PRATHAM: Parallel Thermal Hydraulics Simulations using Advanced Mesoscopic Methods*

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INTRODUCTION

Most of the leading three-dimensional (3D) computational fluid dynamics (CFD) software for turbulent flow simulations in geometries of practical interest solves the Reynolds-averaged Navier-Stokes (RANS) equation with closure turbulence models (e.g., k-ε, k-ω, low Reynolds number turbulence model). Though RANS-based turbulence models can provide a reasonably accurate time-averaged behavior for steady state flows, they usually fail to deliver the details and accuracy needed to follow a flow instability transient, model thermal striping physics or capture transient forcing terms in flow-induced structural vibrations in a nuclear reactor.

Several persisting issues in other approaches for turbulent flow simulation [e.g., those related to parallel scalability and very fine grid requirements in large eddy simulation (LES) for incompressible flows] can be resolved by a new kinetic method called the lattice Boltzmann method (LBM) [1], which has better algorithmic parallel scalability and can use a longer time step than Navier-Stokes equation (NSE)-based explicit solvers, resulting in a significant speedup and reduced wall-clock time for large simulations of practical interest. Compared with the NSE-based approaches, use of LBM offers several advantages, including the following.

1. LBM-based turbulent flow simulations are based on a first-order partial differential equation (PDE), the lattice Boltzmann equation, in contrast to the second-order PDE form of NSE. Also, the nonlinear convective term of NSE is avoided by using an advection-collision algorithm in LBM. The nonlinearity is hidden in the quadratic velocity terms of the equilibrium distribution function in LBM. Because of this, LBM simulations are more robust and relatively less prone to numerical instabilities in capturing large gradients.

2. LBM essentially simulates the incompressible flows by using a quasi-compressible approach in which the pressure is given by a density-dependent equation of state. Because pressure is not an independent variable of the simulation, there is no need to solve the elliptic pressure Poisson equation in LBM. Note that because of its elliptic nature, the pressure Poisson equation needs to be iteratively solved in the NSE-based incompressible flow solvers and requires significant global communications for parallel simulations, adversely affecting their scalability for large problems.

3. The time step, dt, and the spatial step, dx, in LBM are strictly coupled through the so-called light-cone condition, dx = c.dt, where c is the constant characteristic speed of the lattice. Because of this, the numerical stability criterion for LBM differs from NSE-based explicit solvers. In LBM, $dt \propto dx$, rather than the $dt \propto dx^2$ of NSE [2], implying that the time steps do not need to reduce quadratically with decreasing mesh size, which indicates a relatively huge time saving for high-resolution simulation of turbulent flows.

PRATHAM CODE

At the Oak Ridge National Laboratory, efforts are under way to develop a 3D, parallel LBM code—called PRATHAM (**P**a**RA**llel **T**hermal **H**ydraulic simulations using **A**dvanced **M**esoscopic Methods)—to demonstrate the accuracy and scalability of LBM for turbulent flow simulations in nuclear applications. The code has been developed using FORTRAN-90, and parallelized using the message passing interface MPI library. Silo library is used to compact and write the data files, and VisIt visualization software is used to post-process the simulation data in parallel. Both the single relaxation time (SRT) [1] and multi relaxation time (MRT) [3-4] LBM schemes have been implemented in PRATHAM. To capture turbulence without prohibitively increasing the grid resolution requirements, an LES approach [5] is adopted allowing large scale eddies to be numerically resolved while modeling the smaller (subgrid) eddies. In this work, a Smagorinsky model has been used, which modifies the fluid viscosity by an additional *eddy viscosity* depending on the magnitude of the rate-of-strain tensor. In LBM, this is achieved by locally varying the relaxation time of the fluid.

