Summary of thesis: Singular behavior near surfaces: boundary conditions on fluids and surface critical phenomena

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Behaviors of a fluid near a solid surface are different from those in a bulk. In hydrodynamics, these behaviors are described as boundary conditions (BCs) on hydrodynamic equations. The BC conventionally used is the stick BC that a fluid at a solid surface has no velocity to it. It has been confirmed over a century of study that the Navier-Stokes equation with the stick BC describes the macroscopic flow with high accuracy. In recent years, there are remarkable developments of experimental techniques for nano- and micro-scale systems, and it becomes possible to quantitatively measure what occurs at these scales. These developments revealed that the fluids may slip on solid surfaces and the BCs are far more complicated than conventionally thought. In this thesis, I study the basic nature and applications of the slip phenomena from the microscopic viewpoint.

In Chapter 2, I attempt to derive the correct BC to replace the stick BC from an underlying microscopic theory. In particular, I focus on Navier's partial slip BC that the slip velocity of the fluid is linearly proportional to a shear rate at the solid surface. The proportional constant is called a slip length. Some of experimental results reported in past two decades are accurately described by Navier's partial slip BC.

I develop two linear response theories for microscopic systems and derive Navier's partial slip BC in two different ways. The first linear response theory describes the relaxation process of the fluid, and the second describes the non-equilibrium steady state. By employing these linear response theories, I derive two microscopic expressions for the slip length. Next, I validate these expressions by employing the linearized fluctuating hydrodynamics with Navier's partial slip BC. By calculating the microscopic expressions of the slip length exactly, I find that both microscopic expressions hold in the fluctuating hydrodynamic description with giving the same value despite their difference in form.

In Chapter 3, I study the slip phenomena beyond the linear response regime. By employing the molecular dynamical simulation, I examine a possible form of the microscopic BCs that are uniquely determined from a microscopic description of the fluid and the wall. Then, I clarify that the microscopic BCs may exhibit the non-linear behavior.

Next, I consider the relationship between the non-linear microscopic BCs and the BCs conventionally used (e.g. stick BC and Navier's partial slip BC). The conventional BCs have been applied to obtain satisfactory results from the macroscopic point of view in many situations. Then, I attempt to derive such BCs by introducing the extent of measurement accuracy as the mathematical concept.

In the macroscopic limit, I may introduce a scaled velocity field by ignoring the higher order terms in the velocity field that is calculated from the Navier-Stokes equation and the microscopic BC. I define macroscopic BCs as the BCs that are imposed on the scaled velocity field. The macroscopic BCs contain a few phenomenological parameters for an amount of slip, which are related to a functional form of given microscopic BC. By considering two macroscopic limits of the non-equilibrium steady state, we propose two different frameworks for determining macroscopic BCs.

In Chapter 4, I consider how the surface connects to the bulk and what kind of critical phenomena and long-range orders are observed. My motivation is to achieve the *in situ* control of the slip length for the dense fluids, which has attracted attention in order to control the flow in small scale tubes. My key idea is to use the order-disorder transition occurring only near the surface, specifically the crystallization of the fluid only near the surface.

As the first step, I investigate the surface critical phenomena of an ideal Bose gas. Specifically, I study a tight-binding Bose gas with a hopping rate enhanced only on a surface. This model has two advantages. The first one is that this model exhibits nontrivial phase transitions, and the second one is that all quantities can be exactly calculated. By exactly calculating the free energy, I provide a simple picture that diverse critical phenomena at the surface may be caused by competition between pure two-dimensional effects and the interaction through the bulk. Although the phase transitions in this model are rather special, I expect that such structure is universal.

In summary, I propose novel theoretical methods for studying singular behaviors near surfaces.