Advanced Research Computing Coursework Report

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Introduction

Conway's Game of Life first made an appearance in public discourse in 1970, when Martin Gardner wrote a brief article introducing the concept in his column Mathematical Games in Scientific American[1]. The piece briefly describes game, stating its rules, and displaying various diagrams of interesting simple behaviours such as periodicity and indefinite movement across the board. It is notable that Gardner starts by suggesting that readers use 'counters and a board', or failing that, 'pencil and graph paper', to see a demonstration of the game in action. This is in stark contrast to the situation today, where plenty of computer simulations are easily accesible online [2], enabling the game's interesting behaviours at scale to be easily explored. This project seeks to take the ease of implementing this simulation with modern computing tools a step further, by treating it as an exercise in developing highly optimised and parallelised code, with a focus on maximising the performance of the simulation algorithm when run at scale.

The Game of Life consists of a large orthogonal grid of cells which exist in either one of two states: 'dead' or 'alive'. At each stage or 'tick' of the simulation, the state of each cell is updated according to its own current state, and the current state of the cells adjacent (including diagonally) to it. The only state changes occur when:

- an 'alive' cell fewer than two or more than three 'alive' neighbours will become 'dead' in the next tick, and
- a 'dead' cell with exactly three 'alive' neighbours will become 'alive' in the next tick [1].

The evolution of the state of any cell within the simulation is thus bound by a deterministic rule that only depends on the current state of the simulation in a localised area. This makes it akin to physical simulations of the real-world, for instance discrete numerical techniques to solve PDEs that relate to fluid dynamics. In this sense, it is a suitable choice of problem to demonstrate the role of high-performance computing at the frontier of scientific research.

While the focus of this project was to produce highly optimised code, care was taken to balance this with traditional best practices in software development. The general approach in the first instance was to create code that was readable and verified via unit tests, and only once this stage was

reached was the code then iteratively re-factored to be increasingly optimised. This ensured that the maintainability and robustness of the earlier code could be preserved as much as possible, despite the tendency of optimisation to reduce these qualities. In summary, the strategy of development sought primarily to demonstrate sophisticated optimisation techniques, while not losing sight of computer scientist Donald Knuth's sage advice [3]:

> "Premature optimization is the root of all evil."

Algorithm Design and Early Development

The simulation primarily consists of a large orthogonal grid of cells, each of which changes state over time. Therefore the first consideration in carrying out this simulation computationally was the abstraction and storage of this grid in memory. Conceptually, operations need to occur at two levels of abstraction:

- the level of matrix operations, including reading the state (stored in binary) of a cell and counting the number of alive neighbours; and
- the level of simulation operations, such as evolving the simulation, storing how many ticks have passed, and displaying the result.

Therefore, both a `Matrix` and a `World` class were created to store methods and attributes relevant to these respective levels. `World` objects store two `Matrix` objects as members, to represent the current state of the simulation, and the next state. The higher-level `World` objects also store an `age` attribute to keep track of the progress of the simulation, and whose parity determines which of the two grids stores the current state. The `Matrix` class stores, among others, a `count_neighbours` method, the first prototype of which is shown below:

```
1 Matrix matrix::count_neighbours(Matrix A) {
2     Matrix B = Matrix(A.n_rows - 2, A.n_cols - 2);
3
4     for (int i = 1; i < A.n_rows - 1; i++) {
5         for (int j = 1; j < A.n_cols - 1; j++) {
6             for (int p = -1; p < 2; p++) {
7                 for (int q = -1; q < 2; q++) {
8                     B(i - 1, j - 1) += A(i + p, j + q);
9                 }
```

```
            }
            B(i - 1, j - 1) -= A(i, j);
        }
        std::cout << std::endl;
    }
    return B;
}
```

