§20. Large Scale MD Simulation of Gas-liquid Flows

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Gas-liquid flows are important phenomena in many fields of industry. It is especially important for thermal engines and energy transportation. Thus, a study of gas-liquid flow by computer simulations much contributes to the progress of the related fields of industry. Such a study of complex gas-liquid flows by computer simulations, however, involves a fundamental problem.

Here, we are interested in complex gas-liquid flows such as a boiling flow. A boiling flow often shows transition from a bubble flow to a spray flow. The transition is caused by the increase of the volume fraction of vapor in the flow. The phase transition from water to vapor is a nonequilibrim process and the fragmentation of liquid forming droplets is a nonlinear phenomenon. In many studies of gas-liquid flows published so far, numerical models are composed by a combination of a Navier-Stokes equation and equations describing the transportation of energy and mass. The transport equations in these models are based on assumptions of local equilibrium states or linear nonequilibrium processes. The validity of these assumptions in complex gas-liquid flows, however, has not fully been tested.

A molecular dynamics model is one of the most promising ways to simulate behaviors of complex gas-liquid flows avoiding the above problem. In a case of an MD model, the fluid in a system consists of an ensemble of particles interacting each other, and the time evolution of the system is performed straightforward by solving an equation of motion without introducing any untested assumptions.

The main aim of this study is to gain knowledge of complex gas-liquid flows by numerical simulations of MD models. To achieve this aim, it is important to develop fast computer codes and visualization technique of the simulation results. We also try to solve these technological problems in this study.

In the fiscal year of 2010, we worked for the following themes: Development and estimation of an MD code by H. Watanabe. Numerical analysis of a lattice gas model to study its metastable state in a thermodynamic limit by T. Nogawa. Numerical simulations of explosive gas-liquid flows of a binary Lennard-Jones particle system by H. Inaoka. Numerical simulations of fragmentation of Lennard-Jones liquid droplets by K. Yamada.

Development of an MD code: We developed an MPI-parallelized code by using spatial segmentation. We estimated the performance of the code on the Plasma Simulator with up to 128 nodes. As a result, we found that the performance deteriorates with a larger number of nodes. We think the deterioration is caused by the synchronization of the fluctuation of the computational loads. Since the fluctuation increases with the number of nodes, the computation with a large number of nodes tends to be delayed when the computation is synchronized between the nodes. The source code used to get this estimation is publicly released in the following web site: http://mdacp.sourceforge.net/

Analysis of a lattice gas model: We analyzed simulation results of a lattice gas model using a Wang-Landau method to see the behavior of a metastable state of the model at a thermodynamic limit. The calculation speed can be increased with the square of a node number by this method. Thus, by the use of the Plasma simulator, we were able to analyze a metastable state of a system with about 1 million degrees of freedom. We confirmed that the free energy barrier for bubble nucleation decays with a power law of system size, and we estimated the exponent of the power law.

Simulation of explosive gas-liquid flows: We simulated explosive gas-liquid flows of a binary Lennard-Jones particle system with a system configuration similar to that of a shock-tube model. The model consists of two types of particles with different mass and intensity of interaction. Initially, the tube is divided by a diaphragm at the middle of the tube, and a mixture of two types of particles are put in one side of the diaphragm with high pressure and high temperature, while the other side of the diaphragm is kept vacuum. When the diaphragm is removed, the content of the high pressure region pours into the vacuum region causing an explosive flow. In this flow, creation of bubbles and fragmentation of liquid are caused by the depressurization and the bubble expansion. As a result, the flow shows typical flow regimes such as a bubble flow, a network flow, and a spray flow. We obtained a regime map of the flows in the parameter space of the local particle densities and the temperature.

Simulation of droplet fragmentation: We simulated collision of droplets of Lennard-Jones particles to observe fragmentation of the droplets. This leads to the understanding of the fragmentation process of droplets in a complex gas-liquid flow. We simulated the collisions of droplets with fixed size with various kinetic energy. As a result, we found that there is a critical kinetic energy above which the fragmentation of the droplets occurs. At the critical point, critical phenomena similar to the ones seen with a second-order phase transition are observed.

The publications in the fiscal year 2010 related to this research are as follows:

1) Efficient Implementations of Molecular Dynamics Simulations for Lennard-Jones Systems, H. Watanabe, M. Suzuki, and N. Ito, submitted to Prog. Theor. Phys.

2) Scaling relation and regime map of explosive gas-liquid flow of binary Lennard-Jones particle system, H. Inaoka, S. Yukawa, and N. Ito, submitted to Physica A.