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1 Overview

The codebase `game-of-life`, which can be found at <https://github.com/dgsaf/game-of-life>, consists of the original code provided by Dr Pascal Elahi, with the following additions:

- `src/02_gol_cpu_serial_fort.f90`: a serial GOL code which derives from `src/01_gol_cpu_serial_fort.f90`, but improves loop ordering to match the column-major format of Fortran.
- `src/02_gol_cpu_openmp_loop_fort.f90`: a parallel GOL code which derives from `src/02_gol_cpu_serial_fort.f90`, but implements OMP parallel do loops to yield performance benefits.
- `profiling/`: a directory which includes the profiling results of the `01_gol_cpu_serial_fort` and `02_gol_cpu_serial_fort` versions of the GOL code, as well as a brief summary and comparison of the profiling results. The results were collected for a GOL simulation on a 1000×1000 grid, for 100 steps with no visualisation enabled.
- `gol-job-submission.slurm`: a SLURM script which submits a `sbatch` job request for a GOL simulation with a given set of parameters which include:

```
– version_name
– n_omp
– grid_height
– grid_width
– num_steps
– initial_conditions_type
– visualisation_type
– rule_type
– neighbour_type
– boundary_type
```

An output directory is created for the given set of parameters, with the logging output and statistics of the GOL simulation confined there. If the output directory already exists, the job isn't submitted to prevent repeating work needlessly. Note that the `sbatch` job request is invoked with `--cpus-per-task=16`.

- `gol-job-set-submission.sh`: a bash script which constructs different sets of parameters, and executes `gol-job-submission.slurm` for each parameter set. The default values for the unspecified parameters are:

```
– n_omp = 4,
– initial_conditions_type = 0 (random initial conditions),
– rule_type = 0 (ordinary 2D GOL rule),
– neighbour_type = 0 (Moore neighbourhood),
```

- `boundary_type = 0` (hard boundary with default state being dead).

The batches of jobs submitted are:

- A verification batch, which submits a job for every version of the GOL simulation, on a 10×10 grid, for 10 steps, with ASCII visualisation. This is intended to allow for visual confirmation that each version produces uniform results. The logging output and statistics are compared to verify this.
 - A scaling batch, which submits a job for every version of the GOL simulation, on a range of grid sizes, $2^n \times 2^n$ for $n = 1, \dots, 14$, for 100 steps, with no visualisation. This is intended to collect data for analysing the scaling behaviour of each version with increasing grid size, with the total elapsed time being compared.
 - An OMP batch, which submits a job for every parallel version of the GOL simulation, for a range of assigned threads, $n_{\text{omp}} = 1, \dots, 16$, on a 10×10 grid, for 10 steps, with ASCII visualisation. This is intended to allow for visual confirmation that each parallel version produces uniform results, independent of the number of threads assigned to the program. The logging output and statistics are compared to verify this.
 - An OMP batch, which submits a job for every parallel version of the GOL simulation, for a range of assigned threads, $n_{\text{omp}} = 1, \dots, 16$, and for a range of grid sizes, $2^n \times 2^n$ for $n = 1, \dots, 14$ with no visualisation. This is intended to collect data for analysing the scaling behaviour of each parallel version, for each number of threads, with the total elapsed time being compared. Analysing this will yield some insight into the cost associated with the overhead of OMP threading. The total elapsed times are compared to investigate this.
- **output/**: a directory which includes subdirectories (for each parameter set submitted), each of which include the logging output and statistics file; that is, `output/<unique_parameter_set>/log.txt` and `output/<unique_parameter_set>/stats.txt`.
 - **gol-data-extract.sh**: a bash script which extracts the final timing data for the two scaling batches of jobs:
 - The scaling batch, which includes a job for every version of the GOL simulation, on a range of grid sizes, $2^n \times 2^n$ for $n = 1, \dots, 14$, for 100 steps, and with no visualisation.
 - The OMP parallel thread scaling batch, which includes a job for every parallel version of the GOL simulation, for a range of assigned threads, $n_{\text{omp}} = 1, \dots, 16$, and for a range of grid sizes, $2^n \times 2^n$, for $n = 1, \dots, 14$, with no visualisation.

A data directory is created for each scaling batch of jobs, and a `.csv` file is created for each unique job, if it doesn't already exist.

- **data/**: a directory which includes a subdirectory for each scaling batch of jobs, each of which contains a set of `.csv` files, consisting of the grid length and timing data, for each of the jobs in the batch.
- **report/**: a directory which includes this `.tex` file and other files suitable for submission of this assignment.

Additionally, some minor modifications have been made to the following files:

- `Makefile`: the make rule `make cpu_serial_fort` has been modified to include `src/02_gol_cpu_serial_fort.f90`.
- `src/common_fort.f90`: the length of the variable `arg` has been increased from 32 to 2000 to allow for larger filenames for the variable `statsfile`.
- `src/01_gol_cpu_serial_fort.f90`: an error in `subroutine game_of_life_stats()` concerning array indexing has been corrected.

2 Code Synopsis

Here, we will provide a synopsis of the most significant changes and additions to the codebase. Small, but important, sections of code will be presented and discussed; the codebase in its entirety is presented in [Appendix A](#).

2.1 Common Code

The entire common code, `src/common_fort.f90`, can be found in [subsection A.1](#).

Only a small modification has been made to `src/common_fort.f90` from the original code provided by Dr Pascal Elahi: the length of the variable `arg` has been increased from 32 to 2000. This is due to the slurm script `gol-job-submission.slurm` providing, as one of the command line arguments, long strings for the variable `statsfile`. This is necessary for proper manipulation of the `*/stats.txt` output file, which was being truncated prior to the change.

The modified code snippet is shown below.

```
156      ! arg length changed from 32 to 2000 to accommodate large statsfilename.
157      character(len=2000) :: arg
```

Listing 1: Modifications to `arg` variable within subroutine `getinput()`.

2.2 Serial Code

2.2.1 Original Serial Code

The entire original serial code, `src/01_gol_cpu_serial_fort.f90`, can be found in [subsection A.2](#). It contained a bug, which indexed the `num_in_state` and `frac` arrays using 1-based indexing rather than 0-based indexing (mandated by the parameters defined in `src/common_fort.f90`), resulting in incorrect statistics being written to the statistics file.

The corrected code snippets are shown below.

```
126      ! num_in_state and frac modified from dimension(NUMSTATES) to
127      ! dimension(0:NUMSTATES-1) to synchronise with the 0-based indexing of
128      ! states mandated in common_fort.f90.
129      integer, dimension(0:NUMSTATES-1) :: num_in_state
130      real*4, dimension(0:NUMSTATES-1) :: frac
```

Listing 2: Modifications to indexing of `num_in_state` and `frac` array variable within subroutine `game_of_life_stats()`.

```
153      ! Loop bounds modified to synchronise with 0-based indexing of frac(:).
154      do i = 0, NUMSTATES-1
155          write(10,fmt, advance="no") "Frac in state ", i, " = ", frac(i), " "
156      end do
```

Listing 3: Modifications to indexing of `frac` array variable within subroutine `game_of_life_stats()`.

2.2.2 Improved Serial Code

The entire improved serial code, `src/02_gol_cpu_serial_fort.f90`, can be found in [subsection A.3](#). It can be observed in `src/01_gol_cpu_serial_fort.f90`, that the nested `do` loops over the variable `grid(:, :)` do not respect Fortran's column major order for multi-dimensional arrays. Hence, it is guaranteed that cache misses are occurring as the program needs to stride over the array in memory to access elements of `grid(:, :)`. By reversing the order of these nested `do` loops, wherever they occur, the program will no longer suffer from these cache misses, and will instead collect large blocks of contiguous memory, yielding performance benefits.

The modified code snippets are shown below.

```

121 ! Loop over current grid and determine next grid.
122 ! Inner and outer loops have been swapped due to Fortran storing arrays in
123 ! column-major order.
124 do j = 1, m
125     do i = 1, n

```

Listing 4: Modifications to order of nested `do` loops within `subroutine game_of_life()`. Mitigates problem of cache misses when accessing and updating `grid(i, j)`.

```

199 ! Calculated the number of cells in each state across the entire grid.
200 ! Inner and outer loops have been swapped due to Fortran storing arrays in
201 ! column-major order.
202 do j = 1, opt%m
203     do i = 1, opt%n

```

Listing 5: Modifications to order of nested `do` loops within `subroutine game_of_life_stats()`. Mitigates problem of cache misses when accessing and updating `grid(i, j)`.