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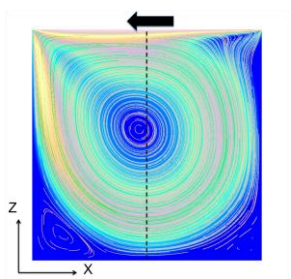
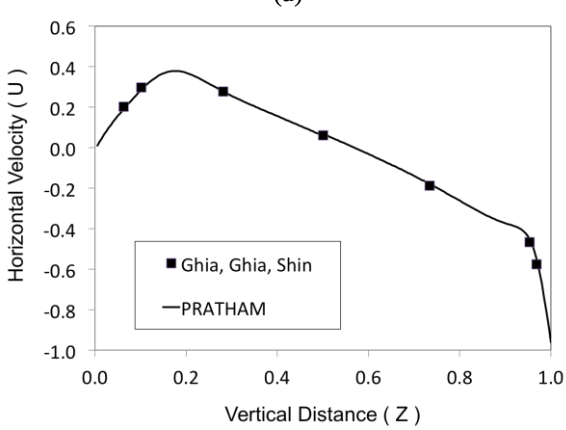
TEST PROBLEMS

To demonstrate the applicability of LBM, and to verify the computational package under development, three test problems have been simulated. The first and second test cases are for flow inside a lid-driven cavity, and the third test case is flow around a cylinder. In both the problems, the most important parameter governing the solutions is Reynolds number, Re = UL/ν, where U is the velocity scale, L is a characteristic length, and ν is the kinematic viscosity of the fluid. The characteristic time scale is defined as t_0 = L/U and the nondimensional time is defined to be $t^* = t / t_0$. Note that PRATHAM is fully 3D, and the two-dimensional (2D) tests were run by collapsing the third dimension to retain only two grid points. Periodic boundaries were used along the third dimension for these 2D simulations.

In a lid-driven cavity problem, a square cavity is completely filled with an incompressible fluid and flow is driven by the motion of the top surface (lid). For this case, L is the cavity length and U is the speed of the lid. Figure 1 illustrates the 2D case.



(a)

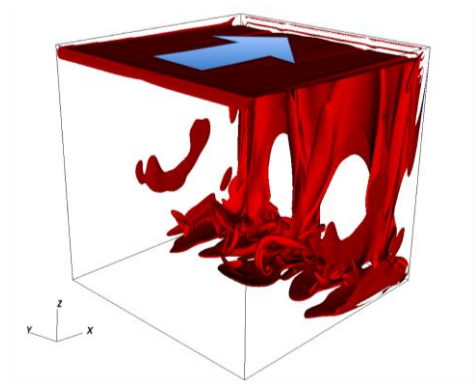


(b)

Fig. 1. PRATHAM simulation of flow inside a two-dimensional lid-driven cavity for Re = 1,000 using a $(200)^2$ lattice: (a) problem schematic, (b) validation of centerline velocity profile with Ghia et al. [6].

Figure 1(a) shows the steady state flow pattern inside the cavity, and one can clearly identify the primary vortex and secondary vortex. In Fig. 1(b), the normalized X-velocity on the vertical centerline of the cavity [dashed line in Fig.1(a)] for Re = 1,000 using PRATHAM is compared with the benchmark numerical results of Ghia et al. [6], obtained using a stream-function vorticity approach. The LBM result agrees well the benchmark solution.

In Fig. 2, preliminary results for a 3D lid-driven cavity flow at Re = 10,000 are shown to highlight the 3D transient capabilities of PRATHAM. In general, the 3D lid-driven cavity problem has several features that make it more challenging than the 2D problem. For example, the side walls cause the flow to have significantly different flow features, as indicated by the enstrophy[†] contours in Fig. 2(a). Also, the 3D flow spans the entire cavity, meaning that all fluid particles travel through every point of the cavity. This is in contrast to the 2D flow, where flow is separated into several vortices, with particles in one vortex restricted to that portion of the flow domain. The instantaneous streamlines shown in Fig. 2(b) provide additional insight into the complexity of the flow field. This simulation was run using a $(400)^3$ lattice on 480 computing cores, and exhibited very good scaling performance. Parallel speed up and efficiency results for PRATHAM will be reported later. [[†]Enstrophy is a measure of the local rotational kinetic energy, and defined as the square of flow vorticity.]



