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Multigrid lattice Boltzmann method for accelerated solution of elliptic equations

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ABSTRACT

A new solver for second-order elliptic partial differential equations (PDEs) based on the lattice Boltzmann method (LBM) and the multigrid (MG) technique is presented. Several benchmark elliptic equations are solved numerically with the inclusion of multiple grid-levels in two-dimensional domains at an optimal computational cost within the LB framework. The results are compared with the corresponding analytical solutions and numerical solutions obtained using the Stone's strongly implicit procedure. The classical PDEs considered in this article include the Laplace and Poisson equations with Dirichlet boundary conditions, with the latter involving both constant and variable coefficients. A detailed analysis of solution accuracy, convergence and computational efficiency of the proposed solver is given. It is observed that the use of a high-order stencil (for smoothing) improves convergence and accuracy for an equivalent number of smoothing sweeps. The effect of the type of scheduling cycle (V- or W-cycle) on the performance of the MG–LBM is analyzed. Next, a parallel algorithm for the MG–LBM solver is presented and then its parallel performance on a multi-core cluster is analyzed. Lastly, a practical example is provided wherein the proposed elliptic PDE solver is used to compute the electro-static potential encountered in an electro-chemical cell, which demonstrates the effectiveness of this new solver in complex coupled systems. Several orders of magnitude gains in convergence and parallel scaling for the canonical problems, and a factor of 5 reduction for the multiphysics problem are achieved using the MG–LBM.

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1. Introduction

An important and challenging aspect of a numerical solution procedure is its computational efficiency. With the advent of the multicore central-processing units (CPUs) and graphical-processing units (GPUs) technologies, the available computational resources are growing and enabling the scientific community to solve challenging problems of interest. At the same time, ensuring the computational effectiveness, i.e. accelerating the convergence of the underlying algorithms used in the numerical solution of the physical problem is an equally important challenge. Indeed, the development of fast and accurate numerical schemes in computational fluid dynamics (CFD) and various other fields remains one of the main active areas of research.

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Optimal solution of complex problems arising from the discretization of the partial differential equations (PDEs) with a computational complexity of $O(N)$, i.e. when the operation count is only proportional to the number of grid nodes N, often requires the use of multigrid (MG) procedures [1–5]. Multigrid methods generally work by rapidly smoothing the high frequency error components in solutions on fine grids by a few relaxation sweeps, which are then transferred to coarse grids recursively to deliver error corrections that achieve convergence acceleration in an optimal sense together with highly accurate numerical solutions. Multigrid techniques have been implemented in the past for various problems, including those involving the solution of the continuum based Navier–Stokes (NS) equations in the context of the classical CFD (see e.g. [6–9]). Various elements and details on the multigrid approach have been presented in monographs on the topic, e.g. [2,4,10]. Often the solution of the NS equations involves the Poisson equation for the pressure field, which is an elliptic PDE. Furthermore, various other complex multiphysics problems involve Poisson and other elliptic equations, e.g. in the solution of the electro-static potential in electro-chemical systems, a subject of present interest. Thus, the development of fast multigrid solvers for such problems becomes important. With the availability of large parallel clusters, the ability of MG approaches to scale well in a multicore environment also assumes as a key criterion for their further development.

The lattice Boltzmann method (LBM) is a more recent computational approach based on kinetic theory for fluid dynamics and other problems. It involves the solution of a discrete form of the Boltzmann equation with a simplified collision term – the lattice Boltzmann equation (LBE) and may be characterized as a mesoscopic method. In general, the LBM computes locally the effect of collision as a relaxation process (the collision step) and subsequently the outcomes, i.e. the discrete distribution functions, are communicated to the respective neighboring points along characteristic directions (the streaming step). The emergent macroscopic fields are then computed by taking the discrete moments of the distribution functions. On the other hand, the pressure, for example, can be obtained locally from an equation of state. The 'collide and stream' algorithm makes the LBM a suitable candidate for efficient parallel computations using a domain-decomposition technique on both CPUs and GPUs. However, the traditional LBM is time marching in nature (either in physical or pseudo time) and is prone to a slow rate of convergence to the desired solution, e.g. steady state. In the past, researchers have proposed to address this issue by suggesting and demonstrating some improvement techniques for convergence of the LBM solutions for certain flow problems. For example, convergence acceleration using preconditioning techniques has been studied [11–13]. Another approach is to use composite grids consisting of multiple-blocks in the lattice Boltzmann framework [14] or local time step method [15]. The utility of a nonlinear MG procedure with an implicit second-order finite-difference scheme for the discrete Boltzmann equation was demonstrated in Ref. [16]. Furthermore, a new nonlinear MG–LBM procedure that conforms with the "collide and stream" nature of the classical formulations allowing efficient implementation was developed and demonstrated for accelerated solution of steady state flow problems in Refs. [17,18].

In this work, we develop a new multigrid (MG) lattice Boltzmann (LB) approach for the fast numerical solution of second-order elliptic PDEs, especially the Laplace and Poisson equations of different characteristics over a rectangular domain. It may be noted that the exact solutions to the Laplace equation are harmonic and may describe electric, gravitational, and fluid potentials. On the other hand, the Poisson equation is encountered in various practical situations e.g. in electro-statics, to solve for the electric potential with a given charge distribution referred to as the Poisson–Boltzmann equation (PBE) and often has a variable coefficient form. Numerical solution to the PBE is also important to analyze the protein-folding problem and to design better drugs [19]. In this article, one set of numerical examples describes, therefore, the MG–LB solution to such a variable coefficient Poisson equation.

Among recent works, multigrid has been applied to solve the Poisson equation [20–24] and solutions to the variable coefficient Poisson equation with jump conditions are discussed in Refs. [25–28]. These works primarily used finite-difference methods to discretize the governing equation on multiple grid-levels. Other numerical methods such as finite-element [20] or finite-volume [29] have also received attention. It is shown in these and other studies that MG is a rapidly convergent as well as an accurate technique to solve elliptic PDEs. To our knowledge, there is no literature available on the development and application of the MG technique in the LB framework for solutions of Poisson type equations and the present work addresses this subject.

Earlier work [30–33] has focused on the development of the LBM for Poisson equation encountered mainly in electrochemical systems in a single grid context. As noted in Ref. [34], there are shortcomings of the earlier methods for the Poisson equation as the final equation used is a time-dependent diffusion equation and the errors are prone to the initialization employed. The undesirable time-derivative term which is present in such methods has been eliminated in the formulation given in Ref. [34]. Other more recent studies involving the LBM for the solution of the Laplace as well as Poisson equations include Refs. [35,36]. All these formulations inherit the shortcomings of the traditional single-grid LBM as the convergence rates are dependent on the problem size leading to slow and inefficient solution procedures, when compared to certain solvers based on the direct discretization of the corresponding PDEs. In this article, the single-grid formulation of Ref. [34], which is an explicit pseudo-time marching approach, is used as a framework for further development involving multigrid techniques.

Furthermore, to the best of the author's knowledge, any parallel algorithm of the multigrid LBM, which could allow simulation of large problems, and their performance analysis has not been discussed in the literature. Hence, in this article, we also present a parallel algorithm of the MG and its performance on an in-house multi-core cluster. Here, the inter-processor communications of the operating variables need to be and are carried out only on the finest grid of the hierarchy, as the multigrid involves transfer of variables across its grid levels according to the scheduling cycles.

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