2.2.3 Profiling Comparison

The two serial codes, `src/01_gol_cpu_serial_fort.f90` and `src/02_gol_cpu_serial_fort.f90` were compiled with profiling turned on, and performed a GOL simulation on a 1000×1000 grid, for 100 steps, with no visualisation. The profiling results are located in `profiling/analysis_*.txt` and a brief summary of these results, and the relevant source code snippets, are included in `profiling/profiling-summary.txt`.

The original serial code took 4.906s to complete. Cumulatively $\sim 45\%$ of the time was spent calculating the number of living neighbours of a given cell in `subroutine game_of_life()`, while cumulatively $\sim 40\%$ of the time was spent calculating the number of grid cells that were in a given state in `subroutine game_of_life_stats()`. That is to say, $\sim 95\%$ of the time was spent accessing elements of `grid(:, :)`. This clearly shows that the vast majority of the time spent in the GOL simulation concerns accessing elements of `grid(:, :)`, and that improving the efficiency of these access operations ensures improved code performance.

The improved serial code took 2.949s to complete. Cumulatively $\sim 65\%$ of the time was spent calculating the number of living neighbours of a given cell in `subroutine game_of_life()`, while cumulatively only $\sim 5\%$ of time was spent calculating the number of grid cells that were in a given state in `subroutine game_of_life_stats()`. It is clear that reversing the order of the nested `do` loops has yielded a significant performance increase, with a $\sim 40\%$ reduction in time taken. Furthermore, the percentage of time spent accessing elements of `grid(:, :)` has been reduced from $\sim 95\%$ to $\sim 70\%$, indicating that the access operations are less of a bottleneck.

Note that in `subroutine game_of_life()`, for every update operation performed on an element of `grid(:, :)`, 4 to 8 access operations are performed.

2.3 Parallel Loop Code

The entire parallel loop code, `src/02_gol_cpu_openmp_loop_fort.f90`, can be found in [subsection A.4](#). It is derived from `src/02_gol_cpu_serial_fort.f90` but with modifications to incorporate parallelism.

The OpenMP worksharing construct, `parallel do`, has been introduced to parallelise the segments of the GOL simulation code which can be parallelised to yield performance improvements. From the profiling analysis, discussed in [subsection 2.2.3](#), it was observed that the majority of time is spent accessing elements the variable `grid(:, :)`. Hence, the segments of code which are likely to result in the best performance improvements when parallelised, are those that involve access operations on `grid(:, :)`; namely, the nested loops over `grid(i, j)` in `subroutine game_of_life()` and `subroutine game_of_life_stats()`.

The parallelised code snippets are shown below.

```

121 ! Loop over current grid and determine next grid.
122 ! Inner and outer loops have been swapped due to Fortran storing arrays in
123 ! column-major order.
124 !
125 ! OMP parallel do
126 ! - A static scheduler is chosen as the expected work per iteration should be
127 !   approximately constant. Thus load balancing is unlikely to be an issue,
128 !   while minimising overhead is of particular concern - making a static
129 !   scheduler the optimal choice.
130 ! - The nested loops are not collapsed as testing revealed that including a
131 !   'collapse(2)' clause leads to a ~10% slower execution time.
132 !
133 !$omp parallel do &
134 !$omp   schedule (static) &
135 !$omp   shared (n, m, current_grid, next_grid) &
136 !$omp   private (i, j, n_i, n_j, k, neighbours)
137 do j = 1, m
138   do i = 1, n

```

Listing 6: Inclusion of OMP parallel do worksharing constructs within subroutine game_of_life().

```

213 ! Calculated the number of cells in each state across the entire grid.
214 ! Inner and outer loops have been swapped due to Fortran storing arrays in
215 ! column-major order.
216 !
217 ! OMP parallel do
218 ! - A static scheduler is chosen as the expected work per iteration should be
219 !   approximately constant. Thus load balancing is unlikely to be an issue,
220 !   while minimising overhead is of particular concern - making a static
221 !   scheduler the optimal choice.
222 ! - The nested loops are not collapsed as testing revealed that including a
223 !   'collapse(2)' clause leads to a ~10% slower execution time.
224 ! - A reduction clause is included for the num_in_state(:) variable as it can
225 !   be reduced across all iterations. Without this clause, the parallel do is
226 !   actually slower than the non-parallel do, however including it leads to
227 !   performance benefits.
228 !

```

```

229  !$omp parallel do &
230  !$omp    schedule (static) &
231  !$omp    shared (opt, current_grid) &
232  !$omp    private (i, j, state) &
233  !$omp    reduction(+:num_in_state)
234  do j = 1, opt%m
235      do i = 1, opt%n
236          state = current_grid(i,j)
237          num_in_state(state) = num_in_state(state) + 1
238      end do
239  end do

```

Listing 7: Inclusion of OMP parallel `do` worksharing constructs within `subroutine game_of_life_stats()`.

Static schedulers were chosen for the `parallel do` loops, as the amount of work per iteration (of either loop) is expected to be approximately constant. Thus, any benefit from introducing a dynamic or guided scheduler would be minimal and outweighed by the cost of introducing scheduler overhead. A reduction clause is attached to the variable `num_in_state(:)`, since it is effectively an indexed counter which can aggregate the results of each thread together without concern.

It was determined in some small scale tests that including the clause `collapse(2)`, which would collapse the two perfectly-nested loops into one, generally did not produce a significant performance benefit and in some cases worsened performance. However this was only tested rudimentarily and may be more significant for increasingly large grid sizes.

2.4 Bash Scripts

2.4.1 GOL Job Submission

The entire GOL job submission SLURM script, `gol-job-submission.slurm`, can be found in [subsection A.5](#).

2.4.2 GOL Job Set

The entire GOL job set submission script, `gol-job-set-submission.sh`, can be found in [subsection A.6](#).

2.4.3 GOL Data Extract

The entire GOL data extract script `gol-data-extract.sh`, can be found in [subsection A.7](#).

3 Results

3.1 Uniform Behaviour Verification

All versions of the GOL simulation were executed on a 10×10 grid, for 10 steps, with ASCII visualisation on, and with $n_{\text{omp}} = 4$ for the parallel versions of the code. The behaviour of the different versions can be compared exactly by examining the ASCII visualisation of the grids to show that they are identical, and/or by comparing the statistics of the grids produced.

To compare the ASCII visualisations for each version, using the `diff` command to compare the `output/*ngrid-10x10*/log.txt` output for each version from that of `src/01_gol_cpu_serial_fort.f90` should indicate any differences in behaviour. If each version produces identical grids, the only differences should be timing results.

```

1 original="output/GOL-01_gol_cpu_serial_fort.nomp-4.ngrid-10x10.nsteps-10.\
2 ic_type-0.vis_type-0.rule_type-0.nghbr_type-0.bndry_type-0/log.txt"
3
4 for log in output/*ngrid-10x10*/log.txt; do
5     diff ${original} ${log}
6 done

```

Similarly, to compare the statistics, we again use the `diff` command to compare the `output/*ngrid-10x10*/stats.txt` output for each version from that of `src/01_gol_cpu_serial_fort.f90`.

```

1 original="output/GOL-01_gol_cpu_serial_fort.nomp-4.ngrid-10x10.nsteps-10.\
2 ic_type-0.vis_type-0.rule_type-0.nghbr_type-0.bndry_type-0/stats.txt"
3
4 for stats in output/*ngrid-10x10*/stats.txt; do
5     diff ${original} ${stats}
6 done

```

Using both methods on the data collected in `output/`, we have verified that the different versions produce identical grids and statistics.

3.2 Scaling Behaviour

All versions of the GOL simulation were executed for 100 steps, with no visualisation, and for a range of grid sizes, $2^n \times 2^n$ for $n = 1, \dots, 14$. For the parallel versions of the GOL simulation, $n_{\text{omp}} = 4$ was selected.

The time taken for each version to complete the simulation was extracted for each grid size, and the results are presented in [Figure 1](#).

It can be seen that all versions of the code run for approximately less than a 1 s, with rather irregular comparative behaviour between each version, until a grid size of $2^9 \times 2^9 = 512 \times 512$ is reached, at which point the scaling behaviour becomes significantly more regular. Past this point, the original serial code is approximately an order-of-magnitude slower than the parallel loop code, while the improved serial code is only half an order-of-magnitude slower than the parallel loop code.

