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Coupled numerical approach combining finite volume and lattice Boltzmann methods for multi-scale multi-physicochemical processes

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ABSTRACT

A coupled (hybrid) simulation strategy spatially combining the finite volume method (FVM) and the lattice Boltzmann method (LBM), called CFVLBM, is developed to simulate coupled multi-scale multi-physicochemical processes. In the CFVLBM, computational domain of multi-scale problems is divided into two sub-domains, i.e., an open, free fluid region and a region filled with porous materials. The FVM and LBM are used for these two regions, respectively, with information exchanged at the interface between the two sub-domains. A general reconstruction operator (RO) is proposed to derive the distribution functions in the LBM from the corresponding macro scalar, the governing equation of which obeys the convection–diffusion equation. The CFVLBM and the RO are validated in several typical physicochemical problems and then are applied to simulate complex multi-scale coupled fluid flow, heat transfer, mass transport, and chemical reaction in a wall-coated micro reactor. The maximum ratio of the grid size between the FVM and LBM regions is explored and discussed.

1. Introduction

Multi-scale phenomena widely exist in material science, electrical and mechanical engineering, chemistry processes and energy and environmental science [1]. Such phenomena are usually caused by large size ratio between different components in a device or induced by complex fluid flow in confined domains (such as interfacial interactions among phases, and hydrodynamics and transport processes in local complex porous media). Generally, the multi-scale phenomena possess a number of prominent characteristics. The first and most important one is the large range of relevant length or time scales, which can vary up to several orders of magnitude. Second, the dominant processes change with the length or time scale [1]. For example, the surface and interfacial phenomena become increasingly important as the size of the system decreases [2]. Third, multi-scale phenomena usually involve intrinsic multiphysics consisting of coupled multiple physicochemical processes [3]. For example, in a proton exchange membrane fuel cell (PEMFC), coupled fluid flow, heat transfer, mass transport, electron and proton conduction, as well as electrochemical reactions simultaneously take place [4].

From the computational physics point of view, multi-scale phenomena in the thermal and fluid science and engineering may be classified into two categories: multi-scale systems and multi-scale processes [5,6]. A multi-scale system refers to a system that is characterized by large variation in length scales in which the processes at different length scales often have

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the same governing equations and are not closely related. The cooling problem of a data center is a typical multi-scale system. The cooling process from the room to the chip involves an extended span of length for about 11 orders of magnitude. In a multi-scale process, the overall behavior is governed by processes that occur at different length and/or time scales which are closely coupled with each other [5,6]. Transport process in proton exchange membrane fuel cell and turbulent flow and heat transfer are two typical examples of multi-scale process. In a PEMFC, processes of fluid flow, heat transfer, mass transport and electronic charge conduction take place in components with different scales and are closely related to each other, and the overall cell performance is a combined result of these coupled processes [7].

There have been an increasing number of studies focusing on the modeling and simulation of the multi-scale phenomena. Due to more complication and coupling involved, the multi-scale process is more challenging to simulate than the multi-scale system [5,6,8,9]. Currently, two types of numerical approaches exist in the literature for the simulation of multi-scale processes in engineering thermal and fluid science [5]. One can be described as "Using uniform governing equation and solving for the entire domain", among which direct numerical simulation (DNS) is a typical example [10]. The second approach is described as "Solving problems regionally and coupling at the interfaces" (hereafter called coupled modeling approach) [11–28]. In such an approach, instead of pursuing a single uniform numerical method for the entire domain, a coupled modeling strategy is proposed, in which different numerical methods are used to predict transport processes in different local regimes and information is exchanged at the interface between neighboring regimes following certain principles. Different numerical methods have their own advantages and disadvantages depending on specific applications. For example, the conventional top-down numerical methods, such as finite volume method (FVM), finite element method (FEM) and finite difference method (FDM), are suitable for large scale simulations with good computational efficiency, while the bottom-up numerical methods, such as the lattice Boltzmann method (LBM) is able to capture local transport details involving complex structures or interfacial behaviors. The goal of the coupled modeling approach is to combine the advantages of different numerical methods leading to an accurate yet efficient numerical approach, and there have been increasing studies dedicated to this problem in recent years [11–28]. For the coupling of the LBM and FVM/FEM/FDM, the LBM is applied in sub-domains where small scale effects, porous transport processes, or interface phenomena are more relevant and FVM/FEM/FDM is used in the remaining domains.

