Competition and Synergy of Macro- and Micro-scale Physics – Status and Prospects of Macro-Micro Interlocked Simulation –

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Multi-scale phenomena are now crucial issue in the wide range of research fields, not only plasma physics, but also chemistry, astrophysics, geo-science, bio-science and so on. For the last decade, aiming to understand the interaction between macro-scale and micro-scale dynamics, several new methodologies for numerical simulations have been quickly developed. Macro-Micro Interlocked (MMI) Simulation is one of such new simulation frame-works. The MMI simulation is performed by the two-way connection of different numerical models, which may handle macroscopic and microscopic dynamics, respectively. The application of the MMI simulation to different multi-scale phenomena, for instance, cloud formation, gas detonation, and plasma dynamics, is investigated. The results of all the applications demonstrates that the MMI simulation is a prospective methodology for multi-scale studies.

Keywords: multi-scale, simulation, plasma, cloud, detonation

1 Introduction

Multi-scale phenomena, in which the micro-scale elementary process and the macro-scale system dynamics mutually influences each other, are now a crucial issue in vastly different research fields, not only plasma physics, but also chemistry, astrophysics, geo-science, bio-science, material science, mechanical engineering, and so on. However, fundamental difficulty arises for the research of the multi-scale processes, because physical processes in different scales are governed by different physical laws, for instance, the molecular dynamics in micro-scale and the continuum dynamics in macro-scale.

Although computer simulation must be a powerful tool for the understanding and the predicting the complex nonlinear phenomena, the applicability of simulation cannot get rid of restriction of the scale, because computer simulation is usually formulated on the basis of the theoretical description like partial differential equations, which is valid only in some limited scale. Therefore, the applicability of each simulation model is also limited to the scale where the basic theory is valid.

To conquer this limitation, several new frameworks are proposed recently. So far, the multi-scale simulations have been developed by 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 caused by micro-scale turbulence in high-temperature plasmas and the bulk cloud parameterization in atmospheric global circulation model. However, since the phenomenological parameterization is not guaranteed to work well in unknown circumstances, the applicability of such a method must be restricted by given knowledge.

Another approach is the large-scale microscopic simulation, whereby the macroscopic phenomena are attempted to be built from the elementary block of micro-scale processes. The large-scale molecular dynamics (MD) simulation is the typical example of that. However, it is computationally so demanding. Since the scale which we can directly calculate with the MD model is limited to the order of micron meter, even using the world largest super-computer [4], we need the 10^{24} ($= 10^{6 \cdot 4}$) times faster computational capability than the current super computer. It would not be feasible at least in near future.

The limitation of the computational feasibility requires that a new type of software and mathematical frame-work should be developed to conquer the difficulty of multi-scale simulation. In fact, several new numerical models have been proposed recently for this purpose. One of the most promising concept is given by the interconnection of different numerical models. [1] developed a new way to make the interconnection between the finite-element, molecular dynamics and semi-empirical tight-binding

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representations, and demonstrated that the connection model, called MAAD (macroscopic, atomistic, ab initio dynamics), is effective as the methodology for the study of brittle crack propagation in silicon. On the other hand, [13] proposed the concept of heterogeneous multi-scale method (HMM) as a general methodology for multi-scale modeling. In the HMM, scale separation is exploited so that coarse-grained variables can be evolved on macroscopic spatial/temporal scales using data that are predicted based on the simulation of the microscopic process. Similar model was proposed also for meteorological simulation, which is called "super-parameterization," by [3] and [7]. Super-parameterization is performed by the mutual connection between atmospheric global circulation model (AGCM) and cloud system- resolving (CSR) model. In the super-parameterization, the CSR models are embedded inside each grid cell of AGCM, and the results of them are used for the cloud parameterization of AGCM.

Macro-Micro Interlocked (MMI) Simulation was proposed by [8] as a new methodology for the multi-scale simulation. The fundamental principle of the MMI simulation is in common with the heterogeneous multi-scale method (HMM) and the super-parameterization. The MMI simulation consists of the macro- and micro-simulation models, which are carried out simultaneously and interconnected to each other. The micro-model is performed under the environmental condition calculated by the macro-model, and the microscopic information is fed back to the macro-model [6]. Originally, the MMI simulation has been proposed as a computational algorithm suitable to the hardware of heterogeneous architecture, called MMI simulator, in which different types of architecture fitting respectively to the numerical models of macro- and micro-scales are interconnected. In particular, heterogeneous vector/scalar architecture is the most promising design of the MMI simulator, and we have developed several applications for that.