While it should be noted that the parallel loop code is slightly slower for smaller grid sizes, as a result of the memory overhead associated with spawning and destroying threads, the total time difference is negligible, while for the larger grid sizes the parallel loop code is much faster with significant improvements in total elapsed time.

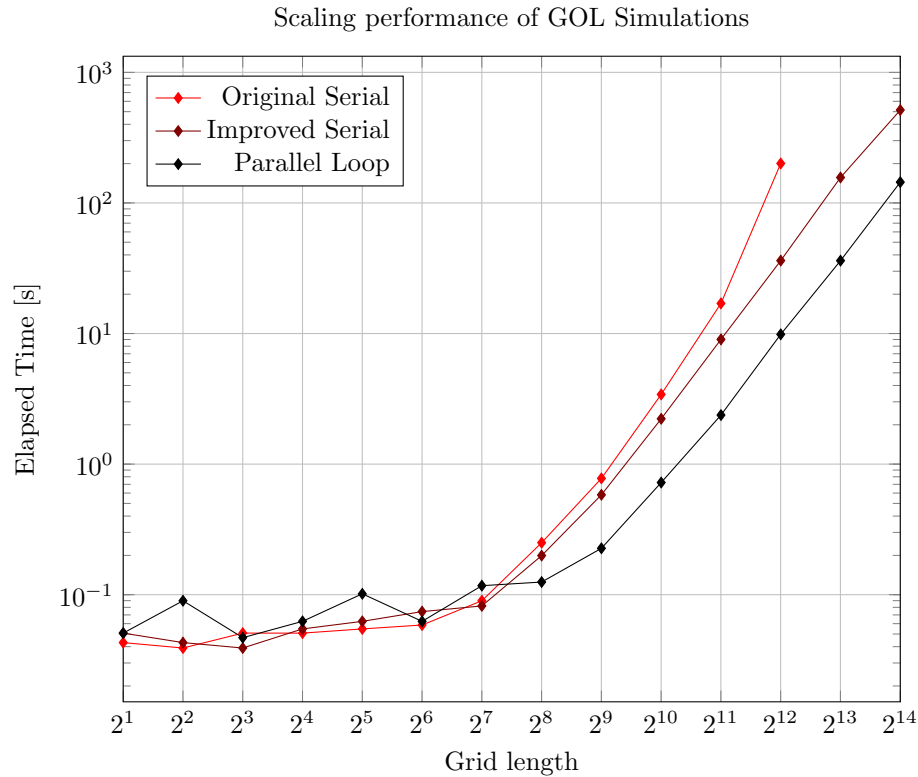


Figure 1: The scaling performance of the original serial, improved serial, and parallel loop (with $n_{\text{omp}} = 4$) versions of the GOL simulations, for 100 steps, with no visualisation, with increasingly large square grids ($n_{\text{grid}} = 2^n \times 2^n$ for $n = 1, \dots, 14$). Note that the x-axis is presented in \log_2 -scale, and the y-axis is presented in \log_{10} scale, to more clearly show the comparative behaviour of each version. Note also that the original serial code failed to complete within 10 minutes for the $2^{13} \times 2^{13}$ and $2^{14} \times 2^{14}$ grids, and therefore those data points were omitted.

3.3 Thread Independence Verification

All parallel versions of the GOL simulation were executed on a 10×10 grid, for 10 steps, with ASCII visualisation on, and for a range of assigned threads $n_{\text{omp}} = 1, \dots, 16$. The behaviour of the different versions can be compared exactly by examining the ASCII visualisation of the grids to show that they are identical, and/or by comparing the statistics of the grids produced.

The ASCII visualisations and statistics can be compared by using the `diff` command in an almost identical way as in [subsection 3.1](#).

```

1 original="output/GOL-02_gol_cpu_openmp_loop_fort.nomp-1.ngrid-10x10.nsteps-10.\
2 ic_type-0.vis_type-0.rule_type-0.nghbr_type-0.bndry_type-0/log.txt"
3
4 for log in output/*openmp*ngrid-10x10*/log.txt; do
5     diff ${original} ${log}
6 done

```

```
1 original="output/GOL-02_gol_cpu_openmp_loop_fort.nomp-1.ngrid-10x10.nsteps-10.\
2 ic_type-0.vis_type-0.rule_type-0.nghbr_type-0.bndry_type-0/stats.txt"
3
4 for stats in output/*openmp*ngrid-10x10*/stats.txt; do
5     diff ${original} ${stats}
6 done
```

Using both methods on the data collected in `output/`, we have verified that the parallel versions produce identical grids and statistics, independently of the number of OMP threads assigned.

3.4 Thread Scaling Behaviour

The parallel loop version of the GOL simulation was executed for 100 steps, with no visualisation, for a range of grid sizes, $2^n \times 2^n$ for $n = 1, \dots, 14$, and for a range of the number of OMP threads used, $n_{\text{omp}} = 1, \dots, 16$

The time taken for the parallel loop code to complete the simulation was extracted for each number of OMP threads used, and for each grid size, with the results presented in [Figure 2](#).

Scaling performance of Parallel GOL Simulations for varying OMP Threads

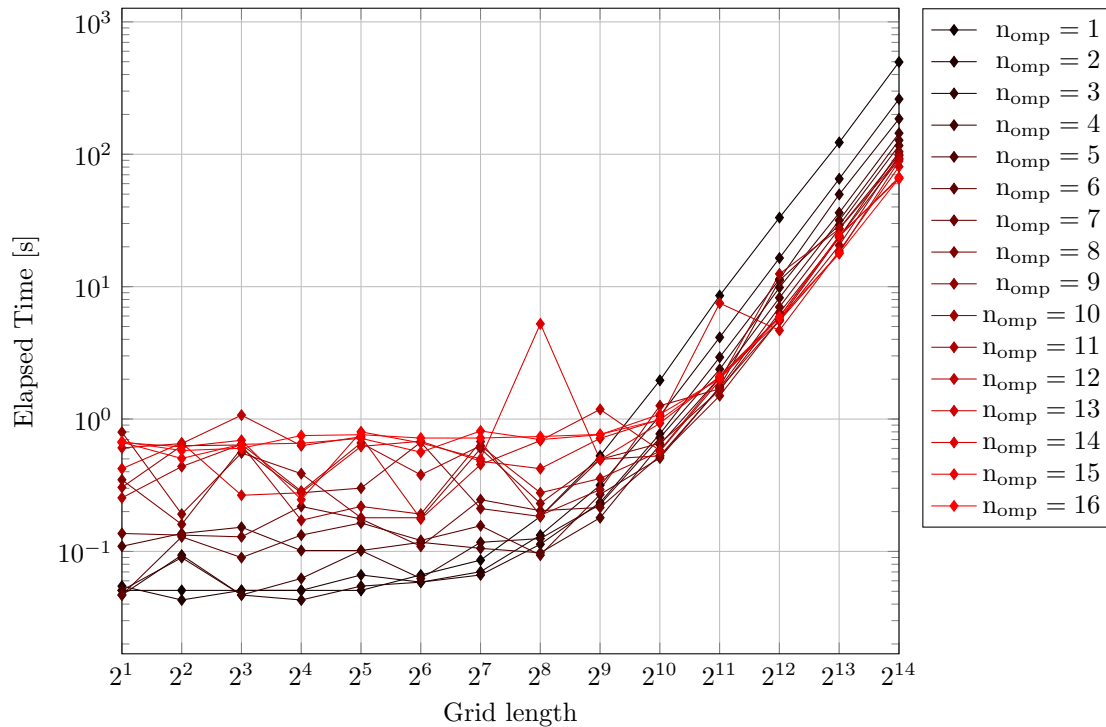


Figure 2: The scaling performance of the parallel versions of the GOL simulations, for 100 steps, with no visualisation, for a range of OMP threads assigned ($n_{\text{omp}} = 1, \dots, 16$), with increasingly large square grids ($n_{\text{grid}} = 2^n \times 2^n$ for $n = 1, \dots, 14$). Note that the x-axis is presented in \log_2 -scale, and the y-axis is presented in \log_{10} scale, to more clearly show the comparative behaviour of each simulation.