The critical task and major difficulty in the coupled modeling strategy is how to exchange information at the interface of neighboring sub-domains (or essentially between different numerical methods). Specially, for the coupling between LBM and FVM/FEM/FDM, it is straightforward to transfer the distribution functions obtained in the LBM framework to macro fluid variables in FVM/FEM/FDM (velocity, density, temperature, concentration and so on) through statistic methods. However, the inverse evaluation of the distribution functions from macro fluid variables is not unique and usually difficult [5,6], since the LBM has more degrees of freedom than the FVM/FEM/FDM. A few recent efforts have been reported to associate the distribution functions with fluid variables in coupling LB-FVM/FEM/FDM simulation strategy [12,15,20,26–28], in which Chapman–Enskog multi-scale expansion skill was widely adopted. FDM and LBM were coupled to simulate 2D pure-diffusion problems in Refs. [12,26], 1D diffusion–reaction problems in Ref. [15], and Poiseuille flow in Refs. [27,28]. FEM and LBM were coupled to simulate wave propagation problems in Ref. [16]. While the simulations in Refs. [12,16,26–28] presented simple examples as a proof-of-concept for the coupled simulation strategy, Christensen and Graham [20] coupled FDM and LBM to simulate a realistic heat transport problem of local phonon transport in crystalline. However, to the best of our knowledge, there has been no studies on coupling the FVM/FEM/FDM and LBM for realistic convective mass (heat) transfer processes, or for transport processes in complex porous media. For pure diffusion–reaction (heat conduction) processes, the only physical variable concerned is concentration (temperature), and the expressions of its corresponding distribution functions only contain concentration (temperature) and its space derivatives. However, when convection is considered, the corresponding expressions of the concentration (temperature) distribution functions will be more complex and also contain density and velocity and their space derivatives. Furthermore, the coupling between FVM/FEM/FDM and LBM will be more complex. Recently, we constructed a reconstruction operator (RO) for deriving the density distribution functions from the macro density and velocity up to the second order [23]. Using this RO in the coupled simulation strategy, we successfully predicted complex fluid flow in a domain with local porous media [21]. Very recently, we proposed a temperature RO [22] and a concentration RO [29] for transferring temperature to temperature distribution functions and concentration to concentration distribution functions, respectively. Using the density RO and concentration RO, transport phenomena in PEMFC are investigated, where FVM is used to simulate transport phenomena in gas channel (GC) and LBM is used to predict transport phenomena in porous gas diffusion layer (GDL) [25,29].

Nowadays, numerical simulations have been widely applied to a variety of fields, such as laminar and turbulence flow, heat and mass transports, chemical reactions, multiphase flow, electrokinetic flows, and so on. In these fields, it is common that the transport phenomena are described by the NS equations coupled with several scalar convection–diffusion (CD) equations [30]. For example, the classical natural convection problem caused by temperature (or concentration) gradient in a cavity is described by NS equations for fluid flow and CD equations for temperature (or concentration) [31]. Another more complex example is the transport processes in PEMFC, which is described by NS equations combined with several CD equations describing temperature, concentration, and electron potential and proton potential [32–34]. Generally, the CD equation can be considered as a scalar transport equation and is similar for different scalars (temperature, concentration, potential, etc.) [30], as will be discussed in detail in Section 2. Therefore, it is desirable to propose a general RO for scalar (the transport of which obeys the CD equation) to develop the coupled simulation strategy.