Mesoscopic Computational Haemodynamics

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Chapter 1

Introduction

Physiology has widely been practised throughout time: along China's Yellow River long before the Chinese Civilisation, by the Indians along the Guanges River and by Egyptians and Nubians along the River Nile. It flourished during the time of Hippocrates (460–370 B.C.), the father of Western medicine and through the period of Aristotle (384–322 B.C.) who tutored Alexander the Great. Galen (130–200 A. D.) developed the first theories of anatomy and physiology and Ibn Sina (980–1037) made further contributions with his *Al-Qanoun*. Ibn Ul -Nafis (1210–1288) became the founder of coronary arteries circulations as we know it today and in his description of pulmonary circulation. He was the main forerunner of Servetus, Vesalius, Colombo and Harvey who in many ways proved the existence of the circulation[1] (Harvey, 1628). From this, a lot is known about how blood flows. The available literature is far too extensive to be cited in a short introduction. The book of Hippocrates on *aphorisms*, that of Aristotle *on the Parts of Animals* (384–322 BC), the Chinese book *Nei Jing* (the Internal Classic) during 472–221 BC, Ibn Ul-Nafis commentaries on medicine, and Harvey's book *On the Circulation of the Blood* (1628) are a few treasures to mention. However, all these attempts described the circulation in a qualitative way. The rules of mechanics were not yet formalised.

The seventeenth and the eighteenth centuries witnessed considerable development in mathematics, physics and related sciences. The concepts of calculus, instantaneous velocity and acceleration were introduced. Works on number theory and calculus by Fermat (1601–1665) were published for the first time as was the following three axioms of Newton (1642–1727) who also recorded the concept of viscosity (Newton, 1687). Euler (1769) formulated the use of differential equations to describe fluid flow. Cauchy (1823) introduced the concept of stress which continues to be at the basis of today's mechanics. Investigations of circulatory function in a Newtonian

[1]Ibn Ul-Nafis' book on *Sharh Tafseer al Qanoun* was translated by Andrea Alpago in 1547. In this book he stated that "The heart has only two ventricles ... and between these two there is absolutely no opening. Also dissection gives this lie to what they said, as the septum between these two cavities is much thicker than elsewhere. The benefit of this blood (that is in the right cavity) is to go up to the lungs, mix with what is in the lungs of air, then pass through the arteria venosa to the left cavity of the two cavities of the heart ..."

sense by Hales[1] established new quantitative and experimental concepts in the field of haemodynamics, the science dealing with blood flow. During the time of the French Revolution, Navier (1822) and Stokes (1845) derived the still accepted Navier-Stokes (NS) partial differential equations that fully describe incompressible viscous fluids. Following this, Poisson developed a theory that also holds for compressible fluids. Meanwhile, the nature of elasticity attracted Thomas Young who studied the relation between the velocity of propagation of the arterial pulse and the elastic properties of arteries.[2]

It did not take long for the Navier-Stokes equations to be accepted as the equations governing fluid flows. Nevertheless, these equations were, and still are very difficult to solve, except for a few idealised cases. Therefore, the approach was still highly theoretical. Moreover, with the NS solution the fluid dynamic limit (at vanishingly small mean free path) is singular at the shock regions. Thereafter, with the development of research in partial differential equations and numerical analysis, it was possible to extract useful information by finding numerical solutions to the NS equations.

During this period, relaxation methods and finite-element-like solutions were reported (Schellbach, 1851). Bessel functions were fully developed by Bessel in 1824. Hagen (1797–1884) and Poiseulle (1797–1869) established the experimental relation between flow rate and pressure gradient for steady viscous flows, which has since been worked out by Hagenbach in 1860 (see e.g. McDonald, 1974) who solved the Navier-Stokes equations for a tube flow. The Webers'[3] works on the influence of vessel elasticity and the dynamics of wave motion on blood flow, together with Moens, Korteweg and Résal has been a great contribution to understanding wave propagation in the circulation (McDonald, 1974). Formation of differential equations for problems of biological interest and attempts to solve them analytically or numerically appeared by the end of the nineteenth century. As the computational need increased, Charles Babbage (1792-1871) proposed the idea of an analytical engine as a computing machine. These are just a few of the great names associated with the historical development of haemodynamics before the start of the twentieth century.

Theories on atomic constituents of matter and sooner, laws of statistical mechanics and thermodynamics were under control since the beginning of last century. Clausius, Maxwell and Boltzmann (1844-1906) are to be regarded as the founders. Statistical mechanics explains how the properties of atoms such as mass, charge, and structure determine the visible properties of matter such as viscosity, thermal conductivity,

[1]Hales, among other achievements, measured the arterial blood pressure (in the horse) for the first time. He also introduced the concept of peripheral resistance. For his many achievements, he deserves the title 'father of haemodynamics', as suggested by McDonald, a pioneer in haemodynamics of the last century.