The objective of this paper is to present the brief review of the application study of the MMI simulation. In the following section, we will explain the principle and the typical results of each MMI simulations for cumulus cloud formation, gas detonation, and plasma dynamics. Finally, the prospects of the MMI simulation will be summarized in Sec.3.

2 Applications

2.1 Cloud Simulation

Although clouds play a crucial role in any meteorological phenomena like global warming, 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 multiscale-multiphysics processes. The macro-scale processes such as the fluid motion of moist air associated with clouds is called "cloud dynamics", and the micro-scale processes such as the condensation and coalescence of water droplets are called "cloud microphysics". These two processes mutually affect each other.

Although the cloud dynamics simulation has been quickly developed with the achievement of large-scale fluid model, the first-principle simulation of cloud microphysics is still difficult. It is due to the fact that huge number of tiny droplets are involved in cloud processes. Therefore, some empirical approximation called 'bulk-parameterization' has been widely used for cloud modeling. However, the applicability of any empirical model is restricted as mentioned in Sec.1, and we cannot use it for the prediction of unknown phenomena like global warming.

Aiming to overcome this difficulty in the cloud modeling, we recently developed a novel simulation model of cloud microphysics, named Super-Droplet Method (SDM) [10], which is a particle-based cloud microphysics model. The *super-droplet* is defined as computational particle representing multiple real droplets, which have common properties, *e.g.* position, velocity, cloud condensation nuclear (CCN), and electric charge. The motion of each super-droplet is calculated by the equation of motion or by the assumption that each droplet immediately attains terminal velocity. The condensation and the evaporation of droplets can be directly calculated based on Köhler's theory using the properties of super-droplet and the state variable of atmospheric environment. The coalescence of droplets is handled by the stochastic manner just like the Direct Simulation Monte-Carlo (DSMC) method.

The cloud dynamics is simultaneously calculated with SDM using the non-hydrostatic model equations,

$$\rho\frac{D\vec{U}}{Dt} = -\nabla P - (\rho+\rho_w)\vec{g} + \lambda\nabla^2\vec{U}, \tag{1}$$

$$P = \rho R_d T, \tag{2}$$

$$\frac{D\theta}{Dt} = -\frac{L}{c_p\Pi}S_v + \kappa\nabla^2\theta, \tag{3}$$

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\rho, \tag{4}$$

$$\frac{Dq_v}{Dt} = S_v + \kappa\nabla^2 q_v, \tag{5}$$

where ρ is the density of moist air, ρ_w the density of liquid water, $\vec{U}$ the wind velocity, P the pressure, λ the viscosity, R_d the gas constant for dry air, T the temperature, θ the potential temperature, L the latent heat, q_v the mixing ratio of vapor, S_v the source of water vapor, and Π is the Exner function, respectively.

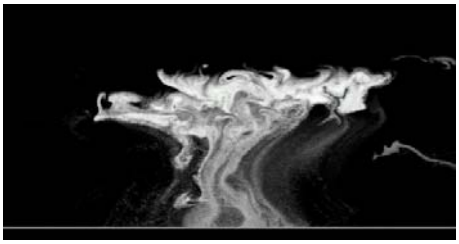

Fig. 1 The simulation results of cloud formation and precipitation using the super-droplet models. Horizontal line on the bottom indicates ground level, and gray-scale represents the cloud droplets.

The density of droplets

$$\rho_w(\vec{x},t) = \sum_i \xi_i m_i(t) w(\vec{x},\vec{x}_i),$$

and the conversion ratio between vapor and liquid

$$S_v(\vec{x},t) = -\frac{1}{\rho(\vec{x},t)}\frac{\partial \rho_w(\vec{x,}t)}{\partial t},$$

are sent to the fluid model, and used in the source terms, where i is the index of super-droplet, ξ_i the multiplicity of super-droplet, m_i the mass of droplet, and w is the shape function of super droplet.