A Appendix

A.1 src/common_fort.f90

```

1  !> Conway's Game of Life - Common
2  !>
3  !> This module provides a common set of functionality which is used across all
4  !> serial and parallel versions of the GOL code.
5  !>
6  !> The only modification to this module has been adjusting the length of the
7  !> 'arg' variable in getinput() from 32 to 2000, to accommodate long statsfile
8  !> filenames.
9  module gol_common
10 !-----
11 !
12 !   Common routines and functions for Conway's Game of Life
13 !
14 !-----

```

```

15  use, intrinsic :: iso_c_binding
16  integer, parameter :: NUMSTATES = 4
17  integer, parameter :: CellState_ALIVE = 0
18  integer, parameter :: CellState_DEAD = 1
19  integer, parameter :: CellState_DYING = 2
20  integer, parameter :: CellState_BORN = 3
21
22  integer, parameter :: NUMVISUAL = 4
23  integer, parameter :: VisualiseType_VISUAL_ASCII = 0
24  integer, parameter :: VisualiseType_VISUAL_PNG = 1
25  integer, parameter :: VisualiseType_VISUAL_OPENGL = 2
26  integer, parameter :: VisualiseType_VISUAL_NONE = 3
27
28  integer, parameter :: NUMICS = 2
29  integer, parameter :: ICType_IC_RAND = 0
30  integer, parameter :: ICType_IC_FILE = 1
31
32  integer, parameter :: NUMRULES = 3
33  integer, parameter :: RuleType_RULE_STANDARD = 0
34  integer, parameter :: RuleType_RULES_EXTENDED = 1
35  integer, parameter :: RuleType_RULES_PROB = 2
36
37  integer, parameter :: NUMNEIGHBOURCHOICES = 2
38  integer, parameter :: NeighbourType_NEIGHBOUR_STANDARD = 0
39  integer, parameter :: NeighbourType_NEIGHBOUR_EXTENDED = 1
40
41  integer, parameter :: NUMBOUNDARYCHOICES = 4
42  integer, parameter :: BoundaryType_BOUNDARY_HARD = 0
43  integer, parameter :: BoundaryType_BOUNDARY_TORAL = 1
44  integer, parameter :: BoundaryType_BOUNDARY_TORAL_X_HARD_Y = 2
45  integer, parameter :: BoundaryType_BOUNDARY_TORAL_Y_HARD_X = 3
46
47  type Options
48      integer :: n, m, nsteps
49      integer :: iictype
50      integer :: ivisualisetype
51      integer :: iruletype
52      integer :: ineighbourtype
53      integer :: iboundarytype
54      character(len=2000) :: statsfile
55  end type Options
56
57  contains
58
59      !  ascii visualisation
60      subroutine visualise_ascii(step, grid, n, m)
61          implicit none
62          integer, intent(in) :: step, n, m
63          integer, dimension(:,,:), intent(in) :: grid
64          character :: cell
65          integer :: i, j
66
67          write(*,*) "Game of Life"
68          write(*,*) "Step ", step
69          do i = 1, n
70              do j = 1, m
71                  cell = ' '
72                  ! could use where

```

```

73         if (grid(i,j) .eq. CellState_ALIVE) cell = '*'
74         write(*,"(A)", advance="no") cell
75     end do
76     write(*,*) ""
77 end do
78 end subroutine
79
80 ! png visualisation
81 subroutine visualise_png(step, grid, n, m)
82     implicit none
83     integer, intent(in) :: step, n, m
84     integer, dimension(:,,:), intent(in) :: grid
85
86 end subroutine
87
88 ! no visualisation
89 subroutine visualise_none(step)
90     implicit none
91     integer, intent(in) :: step
92     write(*,*) "Game of Life, Step ", step
93 end subroutine
94
95 ! visualisation routine
96 subroutine visualise(ivisualisechoice, step, grid, n, m)
97     implicit none
98     integer, intent(in) :: ivisualisechoice
99     integer, intent(in) :: step, n, m
100    integer, dimension(:,,:), intent(inout) :: grid
101    if (ivisualisechoice .eq. VisualiseType_VISUAL_ASCII) then
102        call visualise_ascii(step, grid, n, m)
103    else if (ivisualisechoice .eq. VisualiseType_VISUAL_PNG) then
104        call visualise_png(step, grid, n, m)
105    else
106        call visualise_none(step)
107    end if
108
109 end subroutine
110
111 ! generate random IC
112 subroutine generate_rand_IC(grid, n, m)
113     implicit none
114     integer, intent(in) :: n, m
115     integer, dimension(:,,:), intent(inout) :: grid
116     real :: xrand, rand
117     integer :: i, j
118     do i = 1, n
119         do j = 1, m
120 #if defined(_CRAYFTN) || defined(_INTELFTN)
121             call RANDOM_NUMBER(xrand)
122 #else
123             xrand=rand()
124 #endif
125             if (xrand .lt. 0.4) then
126                 grid(i,j) = CellState_DEAD
127             else
128                 grid(i,j) = CellState_ALIVE
129             end if
130         end do
131     end do

```

```

131         end do
132
133     end subroutine
134
135     ! generate IC
136     subroutine generate_IC(ic_choice, grid, n, m)
137         implicit none
138         integer, intent(in) :: ic_choice
139         integer, intent(in) :: n, m
140         integer, dimension(:, :), intent(inout) :: grid
141         if (ic_choice .eq. ICType_IC_RAND) then
142             call generate_rand_IC(grid, n, m)
143         end if
144     end subroutine
145
146     ! get some basic timing info
147     !struct timeval init_time();
148     ! get the elapsed time relative to start, return current wall time
149     !struct timeval get_elapsed_time(struct timeval start);
150
151     ! UI
152     subroutine getinput(opt)
153         implicit none
154         type(Options), intent(inout) :: opt
155         character(len=2000) :: cmd
156         ! arg length changed from 32 to 2000 to accommodate large statsfilename.
157         character(len=2000) :: arg
158         character(len=2000) :: statsfilename
159         integer :: count
160         integer*8 :: nbytes
161         real*4 :: memfootprint
162         ! get the commands passed and the number of args passed
163         call get_command(cmd)
164         count = command_argument_count()
165         if (count .lt. 2) then
166             write(*,*) "Usage: <grid height> <grid width> "
167             write(*,*) "[<nsteps> <IC type> <Visualisation type> <Rule type> <
Neighbour type> "
168             write(*,*) "<Boundary type> <stats filename> ]"
169             call exit();
170         end if
171
172         statsfilename = "GOL-stats.txt"
173         call get_command_argument(1, arg)
174         read(arg, *) opt%n
175         call get_command_argument(2, arg)
176         read(arg, *) opt%m
177         opt%nsteps = -1
178         opt%ivisualisetype = VisualiseType_VISUAL_ASCII
179         opt%iruletype = RuleType_RULE_STANDARD
180         opt%iictype = ICType_IC_RAND
181         opt%ineighbourtype = NeighbourType_NEIGHBOUR_STANDARD
182         opt%iboundarytype = BoundaryType_BOUNDARY_HARD
183         if (count .ge. 3) then
184             call get_command_argument(3, arg)
185             read(arg, *) opt%nsteps
186         end if
187         if (count .ge. 4) then

```

```

188         call get_command_argument(4,arg)
189         read(arg,*) opt%iictype
190     end if
191     if (count .ge. 5) then
192         call get_command_argument(5,arg)
193         read(arg,*) opt%ivisualisetype
194     end if
195     if (count .ge. 6) then
196         call get_command_argument(6,arg)
197         read(arg,*) opt%iruletype
198     end if
199     if (count .ge. 7) then
200         call get_command_argument(7,arg)
201         read(arg,*) opt%ineighbourtype
202     end if
203     if (count .ge. 8) then
204         call get_command_argument(8,arg)
205         read(arg,*) opt%iboundarytype
206     end if
207     if (count .ge. 9) then
208         call get_command_argument(9,arg)
209         read(arg,*) statsfilename
210     end if
211     if (opt%n .le. 0 .or. opt%m .le. 0) then
212         write(*,*) "Invalid grid size."
213         call exit(1)
214     end if
215     opt%statsfile = statsfilename
216     nbytes = sizeof(opt%n) * opt%n * opt%m
217     memfootprint = real(nbytes)/1024.0/1024.0/1024.0
218     write(*,*) "Requesting grid size of ", opt%n, opt%m
219     write(*,*) " which requires", memfootprint, " GB "
220 #ifndef USEPNG
221     if (opt%ivisualisetype .eq. VisualiseType_VISUAL_PNG) then
222         write(*, *) "PNG visualisation not enabled at compile time,"
223         write(*, *) "turning off visualisation from now on."
224     end if
225 #endif
226     end subroutine
227
228     ! get some basic timing info
229     real*8 function init_time()
230         integer, dimension(8) :: value
231         call date_and_time(VALUE=value)
232         init_time = value(5)*3600.0+value(6)*60.0+value(7)+value(8)/1000.0
233         return
234     end function
235     ! get the elapsed time relative to start
236     subroutine get_elapsed_time(start)
237         real*8, intent(in) :: start
238         real*8 :: finish, delta
239         integer, dimension(8) :: value
240         call date_and_time(VALUE=value)
241         finish = value(5)*3600.0+value(6)*60.0+value(7)+value(8)/1000.0
242         delta = finish - start
243         write(*,*) "Elapsed time is ", delta, "s"
244     end subroutine
245

