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Lattice Boltzmann Methods: A Kinetic Approach for High-Performance CFD

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It is well known that the Navier–Stokes equations in continuum theory can be derived from the Boltzmann equation in the limit of small Knudsen numbers. Solving the Boltzmann equation means computing a particle velocity distribution function f defining the probability that a particle with a microscopic particle velocity $\vec{v}$ will be found at $(\vec{x}, t)$. The first few moments of this distribution function with respect to the particle velocity are macroscopic flow properties, such as density, momentum, energy, and the stress tensor. It is thus possible, in principle, to obtain solutions to the Navier–Stokes equations by solving the Boltzmann equation. The Boltzmann equation being in general much harder to solve, there is nothing at first sight to be gained from such an approach, if concern is limited to hydrodynamics in the context of continuum mechanics. It turns out, however, that the Boltzmann equation can be drastically simplified and still serve as a hyperbolic superset of the Navier–Stokes equations.

Construction of effective and efficient schemes based on kinetic equations requires several approximations. First, the velocity space $\vec{v}$ must be drastically reduced to a finite set of a small number of discrete velocities $\{\vec{e}_j\}$ (see, for example, Figure 1), which leads to b coupled discrete Boltzmann equations for the distribution functions $\{f_i\}$.

The second approximation is to linearize the collision operator. The simplest linearized collision operator, the so-called Bhatnagar–Gross–Krook (BGK) model, approximates the tendency of the system to approach equilibrium by a relaxation process with a constant relaxation time τ.

The third approximation is a coherent discretization of space–time such that the resulting discrete system, the lattice Boltzmann equation (LBE), can be interpreted as a simple two-step evolution procedure for $\{f_i\}$ on a discrete lattice: local collision (i.e., the relaxation process) with constant relaxation times, and advection of the distribution functions from one lattice point to the next according to the discrete velocities.

If the discrete equilibrium distributions are properly chosen as low-order polynomials of the conserved moments of $\{f_i\}$, the LBE can solve the incompressible Navier–Stokes equation with the kinematic viscosity υ as a linear function of the relaxation time τ and the pressure as coupled to the density by an ideal gas equation of state. The lattice Boltzmann equation is in essence an explicit time-marching finite-difference scheme with second-order accuracy in space. The main advantages of the LBE method are very low numerical dissipation, even at scales comparable to the grid spacing, as well as very low dispersion as compared with conventional second-order schemes for the Navier–Stokes equation.

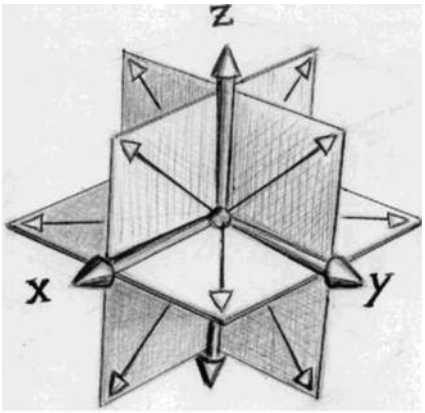

Figure 1. *A set of 19 microscopic velocities spanning a cubic unit cell (D3Q19).*

The lattice BGK scheme sketched here can be improved considerably in terms of stability, and thus computational efficiency, by using a generalized LBE with multiple-relaxation-time models. The generalized LBE is a projection method: The collision process is executed in the moment space spanned by an orthogonal basis, while the advection is performed in the velocity space. Exploiting the maximum number of degrees of freedom in the relaxation process leads to significant improvements in the stability and accuracy of boundary conditions of the LBE method. Numerous extensions in the past two decades have made the LBE method a competitive numerical tool for a wide range of problems, including turbulent flows (see Figure 2), thermal flows, multi-component and multiphase flows, free-surface flows, fluid–structure interactions, viscoelastic fluids, particulate suspensions, colloids, and other complex fluids.

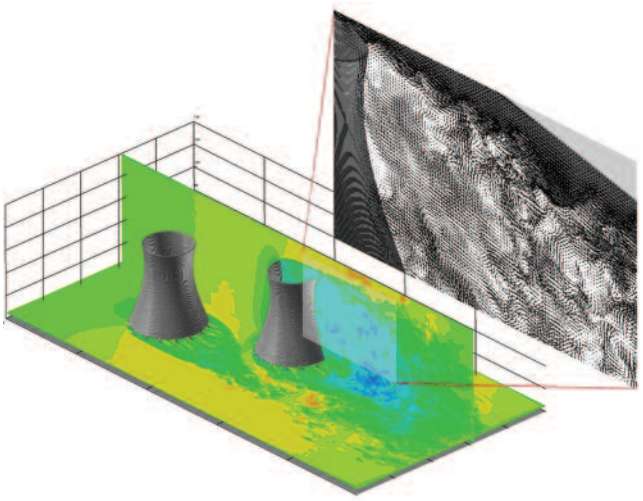

Figure 2. *Snapshot from a large-eddy lattice Boltzmann simulation of turbulent flow around two cooling towers at Re = 10^8 with more than 10^9 degrees of freedom.*

We organized two minisymposia for this year's SIAM Conference on Computational Science and Engineering to present the latest developments in lattice Boltzmann methods. The speakers covered both theoretical developments and practical applications, including direct numerical simulation of turbulence (L.-S. Luo, Old Dominion University), LB methods for magnetohydrodynamics (P. Dellar, Oxford University), use of GPUs for teraflop/s LB computations on a desktop PC (C. Janßen, TU Braunschweig), LB simulations of thermal flows induced by radiative heat transfer (M. Krafczyk, TU Braunschweig), viscous flow and colloid transport in resolved porous media (L. Wang, University of Delaware), large-scale LB simulations of fluid–structure interaction (J. Götz, University of Erlangen), LB simulations of biomedical flows (J. Bernsdorf, NEC Europe), and

multi-species LB models and their application to sustainable energy systems (P. Asinari, Politecnico di Torino). The results presented in the minisymposia demonstrated that the LBE method is highly efficient in terms of parallelization and effective for problems involving multi-physics and complex geometries.

Our minisymposia offered a great opportunity to communicate recent developments in kinetic methods to the SIAM community and have surely paved the way for sessions in this area at future meetings. They also provided a lively forum for the exchange of ideas among scientists working in this area.

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