This routine iterates across all of the entries of A (besides the edges) and then across all neighbours of said entry, summing all of the values to return the results in matrix B - which is easy to understand and debug. Similarly, the first prototype for the routine used to update cells according to the rules was written in an intuitive way:

```
int conway::evaluate_rules(Matrix cells_count, Matrix &
    cells_current,
    Matrix &cells_next) {
    for (int i = 1; i < cells_count.n_rows - 1; i++) {
        for (int j = 1; j < cells_count.n_cols - 1; j++) {
            if (cells_current(i, j) == 1) {
                if (cells_count(i, j) != 2 and cells_count(i,
    j) != 3) {
                    cells_next(i, j) = 0;
                } else {
                    cells_next(i, j) = 1;
                }
            } else {
                if (cells_count(i, j) == 3) {
                    cells_next(i, j) = 1;
                } else {
                    cells_next(i, j) = 0;
                }
            }
        }
    }
}
```

The routine evaluates a set of nested if statements, which first inspects the current state of the cell, and then checks the counts of the neighbouring cells accordingly. Both of these fundamental routines were kept separate from the handling of the periodic boundary. Within the `World` class, the grid of cells was represented as a matrix that had an extra row of cells on each edge. There was then a separate routine to handle the update of these edges to implement a periodic boundary, by copying each 'proper' edge and vertex of the grid to the corresponding opposite 'extra' edge or vertex. Therefore

the evolution of the simulation by one tick is decomposed into updating this boundary first, and then updating the cells.

This modular quality of the code enabled precise verification early on in the project, and indeed developing a suite of unit tests via GoogleTest was the next step after prototyping. This ensured that these core routines behaved as expected, and handled edge cases, forming part of a testing led-development strategy. Creating the test suite involved the anticipation of other important functions that handled the input and output of matrices, for instance. This ensured that the later development was more efficient as the modular organisation of the code, and the role of each routine, had already been planned out. Moreover, the modularity contributed to a more maintanable code, particularly with the separate handling of the boundary, in that different styles of boundaries (such as constant or reflective padding) could be easily implemented later on. This was incidentally beneficial in the later stages of optimisation where these routines could be easily incorporated with the communication of halos during domain decomposition.

Optimisation and Parallelisation

Optimisation was first achieved by single-thread improvements. The focus was on the fundamental simulation routines since the performance of these becomes increasingly important as the scale of the simulation increases. A major improvement in this respect was changing the `count_neighbours` method to exploit the separability of the box blur convolution [4], in the following fashion:

```
1  Matrix matrix::count_neighbours(Matrix &A) {
2      int n_rows = A.n_rows;
3      int n_cols = A.n_cols;
4
5      // Row convolution
6      Matrix B(n_rows, n_cols);
7      for (int i = 0; i < n_rows; i++) {
8          for (int j = 1; j < n_cols - 1; j++) {
9              B(i, j) = A(i, j - 1) + A(i, j) + A(i, j + 1);
10         }
11     }
12
13     // Column convolution
14     Matrix C(n_rows, n_cols);
```

```
15      for (int i = 1; i < n_rows - 1; i++) {
16          for (int j = 1; j < n_cols - 1; j++) {
17              C(i, j) = B(i - 1, j) + B(i, j) + B(i + 1, j);
18          }
19      }
20      return C;
21  }
```

Note that in addition to the separation of the convolution into two one-dimensional kernels, the routine now includes the target cell entry in the count, thereby removing the need to subtract this value in line 17. This reduces the number of operations to compute each count from 10 in the earlier prototype to 6. Additionally, the first row convolution has the extra benefit of accessing both matrices A and B contiguously, since all entries of A accessed in each iteration lie in the same row of the matrix.

The performance gain was documented by the `time_count_neighbours` script, the results of which are found in Table 1. For the largest matrices in the table this optimisation has the effect of a speed up of roughly 8-fold, which increases even further for smaller matrices. It should also be noted that there appears to be a cache-resonance effect for matrices of size larger than 500, significant slow-downs for sizes that are powers of two beyond this number (512, 1024 and so on.). In later timing scripts therefore, these sizes of simulation are avoided, so as not to confound different performance factors.