```



```
246 | end module
```

A.2 src/01_gol_cpu_serial_fort.f90

```

1
2 program GameOfLife
3 !-----
4 !
5 !   This program runs Conway's Game of Life
6 !
7 !   Uses:
8 !
9 !-----
10 use gol_common
11 implicit none
12 interface
13 ! GOL prototypes
14 subroutine game_of_life(opt, current_grid, next_grid, n, m)
15     use gol_common
16     implicit none
17     type(Options), intent(in) :: opt
18     integer, intent(in) :: n, m
19     integer, dimension(:,:), intent(in) :: current_grid
20     integer, dimension(:,:), intent(out) :: next_grid
21 end subroutine
22 ! GOL stats prototype
23 subroutine game_of_life_stats(opt, steps, current_grid)
24     use gol_common
25     implicit none
26     type(Options), intent(in) :: opt
27     integer, intent(in) :: steps
28     integer, dimension(:,:), intent(in) :: current_grid
29 end subroutine
30 end interface
31 type(Options) :: opt
32 integer :: n, m, nsteps, current_step
33 integer, dimension(:,:), allocatable :: grid, updated_grid
34 real*8 :: time1, time2
35
36 call getinput(opt)
37 n = opt%n
38 m = opt%m
39 nsteps = opt%nsteps
40 write(*,*) n, m, nsteps
41 allocate(grid(n,m))
42 allocate(updated_grid(n,m))
43 call generate_IC(opt%iictype, grid, n, m)
44 time1 = init_time()
45 current_step = 0
46 do while (current_step .ne. nsteps)
47     time2 = init_time()
48     call visualise(opt%ivisualisetype, current_step, grid, n, m);
49     call game_of_life_stats(opt, current_step, grid);
50     call game_of_life(opt, grid, updated_grid, n, m);
51     ! update current grid
52     grid(:, :) = updated_grid(:, :)
53     current_step = current_step + 1
54     call get_elapsed_time(time2)
55     time2 = init_time()
56 end do

```

```

57     write(*,*) "Finnished GOL"
58     call get_elapsed_time(time1);
59     deallocate(grid)
60     deallocate(updated_grid)
61 end program GameOfLife
62
63 ! GOL
64 subroutine game_of_life(opt, current_grid, next_grid, n, m)
65     use gol_common
66     implicit none
67     type(Options), intent(in) :: opt
68     integer, intent(in) :: n, m
69     integer, dimension(:,,:), intent(in) :: current_grid
70     integer, dimension(:,,:), intent(out) :: next_grid
71     integer :: neighbours, i, j, k
72     integer, dimension(8) :: n_i, n_j
73
74     ! loop over current grid and determine next grid
75     do i = 1, n
76         do j = 1, m
77             ! count the number of neighbours, clockwise around the current cell.
78             neighbours = 0;
79             n_i(1) = i - 1
80             n_j(1) = j - 1
81             n_i(2) = i - 1
82             n_j(2) = j
83             n_i(3) = i - 1
84             n_j(3) = j + 1
85             n_i(4) = i
86             n_j(4) = j + 1
87             n_i(5) = i + 1
88             n_j(5) = j + 1
89             n_i(6) = i + 1
90             n_j(6) = j
91             n_i(7) = i + 1
92             n_j(7) = j - 1
93             n_i(8) = i
94             n_j(8) = j - 1
95
96             ! loop over all neighbours and check there state
97             do k = 1, 8
98                 if(n_i(k) .ge. 1 .and. n_j(k) .ge. 1 .and. n_i(k) .le. n .and. n_j(k)
99 ) .le. m) then
100                     if (current_grid(n_i(k), n_j(k)) .eq. CellState_ALIVE) then
101                         neighbours = neighbours + 1
102                     end if
103                 end if
104             end do
105
106             ! set the next grid
107             if(current_grid(i,j) .eq. CellState_ALIVE .and. (neighbours .eq. 2 .or.
108 neighbours .eq. 3)) then
109                 next_grid(i,j) = CellState_ALIVE
110             else if (current_grid(i,j) .eq. CellState_DEAD .and. neighbours .eq. 3)
111 then
112                 next_grid(i,j) = CellState_ALIVE
113             else
114                 next_grid(i,j) = CellState_DEAD

```

```

112         end if
113     end do
114 end do
115 end subroutine
116
117 ! GOL stats
118 subroutine game_of_life_stats(opt, step, current_grid)
119     use gol_common
120     implicit none
121     type(Options), intent(in) :: opt
122     integer, intent(in) :: step
123     integer, dimension(:, ::), intent(in) :: current_grid
124     integer :: i, j, state
125     integer*8 :: ntot
126     ! num_in_state and frac modified from dimension(NUMSTATES) to
127     ! dimension(0:NUMSTATES-1) to synchronise with the 0-based indexing of
128     ! states mandated in common_fort.f90.
129     integer, dimension(0:NUMSTATES-1) :: num_in_state
130     real*4, dimension(0:NUMSTATES-1) :: frac
131     character(len=30) :: fmt
132
133     fmt = "(A15,I1,A3,F10.4,A4)"
134     ntot = opt%n * opt%m
135     num_in_state = 0
136     do i = 1, opt%n
137         do j = 1, opt%m
138             state = current_grid(i,j)
139             num_in_state(state) = num_in_state(state) + 1
140         end do
141     end do
142     frac = num_in_state/real(ntot)
143     if (step .eq. 0) then
144         open(10, file=opt%statsfile, access="sequential")
145     else
146 #if defined(_CRAYFTN) || defined(_INTELFTN)
147         open(10, file=opt%statsfile, position="append")
148 #else
149         open(10, file=opt%statsfile, access="append")
150 #endif
151     end if
152     write(10,*) "step ", step
153     ! Loop bounds modified to synchronise with 0-based indexing of frac(:).
154     do i = 0, NUMSTATES-1
155         write(10,fmt, advance="no") "Frac in state ", i, " = ", frac(i), " "
156     end do
157     write(10,*) ""
158     close(10)
159 end subroutine

```

A.3 src/02_gol_cpu_serial_fort.f90

```

1  !> Conway's Game of Life.
2  !>
3  !> A cellular automata program which utilises:
4  !> - a 2D grid with hard, torodial or a hybrid boundary,
5  !> - possible cell states S = {0, 1}; that is, dead or alive,
6  !> - a Moore neighbourhood; that is, where for a given cell, the cells directly
7  !>   and diagonally adjacent are considered its neighbours,
8  !> - Conway's update rule, which updates the state of a cell in accordance with
9  !>   the following behaviour:
10 !>   - any live cell with two or three live neighbours continues to live,
11 !>   - any dead cell with three live neighbours becomes a live cell,
12 !>   - all other live cells die, and all other dead cells stay dead.
13 !>
14 !> This version of the program, 02_gol_cpu_serial_fort, is a serial code, which
15 !> is only modified from the original code, 01_gol_cpu_serial_fort, in the
16 !> following ways:
17 !> - Inner and outer loops over grid(i, j) have been swapped to ensure more
18 !>   efficient array caching (noting that Fortran is column-major).
19 !> - Fixed error in game_of_life_stats() which was indexing states from
20 !>   [1 .. numstates] rather than [0 .. numstates-1].
21 !> - Cosmetic changes, such as adding white space, and including more detailed
22 !>   comments.
23 program GameOfLife
24   use gol_common
25   implicit none
26
27   interface
28     ! GOL prototypes.
29     subroutine game_of_life(opt, current_grid, next_grid, n, m)
30       use gol_common
31       implicit none
32
33       type(Options), intent(in) :: opt
34       integer, intent(in) :: n, m
35       integer, dimension(:,:), intent(in) :: current_grid
36       integer, dimension(:,:), intent(out) :: next_grid
37     end subroutine game_of_life
38
39     ! GOL stats prototype.
40     subroutine game_of_life_stats(opt, steps, current_grid)
41       use gol_common
42       implicit none
43
44       type(Options), intent(in) :: opt
45       integer, intent(in) :: steps
46       integer, dimension(:,:), intent(in) :: current_grid
47     end subroutine game_of_life_stats
48   end interface
49
50   ! GOL main loop variables.
51   type(Options) :: opt
52   integer :: n, m, nsteps, current_step
53   integer, dimension(:,:), allocatable :: grid, updated_grid
54   real*8 :: time1, time2
55
56   ! GOL initialisation.

