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

Inaoka, H. (Uinv. Tokyo)

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 nonequilibrium 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 2011, we worked for the following themes: An attempt of simulating turbulent flows by a system composed of elastic particles by S. Matsumoto. Simulation of boiling by a Lennard-Jones particle system by H. Inaoka. Analysis of a lattice gas model to study bubble nucleation by T. Nogawa. Analysis of bubble nucleation in shear flows by M. Miyama. Development of visualization software with interactive manipulation of the observing particle system by S. Matsumoto.

Simulation of turbulent flows: We attempted to reproduce turbulent behaviors of flows in 2 and 3 dimensional space by numerical simulations using a system composed of particles interacting each other by a simple, elastic potential. The time evolution of the system is performed by integrating an equation of motion starting from an initial state with artificially formed vortexes. As a result, the system reaches to a state where the energy spectrum agrees with a theoretical prediction. This result implies that turbulent behavior of flows can be numerically reproduced by a MD model.

Simulation of boiling: We simulated continuous boiling of a heated fluid by a Lennard-Jones particle system. When the system with the temperature of vapor-liquid coexistence is put in a gravitational field, the gas phase goes up and the liquid phase goes down to form a gas-liquid interface in the system. Starting from this state, we put a heat bath at the bottom of the system to heat the liquid from the bottom. By this simulation, we successfully reproduced successive bubble formations similar to nucleate boiling and film boiling.

Analysis of a lattice gas model: A macroscopic thermodynamic potential cannot describe a metastable state because the potential is a convex function. It is very useful if a dynamics of bubble nucleation can be explained by a thermodynamic description. We developed a method to describe time evolution of a extensive variable of a system from the equilibrium distribution of states with a condition that the extensive variable is constant. We confirmed the applicability of the method by a large scale calculation using Wang-Landau method.

Bubble nucleation in shear flows: As a part of study of gas-liquid transition in nonequilibrium steady state, we observed bubble nucleation in shear flows. Our aim is to study the change of rheological and thermal behaviors of the flow by the bubble nucleation.

Development of visualization software: Because of its drawing algorithm, OpenGL can draw a simple, rotationally symmetric surface of a sphere very fast. By making use of this characteristic, we developed visualization software which can visualize a system with up to 10 million particles. With this software, we can interactively rotate or zoom the system by using a pointing device such as a mouse and freely observe the system.

The publications in the fiscal year 2011 related to this research are as follows:

1) Efficient Implementations of Molecular Dynamics Simulations for Lennard-Jones Systems, Hiroshi Watanabe, Masaru Suzuki, and Nobuyasu Ito, Prog. Theor. Phys. 126 (2011) 203.

2) Scaling relation and regime map of explosive gas-liquid flow of binary Lennard-Jones particle system, Hajime Inaoka, Satoshi Yukawa, and Nobuyasu Ito, Physica A 391 (2012) 423.

3) Static and dynamical aspects of the metastable states of first order transition systems, Tomoaki Nogawa, Nobuyasu Ito and Hiroshi Watanabe, Physics Procedia 15 (2011) 76.

4) Evaporation-condensation transition of the two-dimensional Potts model in the microcanonical ensemble, Tomoaki Nogawa, Nobuyasu Ito and Hiroshi Watanabe, Phys. Rev. E 84 (2011) 061107.