§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 a gas-liquid flow by a computer simulation much contributes to the progress of the related fields of industry. Such a study of a complex gas-liquid flow by a computer simulation, however, involves a fundamental problem.

Here, we are interested in a complex gas-liquid flow 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 the 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 a complex gas-liquid flow avoiding the above problem. In a case of an MD model, the fluid in a system consists of an ensemble of particles interacting with each other, and the time evolution of the system is performed straightforwardly 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 2012, we worked for the following themes: Simulation of boiling of a Lennard-Jones particle system by H. Inaoka. An attempt of simulating turbulent flows with a system composed of elastic particles by T. S. Komatsu.

Simulation of boiling: We simulated continuous boiling of a heated fluid with 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. In the last fiscal year, we successfully reproduced successive bubble formations similar to nucleate boiling and film boiling with our MD model. In this fiscal year, we attempted to reproduce quantitative aspect of boiling with our model. For this purpose, we observed pool boiling curve, and confirmed that the reproduced curve is consistent with observed ones in experiments. This result will be published in Physica A.

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 with each other by a simple, elastic potential. The principal aim of this work is to reproduce a turbulent phenomenon in a comprehensive manner from a scale of thermal dissipation to structures of a turbulent flow such as vortices by an MD model. The maximum simulation we performed in this fiscal year was with a cubic system with its linear dimension of 1000 particle diameters. The number of particles in the system is about 380 million. By the analysis of the simulation result, it became clear that we need to perform longer simulations with a larger system size to confirm a Kolmogrov's spectrum. However, we attempted to compare the energy spectrum obtained by the above simulation to observations of preceding experimental and numerical works. By this research we confirmed following two points. The high frequency part of the energy spectrum of our MD model follows a function form predicted by a law of energy equipartition, and it differs from experimental observation. Howerver, the general function form of the low frequency part of the spectrum, which includes turbulent region and lower frequency part of dissipation region, agrees well with observed spectra of preceding works.

The publications and presentations in the fiscal year 2012 related to this research are as follows:

1) Usefulness of an equal-probability assumption for out-of-equilibrium states: A master equation approach, Tomoaki Nogawa, Nobuyasu Ito, and Hiroshi Watanabe, Physical Review E 86 (2012) 041133.

2) Numerical simulation of pool boiling of a Lennard-Jones liquid, Hajime Inaoka and Nobuyasu Ito, to appear in Physica A.

3) Molecular dynamics simulation of pool boiling of a Lennard-Jones liquid, Hajime Inaoka and Nobuyasu Ito, The 3rd AICS International Symposium, RIKEN Advanced Institute for Computational Science (Feb. 2013).

4) A challenge to turbulence from molecular scale, Teruhisa S. Komatsu, Shigenori Matsumoto, Takashi Shimada, and Nobuyasu Ito, The 3rd AICS International Symposium, RIKEN Advanced Institute for Computational Science (Feb. 2013).

5) 3 more domestic presentations.

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