```

```

57  call getinput(opt)
58
59  n = opt%n
60  m = opt%m
61  nsteps = opt%nsteps
62
63  write(*,*) n, m, nsteps
64
65  allocate(grid(n,m))
66  allocate(updated_grid(n,m))
67
68  call generate_IC(opt%iictype, grid, n, m)
69
70  ! GOL main loop.
71  time1 = init_time()
72  current_step = 0
73
74  do while (current_step .ne. nsteps)
75      time2 = init_time()
76
77      ! Visualise the current state of the grid according to the visualisation
78      ! type selected.
79      call visualise(opt%ivisualisetype, current_step, grid, n, m);
80
81      ! Calculate the statistics of the current state of the grid; that is, the
82      ! fractional occupation of each state across all cells.
83      call game_of_life_stats(opt, current_step, grid);
84
85      ! Calculate the next state of grid according to the Conway update rule.
86      call game_of_life(opt, grid, updated_grid, n, m);
87
88      ! Update the current grid variable.
89      grid(:, :) = updated_grid(:, :)
90
91      current_step = current_step + 1
92
93      ! Write out the time taken for this loop.
94      call get_elapsed_time(time2)
95
96      time2 = init_time()
97  end do
98
99  write(*,*) "Finished GOL"
100
101  ! Write out the time taken for the entire program
102  call get_elapsed_time(time1);
103
104  ! GOL cleanup.
105  deallocate(grid)
106  deallocate(updated_grid)
107 end program GameOfLife
108
109 !> GOL
110 subroutine game_of_life(opt, current_grid, next_grid, n, m)
111     use gol_common
112     implicit none
113
114     type(Options), intent(in) :: opt

```

```

115 integer, intent(in) :: n, m
116 integer, dimension(:,,:), intent(in) :: current_grid
117 integer, dimension(:,,:), intent(out) :: next_grid
118 integer :: neighbours, i, j, k
119 integer, dimension(8) :: n_i, n_j
120
121 ! Loop over current grid and determine next grid.
122 ! Inner and outer loops have been swapped due to Fortran storing arrays in
123 ! column-major order.
124 do j = 1, m
125     do i = 1, n
126         ! Count the number of neighbours, clockwise around the current cell.
127         neighbours = 0;
128
129         n_i(1) = i - 1
130         n_j(1) = j - 1
131
132         n_i(2) = i - 1
133         n_j(2) = j
134
135         n_i(3) = i - 1
136         n_j(3) = j + 1
137
138         n_i(4) = i
139         n_j(4) = j + 1
140
141         n_i(5) = i + 1
142         n_j(5) = j + 1
143
144         n_i(6) = i + 1
145         n_j(6) = j
146
147         n_i(7) = i + 1
148         n_j(7) = j - 1
149
150         n_i(8) = i
151         n_j(8) = j - 1
152
153         ! Loop over all neighbours and check their state. The total number of live
154         ! neighbours is accumulated.
155         do k = 1, 8
156             if(n_i(k) .ge. 1 .and. n_j(k) .ge. 1 .and. &
157                n_i(k) .le. n .and. n_j(k) .le. m) then
158                 if (current_grid(n_i(k), n_j(k)) .eq. CellState_ALIVE) then
159                     neighbours = neighbours + 1
160                 end if
161             end if
162         end do
163
164         ! Set the next grid, according to Conway's update rule.
165         if(current_grid(i,j) .eq. CellState_ALIVE .and. &
166            (neighbours .eq. 2 .or. neighbours .eq. 3)) then
167             next_grid(i,j) = CellState_ALIVE
168         else if (current_grid(i,j) .eq. CellState_DEAD .and. neighbours .eq. 3) then
169             next_grid(i,j) = CellState_ALIVE
170         else
171             next_grid(i,j) = CellState_DEAD
172         end if

```

```

173     end do
174 end do
175 end subroutine game_of_life
176
177 !> GOL stats
178 subroutine game_of_life_stats(opt, step, current_grid)
179     use gol_common
180     implicit none
181
182     type(Options), intent(in) :: opt
183     integer, intent(in) :: step
184     integer, dimension(:, ::), intent(in) :: current_grid
185     integer :: i, j, state
186     integer*8 :: ntot
187     ! num_in_state and frac modified from dimension(NUMSTATES) to
188     ! dimension(0:NUMSTATES-1) to synchronise with the 0-based indexing of
189     ! states mandated in common_fort.f90.
190     integer, dimension(0:NUMSTATES-1) :: num_in_state
191     real*8, dimension(0:NUMSTATES-1) :: frac
192     character(len=30) :: fmt
193
194     fmt = "(A15,I1,A3,F10.4,A4)"
195     ntot = opt%n * opt%m
196
197     num_in_state(:) = 0
198
199     ! Calculated the number of cells in each state across the entire grid.
200     ! Inner and outer loops have been swapped due to Fortran storing arrays in
201     ! column-major order.
202     do j = 1, opt%m
203         do i = 1, opt%n
204             state = current_grid(i,j)
205             num_in_state(state) = num_in_state(state) + 1
206         end do
207     end do
208
209     ! Converted the state occupation from absolute terms to fractional terms.
210     frac(:) = num_in_state(:)/real(ntot)
211
212     if (step .eq. 0) then
213         open(10, file=opt%statsfile, access="sequential")
214     else
215 #if defined(_CRAYFTN) || defined(_INTELFTN)
216         open(10, file=opt%statsfile, position="append")
217 #else
218         open(10, file=opt%statsfile, access="append")
219 #endif
220     end if
221
222     write(10,*) "step ", step
223
224     ! Loop bounds modified to synchronise with 0-based indexing of frac(:).
225     do i = 0, NUMSTATES-1
226         write(10,fmt, advance="no") "Frac in state ", i, " = ", frac(i), " "
227     end do
228
229     write(10,*) ""
230     close(10)

```



```
231 | end subroutine game_of_life_stats
```

A.4 src/02_gol_cpu_openmp_loop_fort.f90

```

1  !> Conway's Game of Life.
2  !>
3  !> A cellular automata program which utilises:
4  !> - a 2D grid with hard, torodial or a hybrid boundary,
5  !> - possible cell states S = {0, 1}; that is, dead or alive,
6  !> - a Moore neighbourhood; that is, where for a given cell, the cells directly
7  !>   and diagonally adjacent are considered its neighbours,
8  !> - Conway's update rule, which updates the state of a cell in accordance with
9  !>   the following behaviour:
10 !>   - any live cell with two or three live neighbours continues to live,
11 !>   - any dead cell with three live neighbours becomes a live cell,
12 !>   - all other live cells die, and all other dead cells stay dead.
13 !>
14 !> This version of the program, 02_gol_cpu_openmp_loop_fort, is a parallel code,
15 !> modified from 02_gol_cpu_serial_fort, to utilise OMP loop parallelisation.
16 !> The following loops have been parallelised
17 !> - In game_of_life(..), over the (i, j) indexes as the updating of each cell's
18 !>   state can be performed independently of any other state.
19 !> - In game_of_life_stats(..), over the (i, j) indexes in calculating the
20 !>   number of cells in a given state.
21 program GameOfLife
22
23   use omp_lib
24   use gol_common
25   implicit none
26
27   interface
28     ! GOL prototypes.
29     subroutine game_of_life(opt, current_grid, next_grid, n, m)
30       use gol_common
31       implicit none
32
33       type(Options), intent(in) :: opt
34       integer, intent(in) :: n, m
35       integer, dimension(:,:), intent(in) :: current_grid
36       integer, dimension(:,:), intent(out) :: next_grid
37     end subroutine game_of_life
38
39     ! GOL stats prototype.
40     subroutine game_of_life_stats(opt, steps, current_grid)
41       use gol_common
42       implicit none
43
44       type(Options), intent(in) :: opt
45       integer, intent(in) :: steps
46       integer, dimension(:,:), intent(in) :: current_grid
47     end subroutine game_of_life_stats
48   end interface
49
50   ! GOL main loop variables.
51   type(Options) :: opt
52   integer :: n, m, nsteps, current_step
53   integer, dimension(:,:), allocatable :: grid, updated_grid
54   real*8 :: time1, time2
55
56   ! GOL initialisation.