The algorithm of SDM, in which particles (droplets) and fluid (moist air) interact with each other, is basically same as particle-in-cell (PIC) plasma simulation, in which particles for electron and ions interact with electromagnetic fields assigned at cells. It is also similar to the plasma simulation that each super-droplet represents multiple number of real droplet.

In order to demonstrate the feasibility of SDM, it has been applied to the simulation of cloud formation and precipitation in maritime cumulus. The simulation system is given by 2-dimensional $x-z$ domain just for simplicity. The initial state consists of un-saturated stratified layer, which is slightly unstable only under 2km in altitude, and number of tiny droplets, which contain soluble substance as Cloud Condensation Nuclear (CCN), are uniformly distributed in the entire domain. As shown in Fig.1, the results indicate that the particle-continuum coupled model may work to simulate the whole process from cloud formation to precipitation without introducing any empirical parameterizations. The new model may provide a powerful tool for the study of cloud-related various problems, although the predictability of SDM should be evaluated more carefully.

2.2 Detonation Simulation

Combustion fluid dynamics is also the typical subject of multi-scale simulation, in which chemical reaction is mutually interacted with the macroscopic flow dynamics. In the conventional methods, the reaction is treated by the Arrhenius rate equation. However, the reaction rate of the equation must be derived from the distribution function assuming local thermal equilibrium (LTE). Although the LTE assumption could be satisfied in normal condition of fluids, when the local Knudsen number, which is defined as the ratio of mean free path to characteristic length scale, is larger than 0.01, the assumption of LTE may not be valid. In the case, the flow should be treated as rarefied gas and we have to solve the Boltzmann equation. Especially, detonation, which is sustained by shock wave driven by combustion wave, is the case, because the thickness of shock may be comparably thin as the mean free path. It implies that the Arrhenius rate equation may not be valid on the shock front.

So, we have developed a novel method for simulation of combustion by connecting a microscopic molecular model and a macroscopic continuum model, those are based on the Boltzmann equation and the Navier-Stokes equation, respectively. We adopted non-steady DSMC method for the molecular model, and the continuum model is carried out by the HLLC method.

Our detonation model is an extension of Hybrid Continuum-Atomistic Simulation, which has been developed by many authors [2, 14, 9]. The algorithm to connect the molecular model and the continuum model is summarized as follows: (1) Gradient of pressure is monitored during the simulation by the continuum model, and the molecular model is embedded in the region where the steepness exceed some threshold and the continuum model is failed. (2) Interlocking layers are laid around the outer-most region of the molecular domains, where particles are generated to let the distribution function be able to represent the macroscopic variables; density, velocity and pressure. Numerical flux on the outer-most boundary of the continuum domain is calculated from the particle motion.

Some result of the two-dimensional detonation simulation is shown in Fig.2. It represents the distribution of pressure on the detonation front. The domain between dotted lines corresponds to the region, where the particle-based model is adopted. The smooth connection between fluid and particle-based models indicates that the continuum-atomistic simulation is applicable also to the combustion process.

2.3 Plasma Simulation

Plasma inherently forms a multi-scale system, in which different characteristic scales related to electron and ions mutually interact. The key issue in multi-scale plasma processes is how macroscopic magneto-hydrodynamics (MHD) is related to microscopic particle kinetics. For instance, in magnetic reconnection

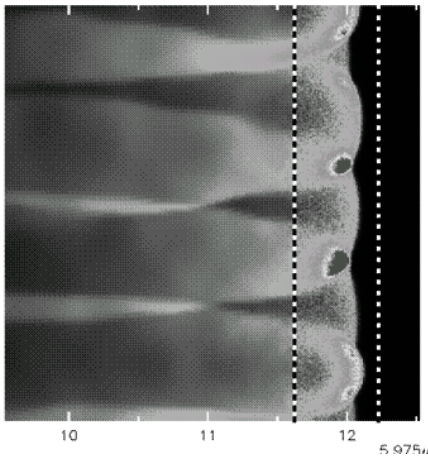

Fig. 2 The pressure distribution of the detonation simulation. The particle-based domain, which corresponds to the region bounded by dotted lines, tracks the detonation front.

