

CRANFIELD UNIVERSITY

JOSÉ OLIVEIRA

DEVELOPMENT OF PHYSICS OR HPC OPTIMISATION
OF A PARALLEL 2D LATTICE BOLTZMANN SOLVER
USING GPUS/CUDA

SCHOOL OF AEROSPACE, TRANSPORT AND
MANUFACTURING
Computational & Software Techniques In Engineering

MSc
Academic Year: 2016–2017

Supervisor: Dr Irene Moulitsas
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Abstract

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List of Abbreviations

CUDA	Compute Unified Device Architecture
CFD	Computational Fluid Dynamics
GPGPU	General-purpose computing on graphics processing units

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Chapter 1

Introduction

Chapter 2

Literature review

In this chapter, we will be taken into the broad field of the Lattice Boltzmann method using the CUDA platform. The topic of this thesis is associated with a number of different study areas, such as Computational Fluid Dynamics, Lattice Boltzmann method, High performance computing and GPGPU. We will then present an extensive literature review on these themes in the remaining of this chapter. Firstly, we will look into Computational Fluid Dynamics and the most commonly used approaches to it. Then we will be giving an overview on the Lattice Boltzmann method. Afterwards we will discuss how it is possible to employ parallelisation techniques in scientific computing. Finally we will review some previous works in this area.

2.1 Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) comes from the need to model fluid flows and associated processes. A wide range of applications come from studying CFD, notably:

- Aircraft design [4]
- Solid particle erosion [13]

- Wind flow simulation [3]
- Combustion chamber simulations [14]
- Environmental and weather prediction [15]
- Automotive and motor sports [16, 5]

CFD can be used as a design and troubleshooting tool, as well as making the process dynamics easier to understand. It is used extensively by scientists and researchers, but it also has innumerable applications in the industry. CFD simulations is a viable tool for manufacturing because it eliminates expensive simulations.

As such, it is the science of determining a solution to fluid flow through space and time [7]. The models needed to calculate the fluid computations include:

- Flow geometry
- Differential (Governing) equations – These describe the physics and chemistry of the flow
- Boundary and initial conditions
- Discretization of the domain

2.1.1 Macroscopic scale

In this approach, the fluid can be seen as a collection of a huge number of particles. To solve these governing equations, one needs to apply conservation of energy, mass and momentum [11]. But since these equations are difficult, or even impossible to solve analytically, discrete schemes, boundary and initial conditions are used to convert these equations into a system of algebraic equations. These equations can then be solved until an appropriate solution is produced.

These problems are usually solved using Navier-Stokes equations that describe the fluid being solved as a continuum, which apply Newton's second law to fluid motion.

2.1.2 Microscopic scale

If we consider the fluid to be represented by individual particles then we will fall under the microscopic approach. In this approach, there is no definition of temperature or viscosity and collision between particles needs to be considered. Thus one needs to solve the differential equation of Newton's second law [11]. Hence, the location and velocity of each particle needs to be taken into account.

We can easily see that this approach becomes unfeasible for normal fluid sizes as the number of equations needed to be solved grows to the order of billions (consider that one mole of water contains more than 6×10^{23} molecules).

2.2 Lattice Boltzmann Method

The Lattice Boltzmann method (LBM) is a mesoscopic scale approach to CFD. It is used to describe a fluid based on probabilities using the Maxwell-Boltzmann equation in the fluid's equilibrium state [11].

In this method, we do not consider the individual characteristics of each particle. By grouping particles together in a D2Q9 (nodes containing 9 particles for 2D problems - Fig 2.1) or in a D3Q19 (nodes containing 19 particles for 3D problems - Fig 2.2) model, we can analyse the behaviour of the particles collectively [11].