```

```

57  call getinput(opt)
58
59  n = opt%n
60  m = opt%m
61  nsteps = opt%nsteps
62
63  write(*,*) n, m, nsteps
64
65  allocate(grid(n,m))
66  allocate(updated_grid(n,m))
67
68  call generate_IC(opt%iictype, grid, n, m)
69
70  ! GOL main loop.
71  time1 = init_time()
72  current_step = 0
73
74  do while (current_step .ne. nsteps)
75      time2 = init_time()
76
77      ! Visualise the current state of the grid according to the visualisation
78      ! type selected.
79      call visualise(opt%ivisualisetype, current_step, grid, n, m);
80
81      ! Calculate the statistics of the current state of the grid; that is, the
82      ! fractional occupation of each state across all cells.
83      call game_of_life_stats(opt, current_step, grid);
84
85      ! Calculate the next state of grid according to the Conway update rule.
86      call game_of_life(opt, grid, updated_grid, n, m);
87
88      ! Update the current grid variable.
89      grid(:, :) = updated_grid(:, :)
90
91      current_step = current_step + 1
92
93      ! Write out the time taken for this loop.
94      call get_elapsed_time(time2)
95
96      time2 = init_time()
97  end do
98
99  write(*,*) "Finished GOL"
100
101  ! Write out the time taken for the entire program
102  call get_elapsed_time(time1);
103
104  ! GOL cleanup.
105  deallocate(grid)
106  deallocate(updated_grid)
107 end program GameOfLife
108
109 !> GOL
110 subroutine game_of_life(opt, current_grid, next_grid, n, m)
111     use gol_common
112     implicit none
113
114     type(Options), intent(in) :: opt

```

```

115 integer, intent(in) :: n, m
116 integer, dimension(:, :), intent(in) :: current_grid
117 integer, dimension(:, :), intent(out) :: next_grid
118 integer :: neighbours, i, j, k
119 integer, dimension(8) :: n_i, n_j
120
121 ! Loop over current grid and determine next grid.
122 ! Inner and outer loops have been swapped due to Fortran storing arrays in
123 ! column-major order.
124 !
125 ! OMP parallel do
126 ! - A static scheduler is chosen as the expected work per iteration should be
127 !   approximately constant. Thus load balancing is unlikely to be an issue,
128 !   while minimising overhead is of particular concern - making a static
129 !   scheduler the optimal choice.
130 ! - The nested loops are not collapsed as testing revealed that including a
131 !   'collapse(2)' clause leads to a ~10% slower execution time.
132 !
133 !$omp parallel do &
134 !$omp   schedule (static) &
135 !$omp   shared (n, m, current_grid, next_grid) &
136 !$omp   private (i, j, n_i, n_j, k, neighbours)
137 do j = 1, m
138   do i = 1, n
139     ! Count the number of neighbours, clockwise around the current cell.
140     neighbours = 0;
141
142     n_i(1) = i - 1
143     n_j(1) = j - 1
144
145     n_i(2) = i - 1
146     n_j(2) = j
147
148     n_i(3) = i - 1
149     n_j(3) = j + 1
150
151     n_i(4) = i
152     n_j(4) = j + 1
153
154     n_i(5) = i + 1
155     n_j(5) = j + 1
156
157     n_i(6) = i + 1
158     n_j(6) = j
159
160     n_i(7) = i + 1
161     n_j(7) = j - 1
162
163     n_i(8) = i
164     n_j(8) = j - 1
165
166     ! Loop over all neighbours and check their state. The total number of live
167     ! neighbours is accumulated.
168     do k = 1, 8
169       if(n_i(k) .ge. 1 .and. n_j(k) .ge. 1 .and. &
170         n_i(k) .le. n .and. n_j(k) .le. m) then
171         if (current_grid(n_i(k), n_j(k)) .eq. CellState_ALIVE) then
172           neighbours = neighbours + 1

```

```

173         end if
174     end if
175 end do
176
177     ! Set the next grid, according to Conway's update rule.
178     if(current_grid(i,j) .eq. CellState_ALIVE .and. &
179        (neighbours .eq. 2 .or. neighbours .eq. 3)) then
180         next_grid(i,j) = CellState_ALIVE
181     else if (current_grid(i,j) .eq. CellState_DEAD .and. neighbours .eq. 3) then
182         next_grid(i,j) = CellState_ALIVE
183     else
184         next_grid(i,j) = CellState_DEAD
185     end if
186 end do
187 end do
188 !$omp end parallel do
189 end subroutine game_of_life
190
191 !> GOL stats
192 subroutine game_of_life_stats(opt, step, current_grid)
193     use gol_common
194     implicit none
195
196     type(Options), intent(in) :: opt
197     integer, intent(in) :: step
198     integer, dimension(:,,:), intent(in) :: current_grid
199     integer :: i, j, state
200     integer*8 :: ntot
201     ! num_in_state and frac modified from dimension(NUMSTATES) to
202     ! dimension(0:NUMSTATES-1) to synchronise with the 0-based indexing of
203     ! states mandated in common_fort.f90.
204     integer, dimension(0:NUMSTATES-1) :: num_in_state
205     real*8, dimension(0:NUMSTATES-1) :: frac
206     character(len=30) :: fmt
207
208     fmt = "(A15,I1,A3,F10.4,A4)"
209     ntot = opt%n * opt%m
210
211     num_in_state(:) = 0
212
213     ! Calculated the number of cells in each state across the entire grid.
214     ! Inner and outer loops have been swapped due to Fortran storing arrays in
215     ! column-major order.
216     !
217     ! OMP parallel do
218     ! - A static scheduler is chosen as the expected work per iteration should be
219     !   approximately constant. Thus load balancing is unlikely to be an issue,
220     !   while minimising overhead is of particular concern - making a static
221     !   scheduler the optimal choice.
222     ! - The nested loops are not collapsed as testing revealed that including a
223     !   'collapse(2)' clause leads to a ~10% slower execution time.
224     ! - A reduction clause is included for the num_in_state(:) variable as it can
225     !   be reduced across all iterations. Without this clause, the parallel do is
226     !   actually slower than the non-parallel do, however including it leads to
227     !   performance benefits.
228     !
229     !$omp parallel do &
230     !$omp    schedule (static) &

```

```
231 !$omp shared (opt, current_grid) &
232 !$omp private (i, j, state) &
233 !$omp reduction(+:num_in_state)
234 do j = 1, opt%m
235   do i = 1, opt%n
236     state = current_grid(i,j)
237     num_in_state(state) = num_in_state(state) + 1
238   end do
239 end do
240 !$omp end parallel do
241
242 ! Converted the state occupation from absolute terms to fractional terms.
243 frac(:) = num_in_state(:)/real(ntot)
244
245 if (step .eq. 0) then
246   open(10, file=opt%statsfile, access="sequential")
247 else
248 #if defined(_CRAYFTN) || defined(_INTELFTN)
249   open(10, file=opt%statsfile, position="append")
250 #else
251   open(10, file=opt%statsfile, access="append")
252 #endif
253 end if
254
255 write(10,*) "step ", step
256
257 ! Loop bounds modified to synchronise with 0-based indexing of frac(:).
258 do i = 0, NUMSTATES-1
259   write(10,fmt, advance="no") "Frac in state ", i, " = ", frac(i), " "
260 end do
261
262 write(10,*) ""
263 close(10)
264 end subroutine game_of_life_stats
```

