMI simulation. So far, we have developed the several models for cloud, plasmas, combustion, friction, fracture, and reaction-diffusion processes, respectively. In this fiscal year 2007, we have continued the development of these models, and extended the applications. The detail report for each topic will be described below.

2. MMI Simulation of Cloud-Atmosphere Coupling

Although clouds play a crucial role in atmospheric phenomena, the numerical modeling for the cloud and atmosphere coupling 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 less demanding cost in computation [3]. A simple SDM for warm rain, which incorporates sedimentation, condensation/evaporation, stochastic coalescence, was established. The methodology to couple SDM and a non-hydrostatic atmospheric model was also developed.

In 2007 FY, we have optimized our simulation code for massively parallel computation and performed the very high-resolution three-dimensional simulation of a shallow maritime cumulus formation (Fig. 1). For this simulation, 624 ×1024 × 1024 spatial grids and 10^{10} computational particles (super-droplets) are included, and it is parallelized by 256 nodes of the Earth Simulator. In our cloud resolving model, the super-droplet microphysics model is coupled to a version of compressible non-hydrostatic model. The validation of the simulation results was performed by comparing with the cloud experiments.

3. MMI Simulation of Plasmas

Plasma inherently forms a multi-scale system, because it consists of different components; ions and electrons. Each the species and the coupling of them generate several characteristic scales corresponding 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. Different 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 performed 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 [4]. In this year, we have developed the three kinds of the interlocked plasma simulations, which are for the particle acceleration on a collisionless shock, auroral arc formation, and solar eruption, respectively [5].

Collision-less shock is believed to be an important accelerator of energetic particles, which are often observed in space and astrophysical plasmas. The fully kinetic approach is necessary for the understanding how the energetic particles are extracted from the thermal population. It is called the injection problem. However, the numerical simulation based on the fully kinetic approach is quite demanding, because the calculation cost is much expensive. On the other hand, because the full kinetics is necessary only around the shock transition region, it is not necessarily needed to calculate the far upstream region by kinetic model. Therefore, we can apply our interlocked simulation model to the shock acceleration process. Our interlocked model of shock consists of the two different hybrid models, which are mutually connected. One is Ion-Particle Hybrid simulation (hereafter Hybrid), in which all ions are kinetically treated, and the another is Energetic-Particle Hybrid simulation (hereafter EP-Hyb), in which only non-thermal energetic ions are kinetically treated and thermal component is treated as fluid.

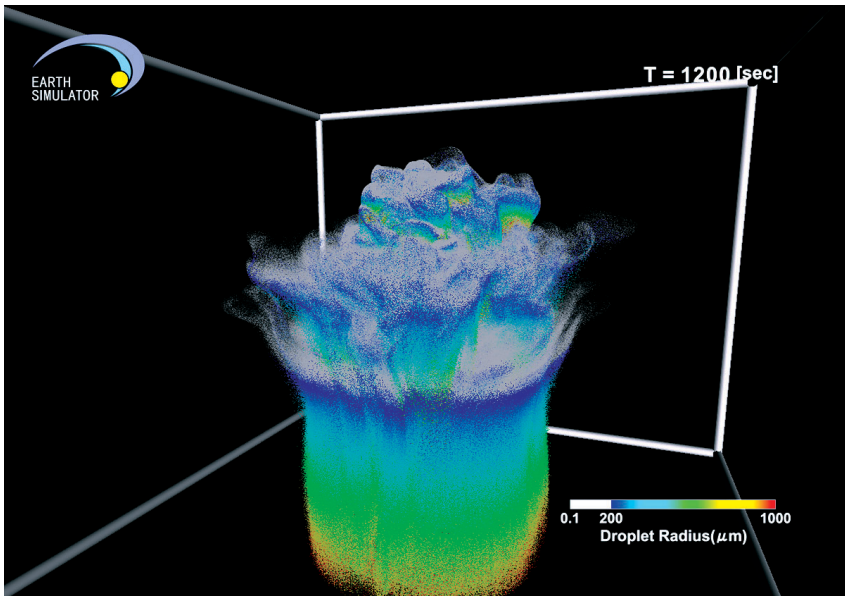

Fig. 1 3-D Simulation of a shallow maritime cumulus formation and precipitation using a coupled model of the Super-Droplet cloud microphysics model and a non-hydrostatic model. This figure was visualized using the special scheme for super-droplets, which has been developed by a collaboration with the Advanced Perception Research Group of the Earth Simulator Center.

