LBM for Rarefied Gas Flows

Seminar Lattice Boltzmann Methods:
Theory, Implementation and Applications

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1 Introduction

If someone tried to sell a Computational Fluid Dynamics software, based on the Lattice Boltzmann Method to, e.g., a car manufacturing industry, he/she would probably have to face the argument "but we successfully use a software that solves the Navier-Stokes equations for many years now!". Indeed, the Navier-Stokes equations are the main tool of the classical approach to the CFD. Yet, they bring with them some important *assumptions*, that restrict their usage in a limited range of applications. The fundamental assumption they pose is the *continuity of the matter*. In the case of the car manufacturer, that has to solve problems mainly in the scales we can see and touch, the matter appears to be continuous, so the application of the NSE is usually legit.

Modern engineers though need to design devices far smaller than cars, in which fluids or gases need e.g. to flow through pipes smaller than hair. Such devices are for example micropumps, micromotors and other Micro-Electro-Mechanical Systems [1]. Micro- and nano-flows are also faced in Chemical Engineering and relevant fields, in devices like microreactors [3], particle separators [1] or in materials with nanopores, like in the shale-gas extraction process (see e.g. [4, 8]). The continuity assumption breaks down in such scales, as e.g. the molecules of the used gases are so rare that interact mainly

with the walls and less with other particles. The same holds also for very low-pressure scenarios as in aero-astronautics applications [5].

In such problems, LBM can be applied, though the Bhatnagar-Gross-Krook, single-relaxation-time approach poses some problems because of the rare collisions of the molecules. Various modifications have been proposed to solve these problems and some of them are going to be presented in this work.

2 Rarefied gas flows

2.1 The Knudsen number

For gases we define their *Mean Free Path* as the average distance that the molecules of this gas are travelling without taking part in collisions. The MFP of a hard-sphere gas in thermodynamic equilibrium is given by the equation [7]:

$$\lambda = \frac{1}{\sqrt{2}\pi \cdot n_\mathrm{g} \cdot d^2} \tag{1}$$

where d is the mean molecular diameter and n_g the number density of the gas. Referring to the mean molecular spacing as δ, $n_\mathrm{g} = \delta^{-3}$. For air at atmospheric conditions ($T = 298\,\mathrm{K}$, $p = 1\,\mathrm{atm}$), $\lambda_\mathrm{air} = 6.111 \cdot 10^{-8}\,\mathrm{m}$ while for the (lighter and smaller) helium $\lambda_\mathrm{He} = 17.651 \cdot 10^{-8}\,\mathrm{m}$. [1]

Knowing the MFP of a gas we can compute the *Knudsen number* for a given scale. This is defined as the ratio of the MFP to the characteristic length L_0 of the geometry:

$$\mathrm{Kn} := \frac{\lambda}{L_0} \tag{2}$$

The length L_0 can also be a limit above which very large variations of a macroscopic quantity Φ_0 may be observed and we can also write:

$$\mathrm{Kn} \approx \frac{\lambda}{\Phi_0} \cdot \left|\frac{\mathrm{d}\Phi_0}{\mathrm{d}L_0}\right| \tag{3}$$

In complex geometries, a local Knudsen number can be chosen to solve the problem of deciding about the characteristic length. Equation 3 gives a good intuition for the relevance of the Knudsen number with the continuity assumption, as in "continuous" scenarios (small Kn) we would expect small variations of macroscopic quantities. We can also relate the Knudsen number to the Mach and Reynolds numbers [7]:

$$\mathrm{Kn} = \frac{\lambda}{L_0} \cdot \sqrt{\frac{\pi\gamma}{2}} \cdot \frac{\mathrm{Ma}}{\mathrm{Re}} \tag{4}$$

where $\gamma := c_p/c_V$ is the specific heat capacity ratio of the gas.

2.2 Division of the gas flow regimes

The Knudsen number can be used to divide different *flow regimes* and a rough, empirical classification can be found in figure 1. [7] The region $\mathrm{Kn} < 10^{-2}$ (or $\mathrm{Kn} < 10^{-3}$, as more recently suggested) is referred to as the *continuum regime*, in which the thermodynamic equilibrium assumptions hold and the application of the Navier-Stokes equations with the usual no-slip boundary conditions is valid. The other part of the range, where $\mathrm{Kn} > 10$, corresponds to the *free molecular regime*. In this area, the molecules almost do not collide with each other.

In between, the gas flow may belong to the *slip-flow regime* ($10^{-2} < \mathrm{Kn} < 10^{-1}$) or to the *transition regime* ($10^{-1} < \mathrm{Kn} < 10$). In the slip-flow regime, methods assuming continuity can still be applied but they will fail near the walls, as there non-equilibrium effects like temperature jump dominate and the no-slip condition cannot be satisfied. In the transition regime, the thermodynamic equilibrium assumptions begin to break down, as the "Knudsen layer" forces a non-linear stress-strain relationship for the flow near the wall.

Which regimes are mainly of practical interest? The term *Rarefied Gas Flows* usually refers to the slip-flow and the transition regime. As an example, $\mathrm{Kn} = 1$ for air is achieved around length scale $L_0 = 65\,\mathrm{nm}$. In some applications, different scales and flow regimes may be paired (*mixed flow regimes*), leading in the need to study transport phenomena in a wide Knudsen range. [1]

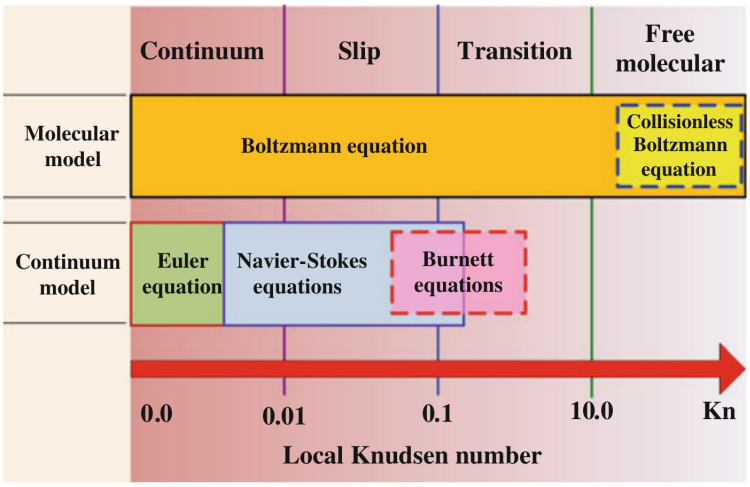

Figure 1: Division of the gas flow regimes in relation to the Knudsen number, along with the limits of different CFD approaches. [7]

3 Breaking down the continuum assumption

Do we need anything more here?

4 Extending the LBM to the slip flow regime

Lorem ipsum.

5 The LBM in the transition flow regime

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6 A stochastic model for finite Knudsen numbers

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7 Conclusion

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