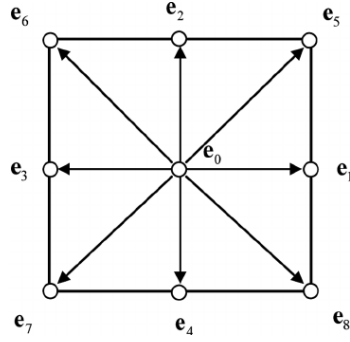


Figure 2.1: 2D LBM model using 9 particles. (D2Q9)

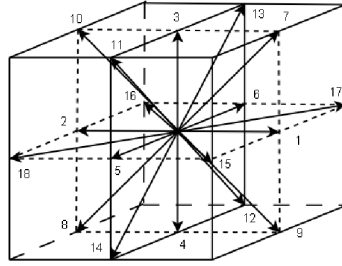


Figure 2.2: 3D LBM model using 19 particles. (D3Q19)

This way we can reap the advantages of both the macro and microscale approaches without the need of high end computers [11]. Since communications between nodes are very limited, LBM also offers the possibility of employing parallel computing to achieve the solution in even faster times.

2.3 High Performance Computing

As humanity evolves, so too does our desire for expanding previous unobtainable goals. As computer technology kept progressing further and further, we soon realised that some problems simply took too many resources to be completed.

Figure 2.3 shows the evolution of computing power over the past 120 years. Moore's

Law states that "processor speeds, or overall processing power for computers will double every two years" [2]. Note that the last 7 most recent data points are NVIDIA GPUs.

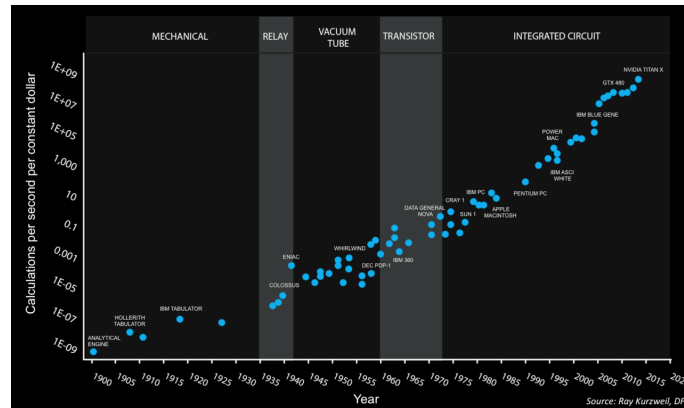


Figure 2.3: Moore's law over 120 years

However, this evolution in computational power could only be achieved by combining CPU cores together. So what if we focused our efforts in splitting the workload, effectively using the multiple cores available to produce a solution?

High performance computing (HPC) comes from the harnessing of computer power to deliver a much higher performance that one could not obtain from a typical computer. To this end, we can talk of HPC as being a collection of computer resources, all of them working simultaneously to achieve a solution of the same problem. Problems that could otherwise take weeks, months or even years can now be solved in minutes, hours or days under these powerful devices. However, different parallelisation strategies for splitting the workload emerge, depending on the underlying hardware.

It is also important to understand that parallel computing is achieved with the help of processors that will execute different calculations or processes simultaneously. To measure the parallelisation's efficiency, it is worth introducing the term Speed-up. The Speed-up is the ratio of the execution time of the parallel algorithm on a single processor

with the execution time of the parallel algorithm on P processors [12]. However, Amdahl's law states that "in parallelization, if P is the proportion of a system or program that can be made parallel (...), then the maximum speed-up that can be achieved using N number of processors is $\frac{1}{(1-P)+\frac{P}{N}}$ " [1]. This means that our parallelisation efforts are limited by the amount of work that can be parallelised and, theoretically, should follow the distribution represented in Figure 2.4.