Incorporating a transposition of matrix `B` was also experimented with, both by including a standalone loop to compute a separate matrix `B_T`, as well as computing `B_T` directly from `A` instead of `B`. Theoretically this could enable both 1D convolutions to be computed as row convolutions, such that they both benefit from contiguous array access. However, this appeared to cause a decrease in performance. This is also a reasonable outcome considering that both the convolution operations and the transposition involve $O(n^2)$ operations with respect to the matrix size n, and so the gain from more efficient usage of the cache is offset by the extra number of total operations from the transposition itself, even at scale. In this way, transposition is much more likely to be fruitful (at scale) in terms of performance in such a scenario if the main algorithm has a computational cost worse than $O(n^2)$.

The `evaluate_rules` function was also optimised to produce the folowing code:

```
1 int conway::evaluate_rules(Matrix &Cells_count, Matrix &
    Cells_current,
2                            Matrix &Cells_next) {
```

Matrix size	Prototype time (ms)	Separable convolution (ms)
2	0.0000658	0.0001272
3	0.003598	0.0001808
4	0.0097835	0.0004059
6	0.0160791	0.0001572
7	0.0210006	0.0002301
8	0.0255929	0.0002429
14	0.0476087	0.0004165
15	0.039723	0.0007573
16	0.0394387	0.0008217
30	0.134101	0.0005995
31	0.115235	0.0007182
32	0.0972259	0.0013144
62	0.431404	0.0018366
63	0.326085	0.0020772
64	0.325566	0.0038449
126	1.48509	0.0319895
127	0.925173	0.0282965
128	1.32786	0.0354224
254	5.63889	0.185919
255	6.37235	0.197116
256	6.23367	0.171525
510	19.1519	0.538269
511	20.3742	0.602934
512	22.1763	0.760738
1022	63.7401	2.37999
1023	67.6161	3.1337
1024	59.022	3.58696
2046	165.155	9.53187
2047	172.047	9.17258
2048	202.097	12.758
4094	608.048	53.6286
4095	554.764	66.2772
4096	580.508	70.9785
8190	1949.4	242.911
8191	2085.35	249.298
8192	1959.89	289.589

Table 1: Mean of 10 timed runs on square matrices, comparing two implementations of `count_neighbours`

.

```
3     for (int i = 0; i < Cells_count.n_rows; i++) {
4         for (int j = 0; j < Cells_count.n_cols; j++) {
5             Cells_next(i, j) =
6                 (Cells_count(i, j) == 3) ||
7                 ((Cells_count(i, j) == 4) && (Cells_current(i
    , j) == 1));
8         }
9     }
10    return 0;
11 }
```

The main improvement compared to the earlier versions of this function is that this routine has no if statements, each of which can cause costly branch mis-predictions in the CP, a problem which scales with the size of the simulation. This updated routine avoids the conditional control flow by employing a masking technique which exploits the binary nature of the cell states. In fact, in this case the optimisation is arguably much quicker to intuit as someone reading the code for the first time; it essentially updates each cell to alive only if there are two adjacent alive cells (in which case the cell could be alive or dead), or if there are three and the cell is currently alive. On a more subtle note, C++ implements short-circuit evaluation of these boolean operators, meaning that the second expression evaluation can be bypassed when the first (true for or, false for and) already determines the overall value of the boolean operator. With this in mind, the more likely condition of 'exactly 2 alive neighbours' is placed before 'exactly 3 alive neighbours and current cell alive', while the less likely condition of 'exactly 3 alive neighbours' is placed before 'current cell is alive', with the aim of minimising the number of boolean expressions that must be evaluated.

The project explored the use of both MPI and OpenMP to make the code parallelised. The main difference between the two interfaces is that unlike OpenMP, MPI 'ranks' do not have access to a shared memory space, instead having separate allocated memory that can be communicated across the ranks. Therefore MPI was used to employ a domain decomposition of the simulation, that is, dividing the simulation grid amongst the ranks to be separately evolved. The main challenge with this is implementing an organised collective communication such that cells on the boundaries of each 'chunk' can be correctly updated with respect to the values of the correct neighbouring cells located on other ranks.