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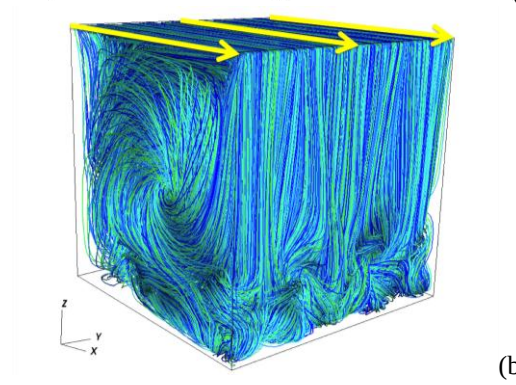
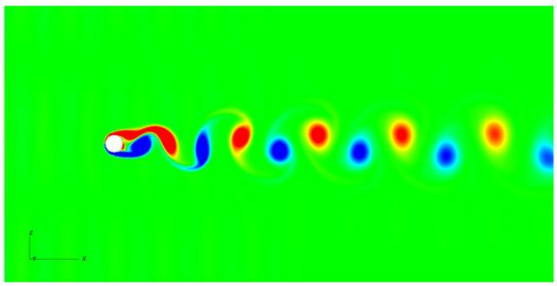


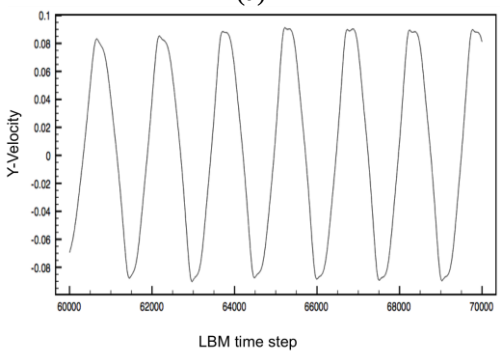
(b)

Fig. 2. PRATHAM simulations of flow inside a three-dimensional lid-driven cavity at Re = 10,000 and t* = 17.5 showing (a) contours of the enstrophy and (b) instantaneous streamlines. This simulation was run for 200,000 time steps using a $(400)^3$ lattice with 480 cores.

Finally, PRATHAM was applied to study flow past a fixed circular cylinder (Figure 3). In this case, L was set equal to the cylinder diameter D and the velocity scale U was the inlet velocity, U_∞, (assumed to be uniform). Zero-gradient conditions were used at the domain outlet. Simulations were carried out for Re = 200, 500, 1000, 5000, 100000 using a lattice size of 1000×2×500.



(a)



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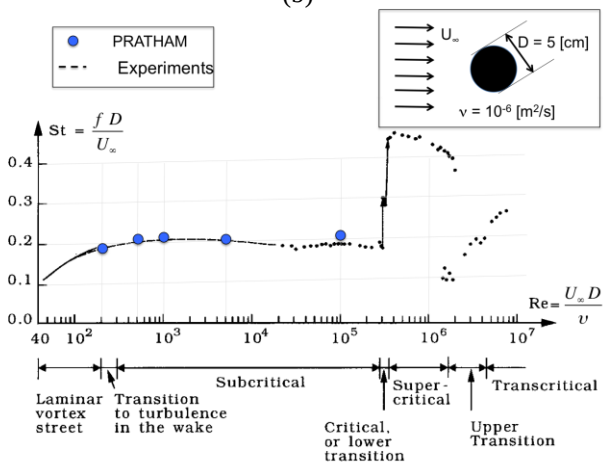

(c)

Fig. 3: Two-dimensional simulation of vortex shedding: (a) vortex shedding downstream of the cylinder; (b) oscillation of the vertical velocity component on the domain centerline, located just downstream of the cylinder; and (c) PRATHAM predictions of the Strouhal number for various Reynolds numbers, showing good agreement with experimental findings (figure adapted from [7]).

In Fig. 3(a), vorticity contours are shown for Re = 200 and t* = 100, where alternate vortices are being shed from the top and bottom of the cylinder. The vortex shedding frequency f is described by the Strouhal number, St = fD/U. Frequency f can be estimated from the PRATHAM solution by selecting a point just downstream of the cylinder and plotting the variation of the Y-velocity component with time [Fig. 3(b)]. Figure 3(c), shows good agreement of the PRATHAM results with the experimental data of Mutlu and Fredose [7].

CONCLUSIONS

A 3-D parallel LBM code, called PRATHAM, is being developed to simulate both the laminar as well as turbulent flows. This code features both the SRT and the MRT LBM approaches, and their corresponding LES models. The code is currently being validated using prior experimental and computational results, and has been scaled up to 480 cores. Ongoing developments including integration of PRATHAM with an in-house Cartesian mesh generator for CAD support and implementation of nonuniform meshing will allow LBM simulations in complex flow geometries.

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