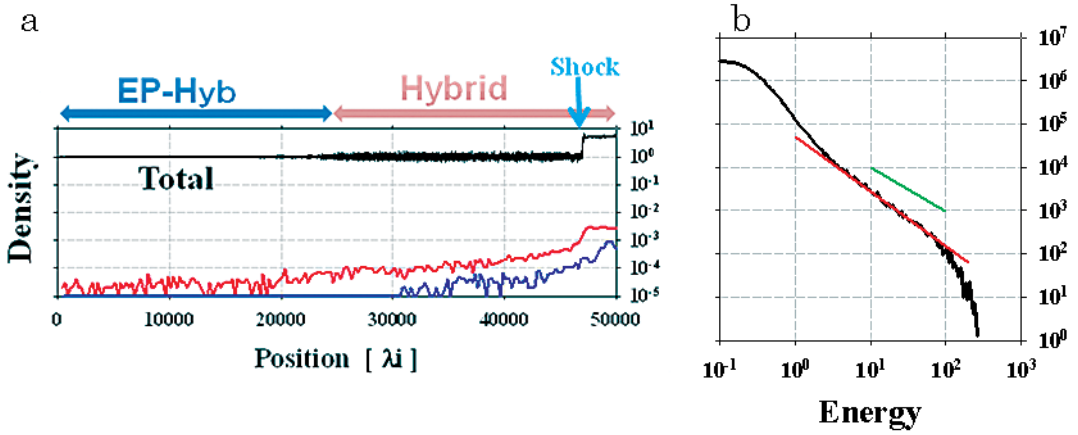

Fig. 2 a: Results from the plasma interlocked simulation of 1D shock process. Black curve represents the distribution of magnetic field, and blue and red curves indicate the density of energetic particles for the initial and the late phases on calculation, respetively. b: Energy spectrum observed in the downstream region of the 1D shock simulation (black lines). The energy is normalized by the shock ram energy. Power-low index is about 1.2 (red line) which is a little bit softer than the index predicted by the DSA theory (green line).

Since energetic particles are only a small fraction compared to thermal component, if thermal ions is replaced by a fluid, we can dramatically reduce the calculation cost. Since the full ion kinetics is necessary only around the shock transition region, the interlocked model is quite useful.

Figure 2a shows the spatial density profile of the 1D simulation system. As shown at the top of the figure, the two different models are connected, and shock is located at the position indicated by the light-blue arrow, where the upstream is the left side of that. Black and red lines show the energetic particle density at the early and late phases of calculation, respectively. As a result, we obtained a power-low energy spectrum in the downstream region, as shown in Fig. 2b. The power-low spectrum indicates the efficiency of the MMI simulation, because it is consistent with the prediction of the diffusive shock acceleration (DSA) theory.

The second subject for the plasma application is solar weather dynamics caused by solar flare eruption. Solar flares and coronal mass ejections (CMEs) are one of the most energetic explosion in the solar system, and they result from the explosive liberation of magnetic energy stored in the solar corona. However, the trigger mechanism of solar flares and the physical relationship between flare and CME are still puzzled, although the accurate modeling of them is strongly required for the forecasting of solar weather disturbance onto geo-space electromagnetic environment.

In this FY, we have started the simulation study to establish the advanced modeling of space weather processes, based on the interlocked technique. We have developed three different simulations, which are able to calculate the trigger of solar flares, the formation of CMEs, and the propagation of them, respectively. As a result, we have successfully performed the first-ever data-driven simulations of solar flare onset and the CME formation, using the data provided by Japanese solar observation satellite HINODE (see Fig. 3). The numerical experiments of the interlocked simu-