[2]It is worth noting that Young, who was a practising physician as well as a physicist, gave an interesting lecture to the Royal Society on the function of the heart and arteries (Young, 1809) in which he said " The mechanical motions, which take place in animal body, are regulated by the same general laws as the motions of inanimate bodies... the circulation of the blood depends on the muscular and elastic powers of the heart and of the arteries, supposing the nature of those powers to be known, must become simply a question belonging to the most refined departments of the theory of hydraulics."

[3]Weber brothers also pioneered in electrophysiology.

pressure, and diffusion. Instrumentation enhanced as a consequence of war demand. In the mean time, a new era of haemodynamics has flourished.

The early twentieth century started with a clear theoretical and experimental idea about the mechanics of the circulation. Manometers capable of measuring pulsatile flow were invented by Otto Frank (1903), leading to a huge accumulation of measured data on pressure pulse. Before and during World War I, sophisticated calculations, with the aid of a Pascal calculator, and reasonably precise measurements of the macroscopic world have been made. The discovery of the string galvanometer and its use in electrocardiography (*het tele-cardiogram*) by Willem Einthoven in 1906[1] opened a new chapter in the study of haemodynamics. Just before World War I, vascular anastomosis and transplantation to treat stenosis and thrombosis were remarkably successful (Carrel[2], 1912). Thereafter, Frank (1927), Womersley (1955a, 1955b; 1955c) and McDonald (1955; 1960) introduced Fourier harmonics and came up with the Womersley solution for pulsatile flow. From there on, theoretical development about pulsatile flow has been completed; the Womersley solution well describes the macroscopic nature of pulsatile flow in arteries. Interests were then shifted towards closer investigation of blood rheology, and fluid-structure interaction. Theories on non-Newtonian fluids and effects were developed and questions on high and low-shear-limits were raised.

Since the middle of the twentieth century, the arterial system has been treated as being in a steady-state oscillation produced by repeated heart beats and the cardiac pulse was represented by its Fourier harmonics.

Computers of the first generation were hardly used by physiologists since they were not widespread. Physiologists, like other researchers in fluid mechanics started to think of modelling flow in more complex geometries. A need for computer simulations was then realised. However, the history of computing during the 1950's and the 1960's is of less importance to the development of haemodynamics, although it is not the case for fluid mechanics. For instance, one of Mark I's applications was to solve ordinary differential equations by the Runge-Kutta method. Iterative solutions of multidimensional partial differential equations were reported (e.g. Stone, 1968).

Numerical fluid dynamics, later called computational fluid dynamics (CFD) was identified (see Garrett Birkhoff in Nash (Ed.), (1990) for extended survey), but mostly engaged in developing and understanding the fluid mechanics of war machines and in space dynamics. However, shortly after the availability of computing facilities, mathematical models and simulations of a biological nature began to develop (e.g. Turing, 1952; Lindermayer, 1968). With the development in computer power, finite difference method and the finite volume method were then ready to solve flow in complex geometries. Primitive versions of the finite-element method were introduced during the 1950's (e.g. Argyris, 1952; Turner *et al.*, 1956; Clough, 1960) and landmarks in its development were established during the 1960's (Przemieniecki *et al.*,

[1]The first cardiogram can be seen at http://www.einthoven.nl/images/fotos/eh002.jpg

[2]Carrel is also known with his "Man the Unknown" book (1935) in which he said "We must arise and move on. We must liberate ourselves from blind technology and grasp the complexity and the wealth of our own nature."

1965). Although the finite difference (e.g. Roache, 1972) and finite volume methods (e.g. Spalding, 1981) were the ones most commonly used, significant difficulties in modelling complex geometries and applying local grid refinement techniques to resolve flow in regions of large velocity gradients were faced until the finite element method was matured in the late 1970's (e.g. Girault and Raviart, 1979). However, it was believed that the finite element method could not be applied to un-symmetric operators, and therefore, use of the methods for solving fluid flow problems was not realised until the first works on solutions of NS equations with the finite element methods appeared (e.g. Oden, 1970; Oden and Somogyi, 1968, Aziz, 1972). Thereafter, the mathematical theory, including priori error estimates was fully developed and from that time the finite element method has become popular in solving many engineering problems.

