Journal of Computational Physics 234 (2013) 8–32

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Development of an immersed boundary-phase field-lattice Boltzmann method for Neumann boundary condition to study contact line dynamics

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ARTICLE INFO

Article history:
Received 5 October 2011
Received in revised form 15 June 2012
Accepted 28 August 2012
Available online 8 September 2012

Keywords:
Immersed boundary method
Phase field method
Lattice Boltzmann method
Multiphase flow
Contact line dynamics
Dirichlet condition
Neumann condition

ABSTRACT

The implementation of Neumann boundary condition in the framework of immersed boundary method (IBM) is presented in this paper to simulate contact line dynamics using a phase field-lattice Boltzmann method. Immersed boundary method [10] is known as an efficient algorithm for modelling fluid–solid interaction. Abundance of prominent works have been devoted to refine IBM [1,11,12]. However, they are mainly restricted to problems with Dirichlet boundary condition. Research that implements the Neumann boundary condition in IBM is very limited to the best of our knowledge. This deficiency significantly limits the application of IBM in computational fluid dynamics (CFD) since physical phenomena associated with Neumann boundary conditions are extremely diverse. The difficulty is attributed to the fact that implementation of Neumann boundary condition is much more complex than that of Dirichlet boundary condition. In the present work, we initiate the first endeavour to implement Neumann boundary condition in IBM with assistance of its physical interpretation rather than simple mathematical manipulation. Concretely speaking, rooted from physical conservation law, the Neumann boundary condition is considered as contribution of flux from the boundary to its relevant physical parameter in a control volume. Moreover, the link between the flux and its corresponding flow field variable is directly manipulated through the immersed boundary concept. In this way, the Neumann boundary conditions can be implemented in IBM. The developed method is applied together with phase field-lattice Boltzmann method to study contact line dynamics. The phase field method [27,39], which becomes increasingly popular in multiphase flow simulation, can efficiently capture complex interface topology and naturally resolve the contact line singularity. Meanwhile, the lattice Boltzmann method is known as an alternative to model fluid dynamics and holds good prospect to simulate multiphase flows with complex geometry [38]. In this context, the developed immersed boundary-phase field-LBM is verified in detail for both steady and unsteady contact line problems. Tests show that the proposed method can correctly reproduce both equilibrium results and dynamic process.

1. Introduction

In fluid mechanics, problems involving interactions between fluid and immersed objects are ubiquitous. To simulate such problems, implementation of boundary conditions, including the Dirichlet and Neumann boundary conditions, is an indispensable task. A straightforward way is to use a body-conformal grid. Specifically, a grid is first generated concerning solid

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http://dx.doi.org/10.1016/j.jcp.2012.08.040

shape as shown in Fig. 1. Subsequently the governing equations are naturally discretized considering solid geometrical information and the boundary conditions can also be readily imposed. In this way, an accurate solution can be yielded [1]. Nevertheless, it is usually difficult to generate a body-fitted grid with good quality, especially when a complex geometry or a moving boundary is presented in the flow field. To overcome this drawback, non-body-conformal methods [2–10] which become increasingly popular, could be employed. Among various non-body-conformal methods, the immersed boundary method (IBM) developed by Peskin [10] has attracted much attention from researchers. Prominent advantages of IBM include easy implementation and robustness to handle complex geometries. In IBM, the governing equations are resolved on a fixed Cartesian (Eulerian) grid. The boundary is presented by a set of Lagrangian points which are independent to the Eulerian grid as shown in Fig. 2. Meanwhile, the influence of boundary on flow field is depicted by adding a force or source term into the governing equations. Hitherto, IBM has undergone continuous development in accurate implementation of boundary conditions. In Peskin's original work, the boundary is treated as being elastic [10]. The relationship between the restoring force and body deformation is governed by the Hook's law, in which a user-defined coefficient is involved. To avoid using the arbitrary coefficient, the direct forcing method is introduced by Fadlun et al. [11]. In their method, the Navier–Stokes (NS) equations are employed to compute the force on the boundary. More recently, a boundary condition-enforced IBM is developed by Wu and Shu [12]. Unlike the previous force calculation schemes, in which the restoring force is pre-calculated and there is no mechanism to enforce the no-slip boundary condition. The newly developed method considers the restoring force as unknown and it is determined in a way that the no-slip boundary condition is enforced. An elegant review of kindred algorithms is provided by Mittal and Iaccarino [1]. Tremendous effort has been devoted to refine IBM. However, most of them are restricted to the Dirichlet boundary condition over decades. To the best of our knowledge, the research that aims at extending the IBM to depict the Neumann boundary condition is very limited. This remarkably restricts the application of IBM in computational fluid dynamics (CFD) since physical phenomena associated with Neumann boundary conditions are extremely diverse. One of the instances is the contact line dynamics in multiphase flow problems. This means that there is a practical demanding to develop an efficient IBM for Neumann boundary condition.

In multiphase flows, when a solid object is brought into contact with two immiscible fluids, a three-phase contact line will be formed. This class of phenomena [13–15] can be referred as contact line dynamics. The contact line dynamics can be numerically modeled by a slip boundary (Dirichlet) condition [16–23] in sharp interface methods or Robin boundary conditions in the phase field method [24–27]. In the phase field method, the no-slip boundary condition is still utilized. Additionally, two Neumann boundary conditions are used to govern variation of composition on a solid boundary [27]. Although the phase field method is relatively a new method, it becomes increasingly popular because of its efficiency to capture interface topology change, natural regularization of the contact line singularity and a sound physical background [24,27–40]. As an interface capturing scheme, the phase field method can be combined with either Navier–Stokes (NS) solver or lattice Boltzmann method (LBM), which is known as an attractive alternative to simulate fluid dynamics. Advantages of LBM [38] include easy implementation and specifically, the potential to bridge widely dispersed scales in multiphase flows. Therefore, in the present work, a phase field-lattice Boltzmann method is used to capture the interface and study the contact line dynamics. Although many works have been done by both phase field-NS solver and phase field-LBM solver, most of the reported results investigate contact line on perfectly smooth surface or, at most, grooved surface with simple geometries represented by straight lines. This is mainly attributed to the intricacies caused by implementation of the Neumann boundary condition on a complex geometry. To overcome this difficulty, an IBM-based algorithm that can handle Neumann boundary conditions will be instrumental. In fact, some attempts have been made, such as the work done by Francois and Shyy [41]. In their work, the immersed boundary method was used to track fluid–fluid interface through interface markers. On

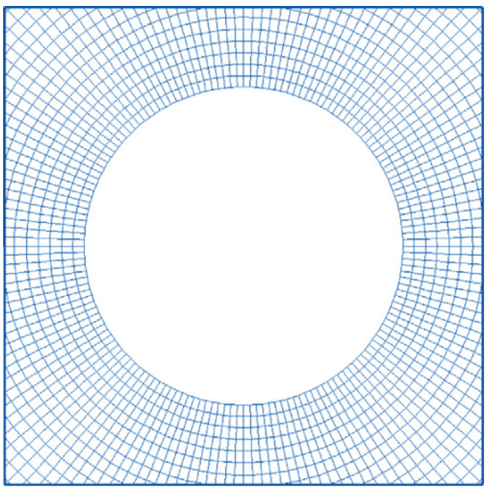

Fig. 1. Sketch of a body-conformal grid.