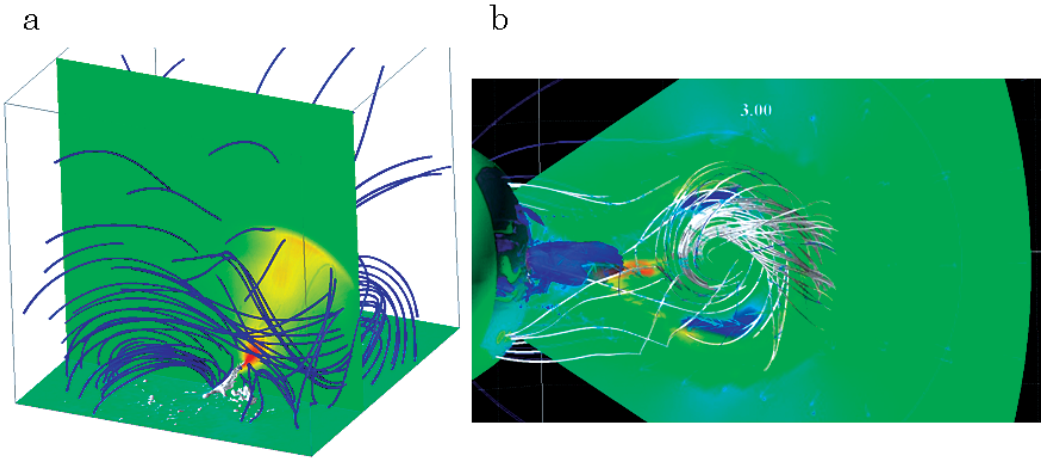

Fig. 3 The results of the data-driven simulations for (a) the solar flare onset and (b) the CME formation. The three-dimensional structure of magnetic field lines is represented with the color scale (blue to red) showing plasma flow speed.

lation, in which all the models are connected to reproduce the consecutive dynamics in the solar and terrestrial connection system, remains as the subject for the next year.

Also the process of quiet auroral arc formation was investigated by the MMI simulation as the another topic of plasma application. The large-scale structure of quiet auroral arc is thought to be formed as a result of the macroscopic interaction between magnetosphere and ionosphere. Ionospheric feedback instability was believed as one of the candidate to explain that. However, auroral energetic electrons, which excited the emission lines in aurora, have to be accelerated by an electrostatic double layer, which should be created by kinetic process in micro-scale instability like the ion-acoustic instability. 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 three years (FY2004–2006).

In this fiscal year, we adopted rigorous ionization and excitation models to the holistic simulation code and investigated the role of accelerated particles in arc formation with this code. The left panel of Fig. 4 shows the distribution of field aligned current density at the top of ionosphere (the color becomes more reddish as the upward current increases and more bluish as the downward current increases). In this panel, there is an intensive current area in 20:00 local time. This longitudinally striated structure was created by the effect of auroral energetic electrons. These electrons ionized atmospheric particles, and increase the ionospheric plasma density. The growth of plasma density enhances the ionospheric conductivity. Therefore, the field aligned current becomes more intensive. The emission intensity is also obtained from the energy spectrum of auroral electron. Right panel of Fig. 4 represents the distribution of the oxygen green line (557.7nm) emission intensity at 110–130 km altitude.

4. 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.

Using the MMI model for the detonation, which had been developed in the last year, we have analyzed the velocity distribution function to clarify the effect of non-thermal particle on the detonation. Figure 5a shows the reaction rate coefficient as a function of temperature defined by the averaged translational energy. The Arrhenius value used in the