Until the middle of 1980's, finite elements methods were not fully formulated to deal with unsteady flow simulations in realistic geometries (van de Vosse, 1987). It is worth noting that till that time, it was not possible to measure time-dependent flow *in vivo* with the available techniques. This gave computational modelling a chance to grow in order to fill this gap. During this period, hypotheses on arterial wall shear stress and its relation to atherosclerosis were tested (e.g. Caro *et al.*, 1969; Zamir, 1977). It may be stated that in vitro, idealised models, and animal experiments were the main modes of cardiovascular investigations during the 1970's.

During and since the 1980's, a new era of computational haemodynamics has been initialised, associating the dramatic increase in computational power, and enhancements in imaging techniques and computational methodology. The localisation of cardiovascular diseases in certain segments of hydrodynamic complexity has been reported (e. g. DeBakey *et al.*, 1985; Thubriker and Robicsek, 1995). Since then, the finite element methods have become adequate and widespread in solving fluid flow problems. In this thesis, most of the cited literature about computational haemodynamics involve the finite element method as a flow solver.

However, the finite element method consumes both memory and computational time. This is attributed to the time consuming generation of the body fitted computational grid, and to the explicit nature of solving the Poison equation. With the development of computer power and advances in parallization methods, the computational time for finite element methods was significantly reduced. Nevertheless, a high demand on interactive simulations is raised. The finite element methods are still far from being interactive. An average simulation time for solving flow in a geometry like the abdominal aorta may take half a day on a single processor of today's technology. Since the computational grid is body fitted, parallization of finite element method is not straightforward as it is for Cartesian grids. Therefore, a tendency to prefer Cartesian grids is slowly growing. In addition, recent years have seen a growing interest in developing numerical algorithms for compressible multi fluids with the need to model multi-component flows. The difficulty in measurement of multi-component flow properties (e.g. Baker, 1991) with traditional computational fluid dynamics solvers, as they are faced with a challenge to produce physically correct solutions (e.g Igra and Takayama, 2002; Fedkiw, 2002) raised a high demand in adopting new robust

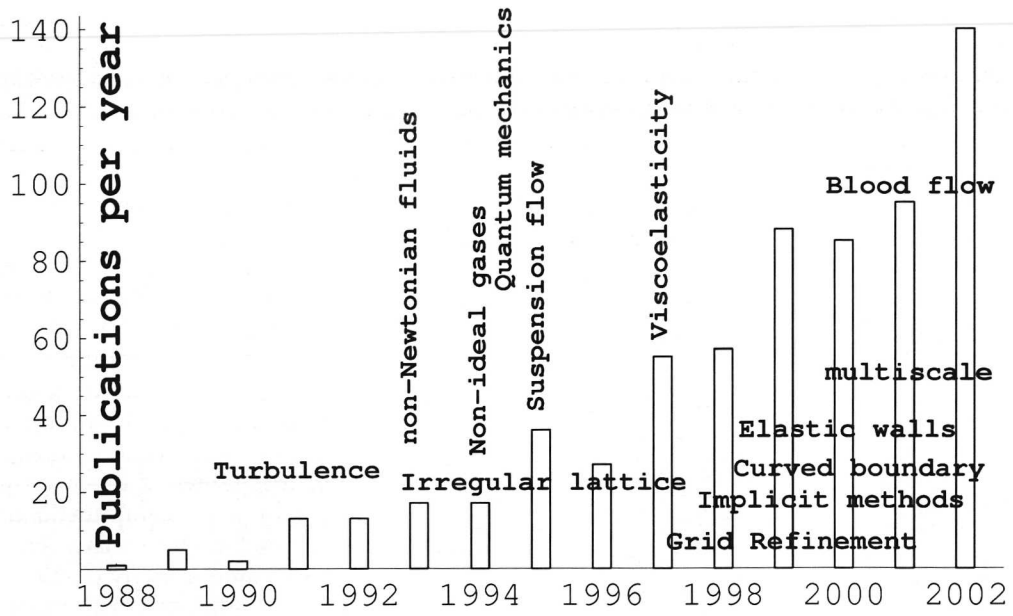

Figure 1.1: Evolution of lattice Boltzmann models in terms of applications (text) and annual number of publications (columns). The graph is generated using the ISI Web of Science and Science Direct digital databases.

techniques. Mixed finite elements techniques (Raviart, 1984) is now being used as a standard way of deriving high-order conservative approximations.

New particle based methods such as dissipative particle dynamics, lattice gases and lattice Boltzmann methods have been developed and matured (McNamara and Zanetti, 1988; Higuera and Succi, 1989; Qian *et al.*, 1992; Aharonov and Rothman, 1993; Behrend, 1995). These mesoscopic techniques have been proved successful in many applications (see Fig. 1.1) and may be quite useful for haemodynamic research, as, among other features, they are more flexible in modelling suspensions.