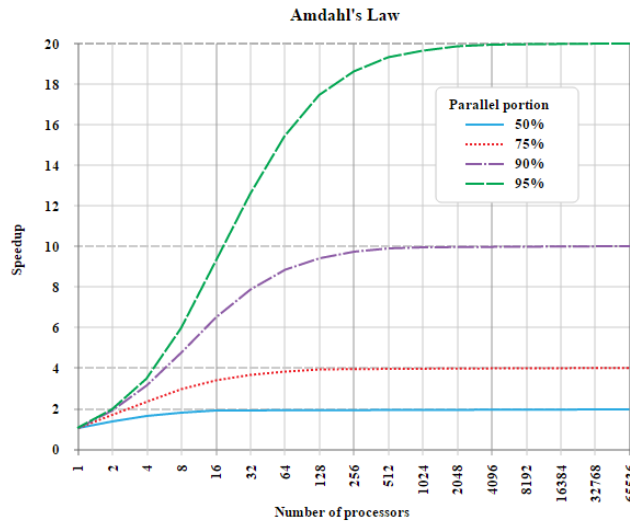


Figure 2.4: A graphical representation of Amdahl's law

2.3.1 Distributed memory

Following a distributed memory architecture for parallel computing means that each processor will have its own independent local memory. In these systems, all the work that one process executes remains local to it, without interfering with the address space of all other processors. Hence, to solve meaningful computations, a communication network needs to be established in order for processes to share data with each other. Such is the case of the Message Passing Interface (MPI).

This means that this architecture is very scalable: with each processor being added to

the system the size of the total memory increases. Also, each processor will be able to access its own memory rapidly and without interference, reducing the usual constraint of memory access penalties.

However, this type of system requires a higher degree of skill from the programmer. The programmer will be the one responsible for most of the details of memory passing between processors and will need to ensure that no race conditions or deadlocks arise from the data communication. Also, whenever data from another processor is needed, the latency of the bandwidth in the network will introduce a heavy time penalty to the computations, as this data will need to be communicated before computations can be performed over it.

2.3.2 Shared memory

2.3.3 GPGPU

General Purpose computing on Graphical Processing Units stands for the use of Graphics Processing unit (GPU) to perform computations on applications normally performed by the CPU. One of the main advantages of using this approach is the amount of cores that a single GPU has. While a typical desktop CPU has up to 4 cores, a GPU can have thousands of cores, allowing users to take advantage of its massively parallel architecture. GPUs can now solve problems that were traditionally solved by the CPU. This is a big improvement, since GPUs are cheaper to acquire and more powerful than CPUs.

NVIDIA then developed CUDA. CUDA code allows programmers to take advantage of GPUs by employing a unified shader pipeline under the familiar C language [8]. Users were no longer required to have specific knowledge of OpenGL or DirectX and could now perform general computations (rather than graphic-specific computations) whilst benefiting from the massive computational power offered by GPUs.

2.4 Previous parallelisation works

This thesis is a continuation of work that started some years ago in Cranfield University. As such, the work from the previous students needs to be analysed.

In 2014, Tamás Józsa and Máté Szőke, adapted two different in-house C and C++ codes into one single C code unifying the advantages of each one of the two original codes [9, 17]. Józsa then parallelised the critical parts of the C code using CUDA and ran tests on the Fermi GPU Cluster from Cranfield, achieving a three times speed-up in general, with a peak of 15 times speed-up [9].

Szőke proposes a CPU APPROACH different parallelisation approach using Unified Parallel C, which is a Partitioned Global Address Space language[17]. This means that it's possible to use shared memory to compute the solution. However, the author verified that a local memory-based approach (like MPI) provided the best results. He also compared the results obtained with the ones obtained by Józsa on the CUDA approach. They found that to achieve the same speed-up as that of a single GPU card, one needs an entire workstation (16 threads in the case of Astral) [17].

In 2015, Ádám Koleszár continued the work and further optimised the parallel version of the LBM method using CUDA [6]. He did an excellent job, resulting in a 10 times faster execution than the previous 2D parallel solver, which means that his new optimised code was 30 times faster than the original, in-house, serial solver.

Finally, in 2016, Maciej Kubat proposed a new version of the LBM solver. Firstly he converts the 2D parallel solver to a 3D parallel solver which entailed a major re-engineering of the code, from data containers to logic cycles [10]. After first trying for a direct adaptation, he found that his code was too slow to produce meaningful solutions. After optimising his own code he was able to reach an almost one hundred times speed-up. However, Kubat states that a lot can be done to improve his code, from boundary

conditions to code readability and maintainability.

Chapter 3

Conclusions

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