

Optimising and Parallelising d2q9-bgk.c

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Abstract

d2q9-bgk.c implements the Lattice Boltzmann methods (LBM) to simulate a fluid density on a lattice. This report outlines the techniques I utilised to optimise and parallelise d2q9-bgk.c, as well as a detailed analysis of those techniques. To do so, this report is split into several sections corresponding to different iterations of my code.

1 Original Code

I compiled the original d2q9-bgk.c using the GNU Compiler Collection (GCC) with the following command:

```
gcc -std=c99 -Wall -O3 d2q9-bgk.c  
-lm -o d2q9-bgk.
```

Table 1: Execution times of the original code

Test Case Size	Time (s)
128 × 128	29.16
128 × 256	58.71
256 × 256	233.32
1024 × 1024	980.89

Figure 1 contains the total time to initialise, compute and collate each of the test cases when running the ELF file produced. It was important to measure the original code, so that I could quantify the performance improvements of my latter implementations. I measured each of the total times by taking an average of 10 runs on Blue-Crystal Phase 4’s (BC4’s) compute nodes. Each of BC4’s compute nodes is a Lenovo nx360 M5, which contains two 14-core 2.4 GHz Intel E5-2680 v4 (Broadwell) CPUs and 128 GiB of RAM [1]. I took an average of multiple runs because of the variation between runs, which exists due to the inconsistent performance of compute nodes. It is important to note that I measured every execu-

tion time in this report in an identical manner to ensure my results were fair and unskewed.

2 Serial Optimisations

2.1 Compiler

Table 2: Execution times after compiler changes, and speedup over the original code

Grid Size	Time (s)	Speedup
128 × 128	22.25	1.31
128 × 256	44.42	1.32
256 × 256	176.69	1.33
1024 × 1024	795.41	1.23

I compiled my serial optimised implementation using the Intel C Compiler as opposed to GCC, since it provides better optimised code for Intel processors. Furthermore, I compiled my code with the `Ofast` option, which set aggressive options to improve the speed of my program, including `O3` optimisations and aggressive floating point optimisations [2].

2.2 Loop Fusion and Pointer Swap

Table 3: Execution times after loop fusion and pointer swap, and speedup over the original code

Test Case Size	Time (s)	Speedup
128 × 128	19.42	1.50
128 × 256	39.21	1.50
256 × 256	155.64	1.50
1024 × 1024	635.61	1.54

LBM is a memory bound problem. As a result of this, there was a significant opportunity to optimise d2q9-bgk.c by decreasing the number of memory accesses. One method I utilised to accomplish this was loop fusion. In the original code,

the entire grid was iterated over in four sequential procedures within each timestep: `propagate`, `rebound`, `collision` and `av_velocity`. By fusing the four loops in these procedures into one, I was able to drastically decrease the number of memory accesses, thereby improving the performance of my program.

Implementing loop fusion offered another significant opportunity to eliminate redundant memory accesses. The original code had a significant quantity of value copying between the `cells` and `tmp_cells` arrays. I was able to eliminate this by writing all new values of cells to a `cells_new` array, and simply swapping the pointers of `cells_new` and `cells` at the end of each timestep. Furthermore, I eliminated the `tmp_cells` array entirely.

2.3 Arithmetic Improvements

Table 4: Execution times after arithmetic improvements, and speedup over the original code

Test Case Size	Time (s)	Speedup
128×128	19.10	1.53
128×256	38.49	1.53
256×256	153.39	1.52
1024×1024	621.52	1.58

Despite the compiler being able to partially optimise the arithmetic within each timestep without making any changes to the code, there were still some manual improvements that I made to improve the performance of the program. Division is a very slow arithmetic operation relative to multiplication. Therefore, to eliminate a large number of unnecessary division operations I pre-calculated several values including:

$$\frac{1}{c^2} = 3 \quad \frac{1}{2c^2} = 1.5 \quad \frac{1}{2c^4} = 4.5$$

where c is the speed of sound. Additionally, I noticed that the number of cells in the grid that were not obstacles `tot_u` was recalculated and then divided by each timestep. I eliminated this inefficiency by counting number of cells that were not obstacles only once (during the initialisation phase). I then saved the reciprocal of this value as a parameter `num_non_obstacles_r`, which I used once per timestep in a multiplicative operation to compute the average velocity.

2.4 Vectorization

Vectorization is the process of converting a scalar implementation to a vector implementation, which enables the compiler to make use of additional registers to perform multiple operations in a single instruction [3].

Table 5: Execution times after vectorization, and speedup over the original code

Test Case Size	Time (s)	Speedup
128×128	5.79	5.04
128×256	11.66	5.04
256×256	40.81	5.72
1024×1024	213.53	4.59

I utilised several techniques to enforce single-instruction-multiple-data (SIMD) vectorization. Firstly, I compiled `d2q9-bgk.c` with the `xAVX2` option to direct the compiler to optimise for Intel processors that support Advanced Vector Extensions 2 (AVX2), which BC4’s compute nodes do [4].

Within my code, I implemented the `#pragma omp simd` pragma to vectorise the inner loop within each timestep. This pragma indicates to the compiler that SIMD instructions can be used to execute iterations of the loop concurrently. The `qopenmp-simd` option is enabled by default at optimisation levels of `O2` or higher to enable OpenMP SIMD compilation [2].

Additionally, I used the `restrict` keyword to assert that the memory referenced by pointers was not aliased and compiled my program with the `restrict` to enable pointer disambiguation. This provided a performance advantage as it prevented the compiler from performing a runtime test for aliasing.

3 Parallelism

3.1 OpenMP

3.2 Scaling

Table 6: Execution times after parallelising (run with 28 threads), and speedup over both the original and vectorized code

Grid Size	Time (s)	Speedup	
		Original	Vectorized
128×128	0.79	36.91	7.33
128×256	0.91	64.52	12.82
256×256	2.85	81.87	14.32
1024×1024	13.43	73.04	15.90

References

- [1] *BlueCrystal technical specifications*. URL: <https://www.bristol.ac.uk/acrc/high-performance-computing/hpc-systems-tech-specs/> (visited on Feb. 19, 2022).
- [2] *Alphabetical List of Compiler Options*. June 12, 2021. URL: <https://www.intel.com/content/www/us/en/develop/documentation/cpp-compiler-developer-guide-and-reference/top/compiler-reference/compiler-options/alphabetical-list-of-compiler-options.html> (visited on Feb. 20, 2022).
- [3] *Using Automatic Vectorization*. June 12, 2021. URL: <https://www.intel.com/content/www/us/en/develop/documentation/cpp-compiler-developer-guide-and-reference/top/optimization-and-programming-guide/vectorization/automatic-vectorization/using-automatic-vectorization.html> (visited on Feb. 21, 2022).
- [4] *Lenovo NeXtScale nx360 M5 (E5-2600 v4)*. URL: <https://lenovopress.com/lp0094-nextscale-nx360-m5-e5-2600-v4> (visited on Feb. 22, 2022).