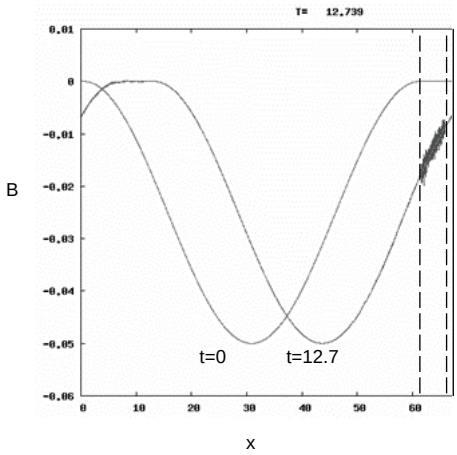

Fig. 3 Magnetic field distribution in the test simulation for Alfvén wave using the PIC-MHD interlocked model. The region between two dotted line corresponds to the part where PIC model is embedded.

that is responsible for explosive energy release in high-temperature plasmas, the kinetics might be important especially in the restricted diffusion region, which is formed when anti-parallel magnetic fluxes collide each other.

So, we have developed the new algorithm for such a multi-scale plasma dynamics. Our model is constituted by 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[11]. This MHD-PIC interlocked model is resembled to the continuum-atomistic simulation, which was explained in the previous subsection. However, it should be mentioned that, in plasma simulation, several characteristics described by PIC model are negated in continuum (MHD) model, in contrast to the hydrodynamic simulations. So, in order to make the smooth interlocking between MHD and PIC models, we have to introduce some special filter, which passes only the MHD mode from the PIC domain to the MHD domain. The filtering process is actualized by the sophisticated sub-cycle procedure. Refer to [11] for the detail.

Figure 3c shows the magnetic wave form in the test-simulation for the one-dimensional Alfvén wave propagation. In this simulation, PIC model is embedded only in a small part of the simulation box, and we examined whether long wavelength Alfvén wave can smoothly propagate in the interlocked system of PIC and MHD. The figure shows that the wave form is scarcely affected by interlocking with the PIC model, as high-frequency modes appear in the PIC domain. It indicates that the particle-continuum connection model is applicable also to plasma simulations.

Recently, [12] applies the interlocked technique to connect different hybrid simulations for the study of particle acceleration on plasma collision-less shock. In that study, the conventional hybrid simulation, in which ions are calculated by particles, is used for the calculation of particle acceleration in shock and is connected to the energetic particle hybrid simulation, which calculates only high energy ions as particles and handles the thermal ion as fluid. Since the computational cost of the energetic particle hybrid model is much cheaper than the ion particle hybrid model, we can dramatically reduce the computational demand using the new interlocked plasma simulation, and it enables the macroscopic plasma simulation including kinetic effects.

3 summary

Three different applications for the MMI simulation are demonstrated. In any examples, the particle-continuum connection technique plays a crucial role. However, it is worthwhile to note that the particle-continuum connection in the cloud simulation is not based on the domain decomposition method, but the application of particle-in-cell technique, unlike the other two applications of plasma and detonation, because cloud is ubiquitous phenomena and we cannot restrict the cloud domain into a limited region. It is a new challenge to embed the cloud microphysics model into the atmospheric global circulation model.

Although the MMI technique is much effective for the multi-scale simulation, in which the micro-scale model is necessary in a limited region, the gap of time-scale between the macro-scale and micro-scale processes is still issue to be resolve, because the micro-scale model is usually time-consuming and it is difficult to calculate the two different models simulta-

neously. Several new technique to fulfill the time-scale gap is now proposed. For instance, equation-free method proposed by [5] tries to accelerate the time integration using extrapolation technique based on the micro-scale calculation.

The MMI simulation is now opening a new world of simulation science, because the new numerical model can cast off the restriction of theoretical description. The MMI simulation is applicable to vastly wide range of fields, and some common technique can be used for the model of even different phenomena. The particle-continuum connection and the particle-in-cell technique are applicable to the simulation of different processes. It demonstrates that the MMI simulation can also play an important role for interdisciplinary communication.

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