

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

Table 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 BlueCrystal Phase 4’s (BC4’s) compute nodes. Each of BC4’s compute nodes was a Lenovo nx360 M5, which contained 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 existed due to the inconsistent performance of compute nodes.

2 Serial Optimisations

I initially implemented a collection of serial optimisations to improve the performance of d2q9-bgk.c.

2.1 Compiler

The first improvement I implemented was compiling with the Intel C Compiler as opposed to GCC, since it produced 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].

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

These changes to the compiler provided a reasonable performance boost, as shown in Table 2.

2.2 Loop Fusion and Pointer Swap

For all the test cases provided, the implementation of LBM in d2q9-bgk was 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 absorbing these four procedures into the `timestep` procedure and fusing the four loops, 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. I eliminated the `tmp_cells` array entirely.

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

Decreasing the number of memory accesses provided further performance improvements, as shown in Table 3.

2.3 Arithmetic Improvements

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 precalculated 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.

These arithmetic improvements provided only a small boost to performance compared to the prior implementation, as shown in Table 4. This was to be expected since the Intel C Compiler had already optimised a large amount of the arithmetic.

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

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]. I utilised several techniques to enforce single-instruction-multiple-data (SIMD) vectorization of the inner loop within each timestep.

Firstly, I converted the `t_speed` structure holding cell speeds from an array of structures (AoS) to a structure of arrays (SoA). Previously, the grid was represented with an array of `t_speed` structures, whereby each structure contained nine vectors. I altered this such that the grid was represented by one `t_speed` structure containing nine pointers, each to an array of floats. Each array of floats contained the values of one vector for each cell within the grid. The SoA format greatly suited vectorization of the inner loop, since it kept memory accesses contiguous when vectorization was performed over structure instances [4].

Having altered the data layout to suit vectorization, I utilised several other techniques to enforce vectorization. Within my code, I implemented the `#pragma omp simd` pragma to vectorise the inner loop within each timestep. This pragma indicated to the compiler that SIMD instructions could 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.

Processors are designed to efficiently move data located on specific byte boundaries, and the compiler is able to perform optimisations when data access is known to be aligned by 64 bytes [5]. To align the `cells`, `cells_new` and `obstacles` vari-

ables, I replaced calls to the `malloc` and `free` procedures with the alignment specific replacements: `_mm_malloc` and `_mm_free`, respectively. I used the `__assume_aligned` procedure and the statement `__assume(params.nx % 16 == 0)` to inform the compiler that the dynamically allocated variables were aligned. Doing so prevented the compiler from generating conservative code, which would have been detrimental to performance.

Once I had utilised these techniques to enforce efficient vectorization of the inner loop, 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), as BC4’s compute nodes do [6].

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

Test Case Size	Time (s)	Speedup
128×128	5.77	5.05
128×256	11.57	5.07
256×256	41.55	5.62
1024×1024	215.52	4.55

Vectorization provided the largest performance improvement of any optimisation that I had implemented to this point, as shown in Table 5.

3 Parallelism

3.1 OpenMP

OpenMP implements parallelism by launching a set of threads that execute portions of code concurrently [7]. I utilised OpenMP’s `#pragma omp parallel` pragma to direct the compiler to parallelise the outer loop in the `timestep` procedure. Furthermore, I compiled my code with the `qopenmp` option, which enabled the parallelizer to generate multi-threaded code based on OpenMP directives, as that which I defined. Since the `tot_u` variable needed to contain the total velocities of each cell, I used the clause `reduction(+:tot_u)` to prevent race conditions. This informed the compiler to create a copy of the `tot_u` variable for each thread (initialised to zero), and to sum the local results when the outer loop terminates.

3.2 Non-Uniform Memory Access (NUMA)

NUMA is a computer memory design in which memory access time depends on the memory lo-

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	1.30	22.43	4.44
128×256	1.48	39.67	7.82
256×256	3.61	64.63	11.51
1024×1024	16.93	57.94	12.73

cation relative to the processor [8]. Memory is allocated to the closest NUMA region to the thread that first touches the data [9]. Since BC4’s compute nodes contain two sockets, the memory access time for a given thread primarily depends on whether the memory is connected to the socket the thread resides in or not. I parallelised the initialisation loops for `cells` and `obstacles` to ensure that each thread touched the same data in both the `initialise` and `compute` procedures. Furthermore, I set the environment variables `OMP_PROC_BIND=true` and `OMP_PLACES=cores` to prevent threads from moving cores.

Table 7: Execution times after writing NUMA-aware implementation (run with 28 threads), and speedup over both the original and vectorized code

Grid Size	Time (s)	Speedup	
		Original	Vectorized
128×128	0.71	41.07	8.13
128×256	0.82	71.60	14.11
256×256	2.64	88.38	15.73
1024×1024	13.47	72.82	16.00

3.3 Scaling

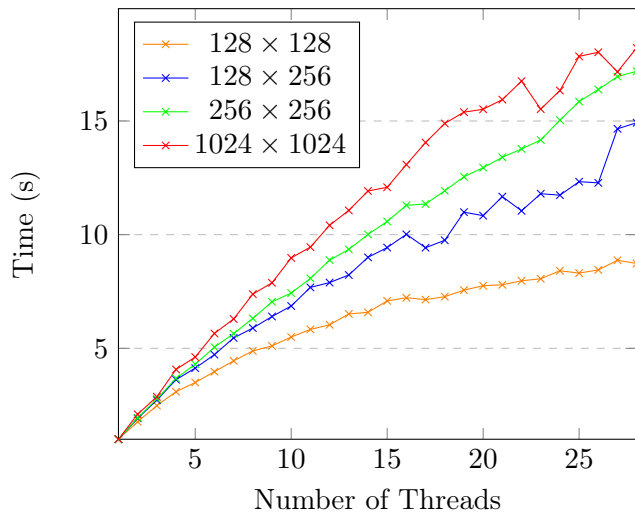


Figure 1: Speedup curves for NUMA-aware implementation

References

- [1] *BlueCrystal technical specifications*. URL: <https://www.bristol.ac.uk/acrc/high-performance-computing/hpc-systems-tech-specs/>.
- [2] *Alphabetical List of Compiler Options*. 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>.
- [3] *Using Automatic Vectorization*. 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>.
- [4] *Memory Layout Transformations*. URL: <https://www.intel.com/content/www/us/en/developer/articles/technical/memory-layout-transformations.html>.
- [5] *Data Alignment to Assist Vectorization*. URL: <https://www.intel.com/content/www/us/en/developer/articles/technical/data-alignment-to-assist-vectorization.html>.
- [6] *Lenovo NeXtScale nx360 M5 (E5-2600 v4)*. URL: <https://lenovopress.com/lp0094-nextscale-nx360-m5-e5-2600-v4>.
- [7] *OpenMP: How it Works*. URL: <https://cvw.cac.cornell.edu/openmp/threads>.
- [8] Joseph Yiu. *The Definitive Guide to ARM Cortex-M3 and Cortex-M4 Processors*. 3rd. Newnes.
- [9] Tom Deakin. “OpenMP and Non-Uniform Memory Access (NUMA)”.