Development of Macro-Micro Interlocked Simulation Algorithm

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The Macro-Micro Interlocked (MMI) simulation, which is performed by the mutual connection of computational models adequate respectively to macroscopic and microscopic processes, is an advanced methodology for the multi-scale simulation. The basic algorithms of the MMI simulation have been developed for the typical multi-scale problems. The first-ever first principle simulation of cloud formation and rainfall is realized using the newly developed algorithm named "Super-Droplet method". The interlocking technique between the magnetohydrodynamic (MHD) model and the particle-in-cell (PIC) model is developed for the simulation of magnetic reconnection, and the direct simulation Monte-Carlo (DSMC) method and the HLLC method are applied to the MMI simulation of detonation. The results of them indicate that the MMI simulation can work as an innovative tool for multi-scale study.

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 any state-of-art research fields, such as material science, plasma physics, chemistry, astrophysics, geo-science, bio-science and so on. Although the Earth Simulator is the ideal tool for the analysis of the complicated nonlinear system and for the prediction of evolution of that, the conventional methodology is not adequate for the simulation of the multi-scale phenomena.

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 the basic theory behind. So far, the multi-scale simulations have been developed by the two different manners. The first is the extension of macroscopic simulation, in which the microscopic effects are included as phenomenological parameters, just like the anomalous resistivity in high-temperature plasma simulations and the bulk cloud modeling in the atmospheric simulations. However, the phenomenological parameterization is not guaranteed to work well in unexpected circumstances, and it is not intrinsically able to provide the primitive information of the microscopic mechanism, which should govern macroscopic phenomena.

Another approach is the large-scale microscopic simulation, whereby we try to rebuild the macroscopic phenomena from the elementary block in the micro-scale. The large-scale molecular dynamics (MD) simulation is the typical example of that. However, it is computationally demanding and the applicability of the direct simulation onto practical phenomena is severely restricted even with the incredible capability of the Earth Simulator.

Macro-Micro Interlocked (MMI) Simulation is the new type of multi-scale simulation, which is recently invented by T.Sato (Sato 2005). The principal framework of the MMI simulation consists of the macro- and micro-simulation models and the interconnection between them. The micro-simulation may help the macro-simulation, when the macro-simulation needs further information, which cannot be handled within the macro-simulation itself. On the other hand, the macro-simulation can provide the environmental information to the micro-simulation, which is therefore able to be performed only in a compact region embedded in the macroscopic domain. By optimizing the information handling between the micro and macro scales, the MMI simulation would greatly reduce the computational demand in the multi-scale simulation.

The objective of this project is to develop the algorithms for the MMI simulation and to demonstrate the applicability of that for typical multi-scale problems. In 2005 FY, that is the second year of this project, we focused on the four typical multi-scale problems, cloud-atmospheric coupling, plasma, combustion, and solid dynamics, and have developed the basic algorithms for them.

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

Although clouds play a crucial role in atmospheric phenomena, for instance global warming and heavy rain, the numerical modeling of cloud is not well established yet. The reason of that is attributed to the fact that the formation of clouds and the development of precipitation are essentially governed by mutiscale-multiphysics processes. The macro-scale processes such as the fluid motion of air associated with clouds is called "cloud dynamics" and the micro-scale processes such as the nucleation growth, and coalescence of water droplets are called "cloud microphysics". These two processes mutually affect each other. Numerical methods to simulate accurately both the processes and the interaction of them are required to understand and predict cloud-related phenomena.

Cloud dynamics model to describe the fluid motion of atmosphere has been well developed so far. However, it is still difficult to perform the accurate simulation of cloud microphysics, though several simulation methods, such as bulk parameterization, spectral (bin) method, and exact Monte Carlo method, have been proposed.

We newly develop a novel simulation model of cloud microphysics, named Super-Droplet Method, which enables accurate calculation for the dynamics, nucleation, and coalescence of all droplets with reasonable cost in computation. The methodology for the coupling between the super-droplets and the non-hydrostatic cloud dynamics is also developed. The practicality of this new cloud model is demonstrated by the regional simulations of cloud formation and precipitation (see Fig. 1). The new model could be useful for weather forecast, the optimization of artificial rain, and the accurate prediction of global warming.