1.0.1 Going Mesoscopic

It is well known that accurate predictions of the behaviour of fluids is possible with the standard macroscopic representation in which the continuum hypothesis[1] and local thermodynamic equilibrium are assumed. The validity of a macroscopic approach holds only if all macroscopic length and time scales are considerably larger (a few

[1]Matter is assumed to occupy every point of the space of interest, regardless of how closely the material is investigated.

hundreds) than the largest molecular length and time scales[1] (e.g. 60 nm and 0.1 sec for nitrogen). The Navier-Stokes equations treat the fluid macroscopicly. Therefore, they are only valid when the length and time scales are such that the fluid is in local thermodynamic equilibrium. With large spatial and temporal gradients, local thermal equilibrium may not be guaranteed over the macroscopic time sclaes and the NS equations would not be an accurate mathematical model to solve. For a better understanding of macroscopic behaviour, and for more accuracy, one may investigate the microscopic world of cells and atoms. The question of whether it is time to go microscopically in haemodynamics may be argued for some time to come, but it may be realised, even now, that microscopic details about rheology of blood and the nature of cardiovascular diseases are needed, and the only way to understand that is by avoiding idealistic simplifications when investigating blood mechanisms. For instance, the non-Newtonian behaviour of blood flow, the chemical interaction with the enzymes produced in the arterial system and the drug-blood relation are all challenging us. It can be argued that this is enough to try different approaches in haemodynamics. Solving the NS equations, which are based on Newtonian mechanics of the macroscopic world, is not enough to handle this problem. Unfortunately, the computational power is far behind performing molecular dynamics simulations[2] even in a tiny arterial segment[3]. As one cannot construct a fully deterministic theory of many particles in motion, the introduction of statistical mechanics by Maxwell (1866) and Boltzmann (1872)[4] provides an alternative approach with which the high abstraction of macromechanics is limited. Statistical mechanics suggests Boltzmann transport equation as an alternative mesoscopic approach to Newton's laws of motion. This has been recognised as a real breakthrough in theoretical physics.

The Boltzmann equation is still hard to solve and only perturbative approximations are used in fluid dynamics (Caflisch, 1983). Numerical solutions of the Boltzmann equation have many applications, ranging from nuclear reactor design, through medical radiation physics, to high energy physics. Both deterministic and stochastic approaches are widespread. Deterministic solutions are fast, but are usually associated with discretization errors. Monte Carlo methods are more accurate but are quite slow. Recently, considerable efforts have been made in both directions.

[1]The length scale is usually taken as the mean free path between collisions while the time scale is represented by the time between successive collisions.

[2]In molecular dynamics, the interaction between individual molecules is computed for the whole system.

[3]For 100k atoms, it takes a week to simulate a nanosecond on an Athlon cluster of 32 processors with NAMD, a molecular dynamics code designed for high-performance simulation of large biomolecular systems. See http://www.ks.uiuc.edu/Research/namd/

[4]Boltzmann was the first to show that the entropy increases with time. His atomic hypothesis gave him a hard time that he didn't survive to see being proved one year after his death.

1.0.2 Choice of the Numerical Method

Just after World War II, the ENIAC computer was built. This changed the world of computing in many aspects. The early Monte Carlo calculations[1] and sampling techniques were made possible (e.g. Richtmyer and Metropolis, 1949) and with the introduction of the cellular automata by von Neumann in 1948 (the universal computing machine, to mimic the complexity of nature), computers have been recognised as a kind of experimental laboratory rather than just number processing devices. Since then, Lattice Gas automata (LGA), a special category of cellular automata, were developed and have been proved to model hydrodynamics in a much simpler way than the conventional computational fluid dynamics solvers. Although it may be considered as a particular class of cellular automata with some additional constraints (Rivert and Boon, 2001), lattice gases can be described, from a physical point of view, as a simple fully discrete microscopic model of a fluid in which fictitious particles reside on finite regions of a regular Bravais lattice. It is therefore a particle-in-cell method, in which the continuous physical domain is broken-up into a number of discrete states. Particles move with discrete velocities, stream to neighbouring sites where they collide under collision rules and stream again in a continuous way till a predefined equilibrium state is reached. Currently there are a considerable number of lattice gas models, being adapted to simulate specific applications. More details on lattice gas hydrodynamics were described in the recent books of Rothman and Zaleski (1997), Chopard and Droz (1998), and Rivet and Boon (2001).

Although they proved successful in returning the elegance of Physics, lattice gas models were met with two major difficulties: they are very noisy due to their Boolean nature[2], and they do not satisfy Galilean invariance[3] due to the velocity dependent density in the equations of motion.