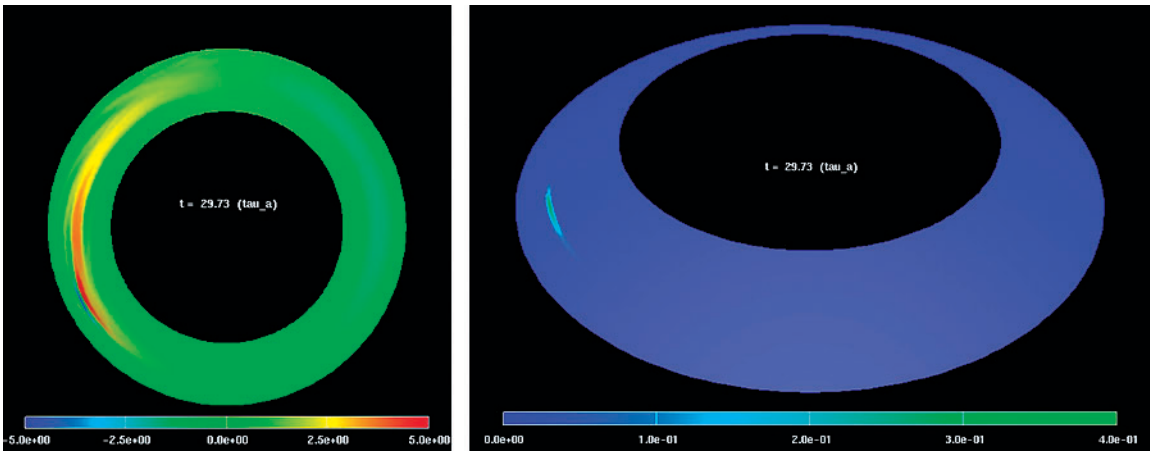

Fig. 4 The result of holistic auroral arc simulation. Left: The distribution of field aligned current density at the top of ionosphere. Right: the distribution of the green line emission intensity.

continuum fluid simulation is also plotted for comparison. This plot shows that the reaction rate coefficient is not a function of temperature due to kinetic effects. In Fig. 5b, we also show the rate coefficients as a function of distance from the wave front. This figure reveals that the reaction proceeds faster than the fluid approximate on the shock front, and reaction occurs even in the upstream region of the shock front where the reaction rate from Arrhenius' formula almost vanishes. These results demonstrate that the fluid description is not valid for the reaction in the vicinity of the detonation front, and the MMI simulation is effective [6].

After some improvement of the computational algorithm and the simulation code, we developed the 3-dimensional particle-continuum interlocked simulation of a gas detonation as shown in Fig. 6. It is shown that complex cell structure caused by interaction of triple lines is reproduced by this simulation.

5. MMI Simulation of Friction and Fracture

Friction and fracture are typical multi-scale phenomena where molecular dynamics and continuum mechanics (elastic dynamics) are strongly coupled. We are developing a macro-micro interlocked simulation scheme, where the two types of simulations run simultaneously exchanging necessary information. For example, in fracture problems, the strain calculated by elastic dynamics simulation is given to molecular dynamics as a boundary condition and then the stress calculated by the molecular dynamics (MD) simulation is used to construct a constitutive law for the elastic dynamics simulation. In this scheme, larger-size MD simulation is needed to give more precise information to elastic dynamics simulation. Therefore, in this fiscal year, we have concentrated on developing a platform for massively paralleled simulation of molecular dynamics. Figure 7 shows a test simulation result of mode I fracture in Lennard-Jones materical, where 10^7

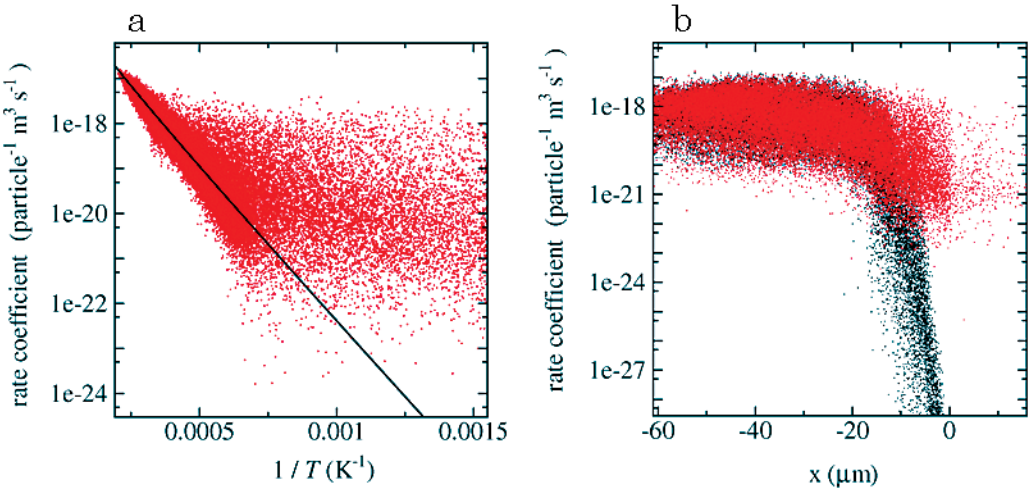

Fig. 5 The reaction rate coefficient plotted as a function of (a) temperature and of (b) position originated at the detonation front. Arrhenius value is also plotted by (a) solid line and (b) black dots.