In the first instance this was done using a 1D topology, dividing the simulation along the vertical dimension.

As previously mentioned, the pre-existing routine for updating the periodic boundary was helpful here. This routine updates every 'ghost' cell at the boundary of the matrix of cell values with the corresponding true inner cell value found on the opposite side of the matrix. Without parallelisation this simply implements the periodic boundary at the extremes of the boundary. But adding this as an extra step before communicating between ranks is also help, as shown in Figure 1. Without this step, vertices must be passed to multiple locations which can make it difficult to keep track of where cell values are communicated, as in Figure 1a. Moreover, there must be separate communications for the edges and vertices.

However,

domain decomposition how it works 1d decomposition, how the single thread development helped give a clean solution 2d decomposition, creating a Cartesian grid

OMP threading with parallel fors (collapsed), barriers,

Hybrid approach

Timing plots.

Summary

Learnings: CSD3, C++, previous C1 things that were useful (e.g. versioning, branches) What went to plan and what didn't: How you could extend: refactoring of the code, niche things like avoiding cache resonance and automatically finding a topology; integrating 1d and 2d decomp.

References

[1] M. Gardner, "The fantastic combinations of john conway's new solitaire game 'life'," *Scientific American*, vol. 223, no. 4, 1970.

[2] E. Martin, "Playgameoflife.com," accessed Mar. 27, 2024. [Online]. Available: https://playgameoflife.com/

[3] D. E. Knuth, "Structured programming with go to statements," *ACM Comput. Surv.*, vol. 6, no. 4, pp. 261–301, dec 1974. [Online]. Available: https://doi.org/10.1145/356635.356640

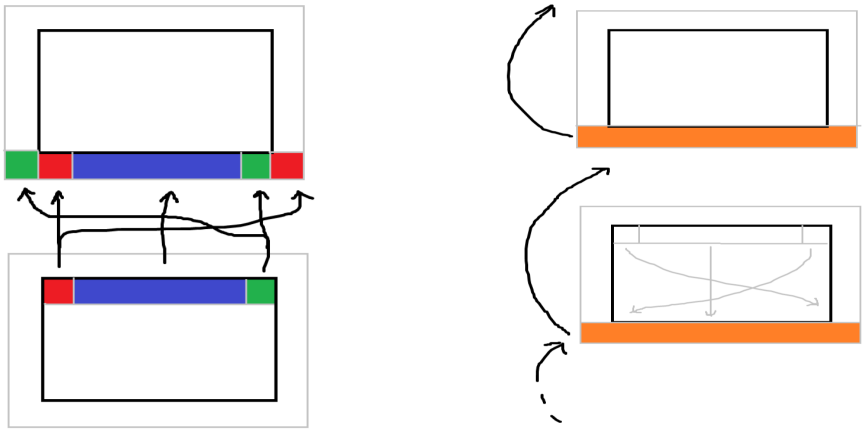
[4] Wikipedia.org, "Separable filter," https://en.wikipedia.org/wiki/Separable_filter, 2022.

A Statement on the use of auto-generation tools

Auto-generation tools, such as GitHub or Microsoft Copilot, were not used at any stage during the development of the code within the repository of this project. Similarly, none of the content of this report was produced – or proofread – by modern Large Language Models such as ChatGPT at any point.

B High-Performance Computing Resources

This work was performed using resources provided by the Cambridge Service for Data Driven Discovery (CSD3) operated by the University of Cambridge Research Computing Service (www.csd3.cam.ac.uk), provided by Dell EMC and Intel using Tier-2 funding from the Engineering and Physical Sciences Research Council (capital grant EP/T022159/1), and DiRAC funding from the Science and Technology Facilities Council (www.dirac.ac.uk).



(a) Required communication (b) Two-step implementation

Figure 1: Illustration of the communication between chunks in 1D topology.