Being established to overcome these problems, the lattice Boltzmann method (LBM) may be considered as an attractive alternative to conventional computational fluid dynamics solvers such as the finite elements and the finite difference methods. This is due to its simple implementation, straightforward parallelism, easy grid generation and its proven capability in simulations of multi-component flows and complex geometry. The lattice Boltzmann method is nowadays considered as a matured computational fluid dynamics flow solver. The method competes with traditional Navier-Stokes solvers by directly obtaining the pressure without a need to solve the Poisson equation and obtaining the stress tensor without using simulated velocity gradients. This strong argument is not yet taken seriously since the method is still developing while the conventional solvers are quite mature.

This motivated us to test the capability of the method in the field of haemodynamics, in which it is hardly used, although it has often been argued that the method has many capabilities that may attract researchers in haemodynamics. Pioneering work

[1] It is believed that Enrico Fermi (1901-1954) was the first to use what was to be called later the Monte Carlo method in studying the moderation of neutrons in 1930's in Rome (see Nash (Ed.), 1990).

[2] The lattice gas intrinsic fluctuations may be used to capture the essentials of actual fluctuations in real fluids. For more details see Rivet and Boon(2001).

[3] A frame of motion is Galilean invariant if the equations of motion do not change in all other frames.

in this direction was done by Krafczyk *et al.* (1998).

1.0.3 Objectives of This Study

As the complex nature of blood flow in the human arterial system is still gaining more attention, and since cardiovascular diseases are considered a leading cause of death in the developed world and are now becoming more prevalent in developing countries (World Health Organisation, 2002), the main objective of this thesis is to better understand the nature of blood flow in realistic geometry (namely patient specific geometry produced from medical scanners) through solving the mesocopic Boltzmann transport equation with a simple to generate grid via the lattice Boltzmann method. Other objectives include testing capabilities, robustness, accuracy and performance of the lattice Boltzmann method for unsteady flows and development of tools to enhance them towards interactive simulations. Relevant flow quantities will be validated through experimental and/or macroscopic numerical data. The outcomes of the study will be used to develop a computer-aided surgical planning environment in a Grid-supported virtual environment.

1.0.4 Thesis Overview

In Chapter 2, we briefly review the basics of haemodynamics, focusing on recent development in mathematical modelling of blood flow circulation. Then we present model considerations. This chapter is based on available literature which may be referred to for further details.
A derivation of the lattice Boltzmann method from the Boltzmann equation and the discussions on its benefits and drawbacks are dealt with in Chapter 3. Formal error analysis and its relation to hydrodynamics non-dimensional parameters for time-dependent flows is presented. The advances in the theory of lattice Boltzmann methods are highlighted with a special focus on features related to time-dependent flows.
As the grid is Cartesian, discretization errors are eliminated in a two-dimensional benchmark simulations, aiming at understanding the error behaviour of the lattice Boltzmann method in detail. This is presented in Chapter 3 which involves steady flow in simple 2D geometries. A comparison with a conventional computational fluid dynamics solver is made.
Although the lattice Boltzmann method is easy to implement, it is not yet fully developed to deal with boundaries different than fluid ones. There are a number of boundary conditions that may be used but they are highly sophisticated and may violate the conservation laws and the stability of the system. However, there are some boundary conditions that are now popular due to their robustness in dealing with complex geometries. In this study, we focus only on those boundary conditions we believe can be used without difficulty in computational haemodynamics. In Chapters 4, 5, 6 and 8 initial and boundary conditions are studied.
In Chapter 5 three-dimensional pulsatile flow benchmarks are investigated. The Womersley solution is recovered within a very high accuracy.

One objective of this thesis is to seek a possibility of using the lattice Boltzmann method as a core for an interactive simulation environment believed to be useful in so called predictive medicine. Reasonably, computational aspects of the standard lattice Boltzmann method are discussed in Chapter 6, while Chapter 7 discusses acceleration techniques for time dependent flows.
Simulation results of steady and unsteady flow in a model of the human aortic bifurcation reconstructed from Magnetic Resonance Angiography are presented in Chapter 8 as a typical haemodynamic application. Velocity profiles and shear stress are presented and visualised. Qualitative and quantitative analysis of the flow fields and the shear stress are presented.
Although some studies on flow in elastic tubes were investigated by the author and others (Hoekstra *et al.*, 2003), results on flow in elastic structures are not discussed in this thesis.
Chapter 9 concludes the thesis with a brief summary, concluding remarks and plans for future work. Acknowledgement is given at the end of the thesis.