3. MHD-PIC Interlocked Plasma Simulation

Plasma is inherently multi-scale system, in which there are different characteristic scales related to electron and ions. Magnetic reconnection, which is widely believed as a key mechanism for the explosive energy conversion in high-temperature plasmas such as solar flares, is one of the typical multi-scale phenomena.

The key issue in reconnection physics is how the macroscopic plasma dynamics as magnetized fluid is related to the microscopic particle motion in the reconnection region, which is formed on magnetic neutral line when anti-parallel magnetic fluxes collide with each other. We develop the new algorithm, which can handle the microscopic plasma kinetics in a limited area like the diffusion region. It consists of the connection of the particle-in-cell (PIC) model and the magnetohydrodynamic (MHD) model, the former of which is embedded in the MHD simulation domain.

The MHD-PIC Interlocked Simulation can well manage both the kinetic effects in the diffusion region and the MHD system evolution. The interlocking between the two models is performed by connecting the electric field, which is derived by the generalized Ohm's law in the MHD model and by the Ampere's law in the PIC model, respectively.

Figure 2 shows the preliminary results of the test-simulation, in which left panel indicates the initial condition of the solitary Alfven wave in X (horizontal)-Y (vertical) plane. The ambient field directs into positive X direction (right). Y-component of the magnetic field is plotted in the color scale con-

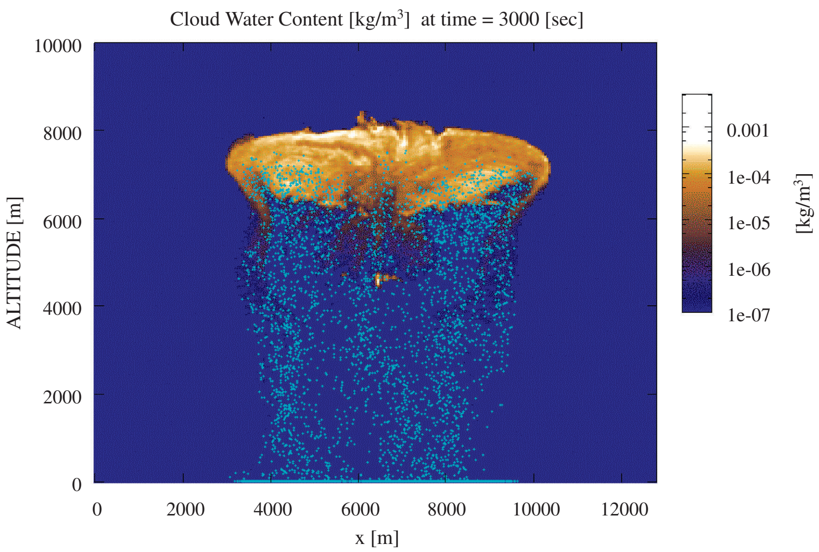

Fig. 1 A novel simulation result for cloud formation and rainfall using the "Super-Droplet Method". It is the first-ever first principle cloud simulation, which is able to resolve the motion, condensation, and coalescence of each droplet.

