

Equations of the Lattice-Boltzmann Method

The Boltzmann equation for any lattice model is an equation for the time evolution of $f_i(\mathbf{x}, t)$, the single-particle distribution at lattice site $\mathbf{x}$:

$$f_i(\mathbf{x} + \mathbf{e}_i, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i(f(\mathbf{x}, t)),$$

where $\Omega_i = \Omega_i(f(\mathbf{x}, t))$ is the local collision operator at that site, $i = 0, 1, \dots, 14$, and Δt is assigned a value of unity. Since the usual aim of lattice methods is to model macroscopic dynamics, the “exact” collision operator is unnecessarily complex and therefore numerically inefficient. Two groups (see Chen *et al.* and Qian *et al.* in the Further Reading) nearly simultaneously suggested that the collision operator be approximated by a single-time-relaxation process in which relaxation to some appropriately chosen equilibrium distribution occurs at some constant rate. In particular the collision term, $\Omega(f)$, is replaced by the single-time-relaxation approximation,

$$\Omega_i(f(\mathbf{x}, t)) = -\frac{f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t)}{\tau}.$$

The appropriately chosen equilibrium distribution, denoted by f^{eq} , depends on the local fluid variables, and $1/\tau$ is the rate of approach to this equilibrium. The relations $\sum_i \Omega_i = 0$ and $\sum_i \mathbf{e}_i \Omega_i = 0$ must be true to conserve mass and momentum, respectively. In order for the fluid to have Galilean-invariant convection and a pressure that does not depend on velocity, an appropriate equilibrium distribution, f_i^{eq} , must be assumed. For a two-dimensional hexagonal lattice, the formula is:

$$f_i^{\text{eq}} = \frac{\rho(1 - \alpha)}{6} + \frac{\rho}{3} \mathbf{e}_i \cdot \mathbf{v} + \frac{2\rho}{3} (\mathbf{e}_i \cdot \mathbf{v})^2 - \frac{\rho}{6} \mathbf{v}^2$$

and

$$f_0^{\text{eq}} = \alpha\rho - \rho\mathbf{v}^2.$$

(The corresponding formulas for the cubic lattice appear in the article by Alexander, Chen, and Grunau listed in the Further Reading.) In these equations the density $\rho(\mathbf{x}, t) = mn(\mathbf{x}, t)$ (where m is the mass of each particle), the number density $n(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t)$, and α is a free parameter related to the sound speed as shown below. For the lattice-Boltzmann method, the particle distribution does not have an upper bound. The only requirement is that $f_i \geq 0$.

To derive the macroscopic equations obeyed by this model, one performs a Taylor expansion in time and space and takes the long-wavelength and low-frequency limit of the lattice-Boltzmann equation for the single-particle distribution. The result is a continuum form of the Boltzmann equation correct to second order in the lattice spacing and the timestep. A scaling expansion argument, the assumption of single-time relaxation, and the neglect of higher-order terms lead to the following final form of the macroscopic equations obeyed by the simulated system

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_\beta)}{\partial x_\beta} = 0, \text{ the equation of mass continuity;}$$

$$\frac{\rho \partial v_\alpha}{\partial t} + \rho v_\beta \frac{\partial v_\alpha}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta} \left[\frac{\lambda}{\rho} \left(\frac{\partial \rho v_\gamma}{\partial x_\gamma} \delta_{\alpha\beta} + v_\alpha \frac{\partial \rho}{\partial x_\beta} + v_\beta \frac{\partial \rho}{\partial x_\alpha} \right) \right] + \frac{\partial}{\partial x_\beta} \left[\mu \left(\frac{\partial v_\beta}{\partial x_\alpha} + \frac{\partial v_\alpha}{\partial x_\beta} \right) \right],$$

the equation of momentum conservation; and

$$p = \frac{1 - \xi}{2} \rho.$$

the equation of state.

In the above equations, v_β is the component of the velocity in the β -direction; p is the pressure; and the sound speed, c_s , is $\sqrt{(1 - \xi)/2}$, where ξ is a free parameter. The shear viscosity, μ , and the bulk viscosity, λ , are given by

$$\mu = \frac{2\tau - 1}{8} \rho$$

and

$$\lambda = \frac{(\tau - 1/2)(2\xi - 1)}{4} \rho.$$

The above equations converge to the exact incompressible Navier-Stokes equations only when the derivatives of the number density in the second viscosity term on the right-hand side of the equation are small. Since the gradients of the density are $O(v^2)$, the unphysical terms in the momentum-conservation equation are correct to order (v^3) . Thus, although the physics of the lattice-Boltzmann method contains compressibility effects, one may come arbitrarily close to solving the incompressible Navier-Stokes equations by reducing the Mach number (through the choice of α) and thereby reducing the simulated flow to very low speed. (Nevertheless the compressibility effects in the lattice-Boltzmann approach are physical and the method can also be used to simulate compressible fluids.)

Traditional methods for solving incompressible flows, such as finite-difference or finite-element, require solution of a Poisson equation for the pressure term, which is induced by the mass-continuity equation and the momentum-conservation equation. In the lattice-Boltzmann approach, this time-consuming step is avoided because the incompressibility requirement has been relaxed and the effects of pressure changes are controlled by an equation of state rather than a Poisson equation. It can be argued that the conventional methods most closely related to the lattice-Boltzmann method are the pseudocompressible algorithms for solving incompressible fluid flows. $\square$