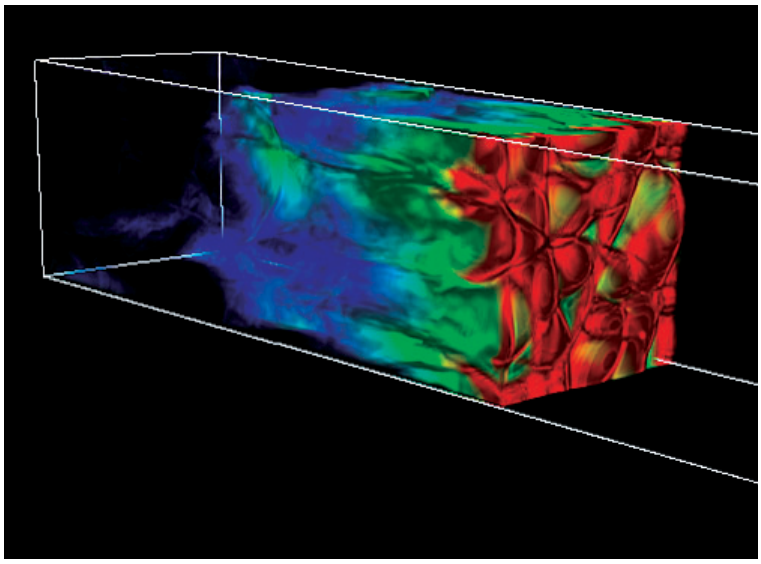

Fig. 6 Pressure distribution in the MMI simulation for detonation.

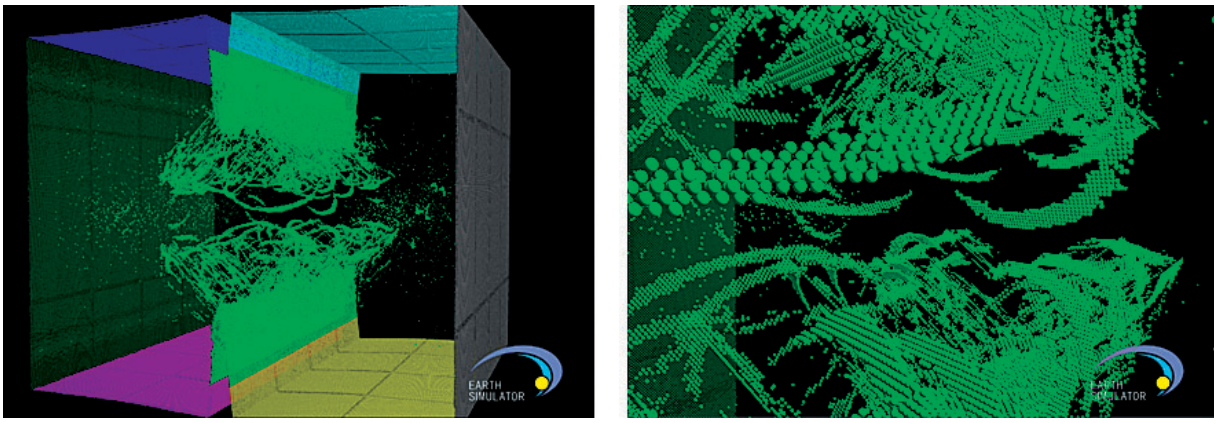

Fig. 7 Molecular dynamics simulation of fracture in Lennard-Jones material. Only atoms of larger potential energy are drawn to show dislocations developing from the tips of cracks. Right panel is a zoom-in view of left.

atoms are incorporated. We have also developed the large-sized MD simulations of friction, where we observed a very complicated interface consisting of many slip surfaces, which cannot be seen in the previous small-sized simulations, appears on a friction region. More extensive work on these microscopic features with large-sized MD simulations are needed to improve our MMI simulation scheme.

6. MMI Simulation of Oscillatory Reaction-Diffusion System

Reaction-Diffusion system is a class of partial differential equation which consists of reaction-term and diffusion-term. Though the form of the equation is simple, they exhibit various types of dynamical patterns, and thus they are widely used to model biological and other pattern formation phenomena. The reaction-diffusion systems is a typical subject for demonstrating and developing the MMI simulation methodology.