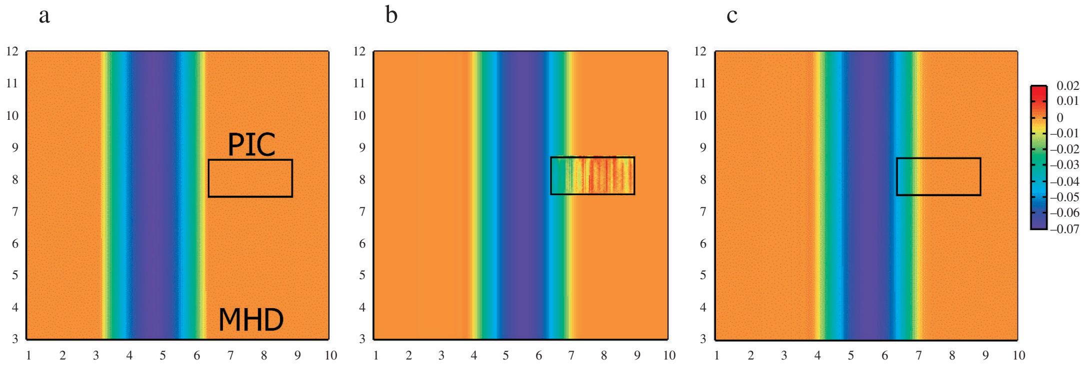

Fig. 2 The distribution of magnetic field variation in the test simulation of the MHD-PIC interlocked model. Alfven wave propagates smoothly into PIC simulation region.

tour (left panel). As time goes, the wave propagates into right direction. On the head of wave, there is the PIC simulation area noted by black rectangle. Even though the solution of the PIC simulation is noisy due to microscopic wave effects (middle panel), we can well calculate the smooth propagation of the MHD wave by the interlocked model (right panel), if the electric field calculated by the PIC model is sent back to the MHD model through some adequate low-pass filter.

4. Interlocked Simulation of Detonation

Combustion fluid dynamics is a typical subject of the macro-micro interlocked simulation, in which the microscopic reaction is mutually interacted with the macroscopic flow dynamics. Especially, in detonation, which is combustion sustained by the interaction between a combustion wave and a shock wave, the multi-scale coupling is crucially important, because the spatial gradient of physical quantities such as temperature and density become so steep in the detonation front that the local thermal equilibrium cannot be maintained, and the macroscopic description of combustion based on the Arrhenius rate law is broken down.

We have been developing a novel method for simulation of combustion connecting a microscopic molecular model and a macroscopic continuum model. In this fiscal year, we have developed each model of the macro and micro simulations and started to research an algorithm to connect them.

Our macro-micro interlocked model consists of a microscopic molecular model based on the Boltzmann equation and a macroscopic continuum model based on the Navier-Stokes equation. We use non-steady direct simulation Monte Carlo (DSMC) method for the molecular model. The continuum model is integrated by the HLLC method and the point-implicit method is applied for the source terms.

The demonstration of the two-dimensional molecular simulation of detonation is shown in Fig. 3. The algorithm to connect the molecular model and the continuum model is summa-

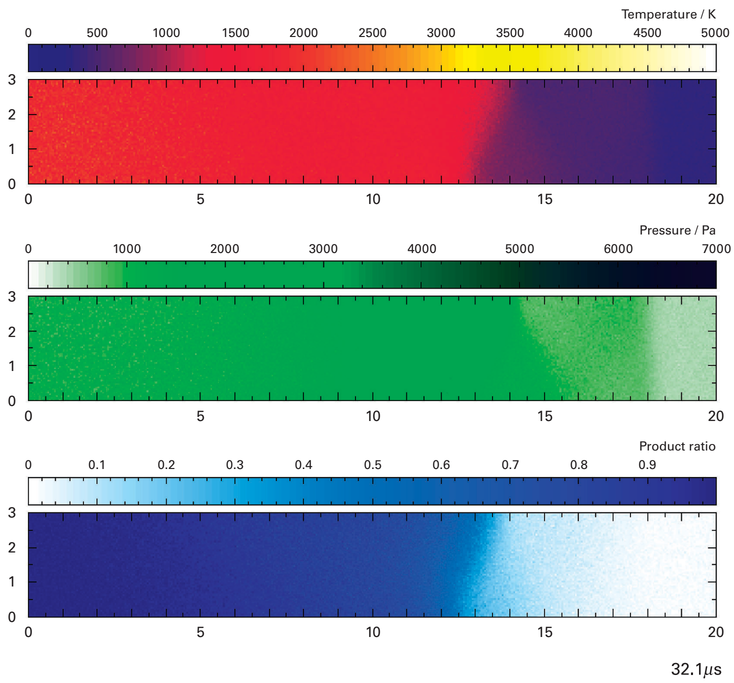

Fig. 3 The results of simulation of detonation formation using DSMC model. Panels from above indicate the distribution of temperature, pressure, and product ratio.

rized as follows: (1) Gradients of physical quantities are monitored during the simulation by the continuum model, and the molecular model is embedded in the region where the gradients exceed some threshold and the continuum model is failed. (2) Interlocking layers are laid around the outer-most region of the molecular domains. The whole system is simulated by sharing the statistical mean values of chemical density, temperature, and energy between the molecular and continuum models in the interlocking layers. The implement of the connection model and the application of that to practical engine design are planed in the next fiscal year.