In 2007 FY, we developed a MMI simulation scheme to simulate oscillatory Reaction-Diffusion system. The scheme consist of the first principle micro-model based on the Complex Ginzburg-Landau (CGL) equation and the macro-model based on the phase-equation, which gives the valid approximation of the CGL equation when the solution approaches to an asymptotic oscillatory phase. Intuitively, however, the phase-equation may not be a good approximation of CGL eq. when any phase singularities are located near by the solution. Our MMI simulation scheme works out with two way communications between the Micro and the Macro region, the former of which covers only the region where the latter cannot work well as the approximation of the CGL equation. Figure 8 shows one of the MMI simulation results. The interaction of two phase singularities is well simulated using the MMI scheme and the result suggests that the MMI simulation methodology is applicable to the simulation of the dynamical pattern formation phenomena that involves phase singularities.

7. Summary

We have instigated the potentiality of the MMI simulation as a new methodology, which should be used to simulate as well as predict the multiscale interaction in different phenomena. We have advanced the development of the MMI simulation algorithm mainly for the physical processes,

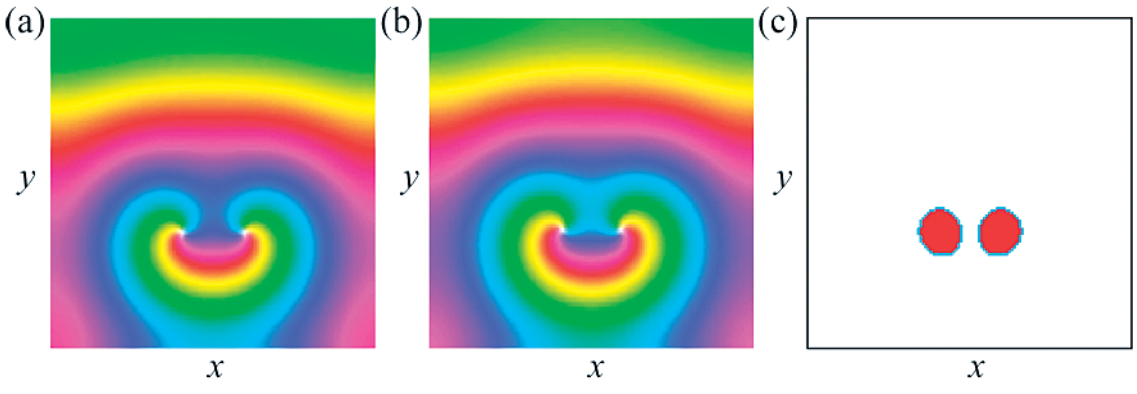

Fig. 8 The simulation results of oscillatory reaction-diffusion system. (a): The result of direct simulation based on the CGL eq. (b) The result of the MMI simulation, and the subset (c) shows the Micro-region in (b) where the CGL eq. is activated automatically. Note that (a) and (b) agree fairly well.

which are relevant to geo-science, space science, material science, and chemistry. However, the applicability of the MMI simulation is not limited only to natural science and engineering. It could be important to investigate the applicability of the MMI simulation to various phenomena related to social sciences as well as ecological science. In fact, we have started the international collaboration with Management School, Lancaster University for the development of MMI economic simulation [7]. This project should be more extended to improve the numerical techniques for the multiscale coupling as well as to deploy them to more practical problems.

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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を複数の計算モデルの連結で捉える「連結階層シミュレーション」は様々な研究分野における新たなマルチスケールシミュレーションの方法論として広く認めらている。我々は地球シミュレータの高速性能を活かし、雲、プラズマ、燃焼、摩擦、破壊、反応拡散系など様々な現象に関する連結階層シミュレーションのアルゴリズム開発を発展させた。その結果、無衝突衝撃波における粒子加速のシミュレーション、デトネーション(爆轟)過程のシミュレーションなどによって、粒子・連続体連結モデルの応用発展性に関する顕著な成果を得ることができた。さらに、超水滴法による本格的な3次元雲形成シミュレーションを実現すると共に、固体間摩擦領域の複雑な原子構造を捉える事ができる大規模分子動力学モデルの開発を行った。また、ランカスター大学との国際共同研究を展開し、マクロ経済とミクロ経済モデルの連結シミュレーション研究に着手すると共に、全国的な宇宙天気モデルリング研究を推進することにより、連結階層シミュレーションの応用性を発展させることができた。

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, プラズマ, 雲, 燃焼, 摩擦, 破壊,
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