5. Solid Dynamics as Multi-scale Phenomena

Solid fracture is one of the typical problems for the application of the macro-micro interlocked simulation. Microscopic simulation by molecular dynamics (MD) model may provide ab initio information about crack tip formation, while macroscopic simulation by continuum model can determine stress distribution around cracks. Since the two dynamics depend strongly on each other, one needs to solve them simultaneously and connect them in a consistent way. Usually the connection is done in a handshaking region where the solution is given by some kind of average of the micro and macro solutions. This method, however, limits the time and length scales to those of the micro simulation, and to overcome the limitation will be the key for the practical use.

This year, as the first step to develop the macro-micro interlocked simulation for solid fracture, we performed various test simulations in both micro and macro scales (see Fig. 4): (i) molecular dynamics simulation with Lennard-Johns potential, (ii) continuum mechanics simulation using moving particle semi-implicit method and (iii) continuum mechanics simulation based on the phase-field model.

6. Summary

The MMI simulation algorithms for the four different multi-scale problems have been developed. The particle-continuum connection technique is the kernel for the MMI simulation of these problems, and we have invented the new methodology for that in the cloud, plasma and combustion simulations. They will be applied to more practical problems in the next fiscal year to demonstrate the operability and the effectiveness of the MMI simulation.

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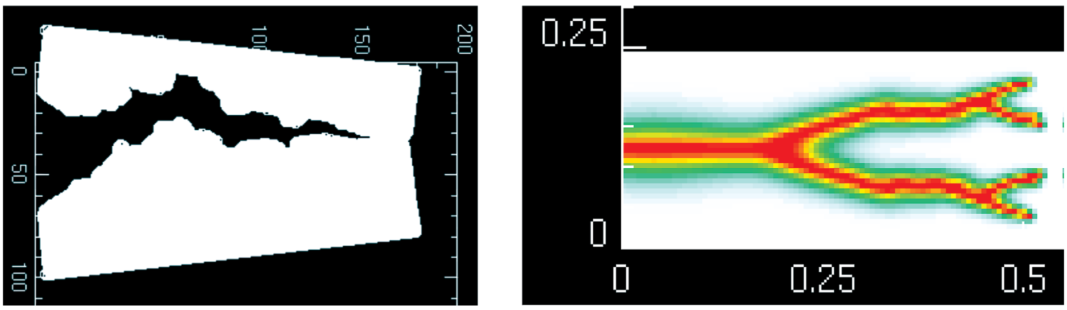

Fig. 4 Test simulations of mode-I fracture. Left: Molecular dynamics simulation with the Lennard-Johns potential. Right: Grid-based (finite difference) simulation using phase-field model.

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クローズアップされている。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、異なる階層の効果を境界条件や経験的なパラメターとして取り込まなければならず、マルチスケール問題を第一原理的に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はなく、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し、マルチスケール問題に対する一般的な方法論を確立することにある。

本年度は、雲微物理を含む大気力学、プラズマ爆発現象とオーロラ発生、高速燃焼流体、固体破壊など典型的なマルチスケール問題に注目し、それらに対する基盤的な連結階層アルゴリズムの開発をそれぞれ進めた。その結果、独自に開発した「超水滴法」を使い、雲生成と降雨に関する第1原理シミュレーションに初めて成功した。また、MHDモデルとPICモデルの連結による磁気リコネクションのシミュレーション、DSMC法とHLLC法の連結によるデトネーションのシミュレーションに関する基礎ソフトウェアの開発を実現した。

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実現可能性を示すものである。今後は、パルスデトネーションエンジンの設計などより現実的な問題への応用研究を進め、連結階層シミュレーションの実問題に対する有効性を実証するための研究を発展させる。