A.5 gol-job-submission.slurm

```

1  #!/bin/bash -l
2
3  # SLURM details
4  #SBATCH --account=courses0100
5  #SBATCH --reservation=courses0100
6  #SBATCH --job-name=GOL
7  #SBATCH --time=00:10:00
8  #SBATCH --export=NONE
9  #SBATCH --nodes=1
10 #SBATCH --tasks-per-node=1
11 #SBATCH --cpus-per-task=16
12
13 # parameters
14 # Redundant when using gol-job-set-submission.sh to export parameter sets into
15 # this script.
16 # version_name="01_gol_cpu_serial_fort"
17 # n_omp=2
18 # grid_height=10
19 # grid_width=10
20 # num_steps=10
21 # initial_conditions_type=0
22 # visualisation_type=0
23 # rule_type=0
24 # neighbour_type=0
25 # boundary_type=0
26
27 # filenames
28 base_name="\
29 GOL-${version_name}.\
30 nomp-${n_omp}.\
31 ngrid-${grid_height}x${grid_width}.\
32 nsteps-${num_steps}.\
33 ic_type-${initial_conditions_type}.\
34 vis_type-${visualisation_type}.\
35 rule_type-${rule_type}.\
36 nghbr_type-${neighbour_type}.\
37 bndry_type-${boundary_type}"
38
39 output_dir="output/${base_name}"
40 log_filename="${output_dir}/log.txt"
41 stats_filename="${output_dir}/stats.txt"
42
43 # load appropriate modules
44 module load gcc/8.3.0
45
46 # program execution
47 export OMP_NUM_THREADS=${n_omp}
48
49 exe="./bin/${version_name}"
50
51 args="\
52 ${grid_height} \
53 ${grid_width} \
54 ${num_steps} \
55 ${initial_conditions_type} \
56 ${visualisation_type} \

```

```
57 ${rule_type} \  
58 ${neighbour_type} \  
59 ${boundary_type} \  
60 \"${stats_filename}\"\  
61  
62 echo "GOL SLURM job submission"  
63 # echo "version_name: ${version_name}"  
64 echo "base_name: ${base_name}"  
65 # echo "log_filename: ${log_filename}"  
66 # echo "stats_filename: ${stats_filename}"  
67 # echo "exe: ${exe}"  
68 # echo "args: ${args}"  
69  
70 # check if the GOL simulation has already been performed for these parameters,  
71 # and if it hasn't, run the GOL simulation.  
72 if [ -d "${output_dir}" ]; then  
73     echo "GOL simulation already performed for these parameters"  
74 else  
75     echo "GOL output directory will be created"  
76  
77     mkdir -p ${output_dir}  
78     touch ${stats_filename}  
79     touch ${log_filename}  
80  
81     echo "GOL simulation will commence"  
82  
83     srun -n 1 -c ${n_omp} ${exe} ${args} > ${log_filename}  
84 fi
```


A.6 gol-job-set-submission.sh

```

1  #!/bin/bash -l
2
3  # kv_string
4  # utility function for converting parameter associative array into an export
5  # string suitable for the command
6  # > parameter_string=$(kv_string parameters)
7  # > "sbatch gol-job-submission.slurm --export=${parameter_string}"
8  function kv_string {
9      local -n array=$1
10
11      str=""
12
13      declare -i counter=1
14      length=${#array[*]}
15
16      for key in ${!array[*]} ; do
17          kv_pair="${key}=${array[${key}]}"
18          if [ ${counter} != ${length} ] ; then
19              str+="${kv_pair},"
20          else
21              str+="${kv_pair}"
22          fi
23          counter+=1
24      done
25
26      echo ${str}
27  }
28
29  # parameter sets
30  version_names_serial="01_gol_cpu_serial_fort 02_gol_cpu_serial_fort"
31  # version_names_parallel="02_gol_cpu_openmp_task_fort 02_gol_cpu_openmp_loop_fort"
32  version_names_parallel="02_gol_cpu_openmp_loop_fort"
33  version_names="${version_names_serial} ${version_names_parallel}"
34
35  grid_lengths="2 4 8 16 32 64 128 256 512 1024 2048 4096 8192 16384"
36  # grid_lengths="10 100 1000 10000"
37
38  n_omps="1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16"
39
40  # parameter associative array with default values
41  declare -A parameters
42
43  parameters[version_name]=" "
44  parameters[n_omp]=4
45  parameters[grid_height]=1
46  parameters[grid_width]=1
47  parameters[num_steps]=1
48  parameters[initial_conditions_type]=0
49  parameters[visualisation_type]=3
50  parameters[rule_type]=0
51  parameters[neighbour_type]=0
52  parameters[boundary_type]=0
53
54  # load appropriate modules and compile code
55  module load gcc/8.3.0
56

```

```

57 # GOL job sets
58 echo "GOL SLURM job set submission"
59 echo
60
61 # GOL uniformity / ascii visualisation
62 # Performing GOL simulations on a 10x10 grid, for 10 steps, with ascii
63 # visualisation. Intended to verify that different GOL versions produce the same
64 # behaviour.
65 echo "GOL ascii jobs"
66 echo "versions: ${version_names}"
67 echo "ngrid: 10x10"
68 echo "nsteps: 10"
69 echo "vis_type: 0 (ascii)"
70 for version_name in ${version_names} ; do
71     parameters[version_name]=${version_name}
72     parameters[grid_height]=10
73     parameters[grid_width]=10
74     parameters[num_steps]=10
75     parameters[visualisation_type]=0
76
77     parameter_string=$(kv_string parameters)
78     # echo "--export=${parameter_string}"
79     sbatch --export=${parameter_string} gol-job-submission.slurm
80 done
81 echo
82
83 # GOL scaling
84 # Performing GOL simulations on increasingly large grids, 2^n x 2^n for n = 1,
85 # .., nmax, for 100 steps, with no visualisation. Intended to determine the
86 # scaling behaviour of the different GOL versions.
87 echo "GOL scaling jobs"
88 echo "versions: ${version_names}"
89 echo "grid lengths: ${grid_lengths}"
90 echo "nsteps: 100"
91 echo "vis_type: 3 (none)"
92 for version_name in ${version_names} ; do
93     parameters[version_name]=${version_name}
94     parameters[num_steps]=100
95     parameters[visualisation_type]=3
96
97     for grid_length in ${grid_lengths}; do
98         parameters[grid_height]=${grid_length}
99         parameters[grid_width]=${grid_length}
100
101         parameter_string=$(kv_string parameters)
102         # echo "--export=${parameter_string}"
103         sbatch --export=${parameter_string} gol-job-submission.slurm
104     done
105 done
106 echo
107
108 # GOL thread independence
109 # Performing parallel GOL simulations with varying numbers of omp threads, on a
110 # 10x10 grid, for 10 steps, with ascii visualisation. Intended to verify that
111 # the parallel GOL versions produce the same behaviour independent of the number
112 # of omp threads.
113 echo "GOL thread independence jobs"
114 echo "versions: ${version_names_parallel}"

```

```

115 echo "ngrid: 10x10"
116 echo "nsteps: 10"
117 echo "vis_type: 0 (ascii)"
118 echo "n_omps: ${n_omps}"
119 for version_name in ${version_names_parallel} ; do
120     parameters[version_name]=${version_name}
121     parameters[grid_height]=10
122     parameters[grid_width]=10
123     parameters[num_steps]=10
124     parameters[visualisation_type]=0
125
126     for n_omp in ${n_omps}; do
127         parameters[n_omp]=${n_omp}
128
129         parameter_string=$(kv_string parameters)
130         # echo "--export=${parameter_string}"
131         sbatch --export=${parameter_string} gol-job-submission.slurm
132     done
133 done
134 echo
135
136 # GOL thread scaling
137 # Performing parallel GOL simulations with varying numbers of omp threads, on
138 # increasing large grids, 2^n x 2^n for n = 1, .., nmax, for 100 steps, with no
139 # visualisation. Intended to determine the scaling behaviour of the parallel GOL
140 # versions, with increasing number of omp threads, and with increasing grid
141 # sizes.
142 echo "GOL thread scaling jobs"
143 echo "versions: ${version_names_parallel}"
144 echo "grid lengths: ${grid_lengths}"
145 echo "nsteps: 100"
146 echo "vis_type: 3 (none)"
147 echo "n_omps: ${n_omps}"
148 for version_name in ${version_names_parallel} ; do
149     parameters[version_name]=${version_name}
150     parameters[num_steps]=100
151     parameters[visualisation_type]=3
152
153     for n_omp in ${n_omps}; do
154         parameters[n_omp]=${n_omp}
155
156         for grid_length in ${grid_lengths}; do
157             parameters[grid_height]=${grid_length}
158             parameters[grid_width]=${grid_length}
159
160             parameter_string=$(kv_string parameters)
161             # echo "--export=${parameter_string}"
162             sbatch --export=${parameter_string} gol-job-submission.slurm
163         done
164     done
165 done
166 echo

```

A.7 gol-data-extract.sh

```

1  #!/bin/bash -l
2
3  # utility function
4  function parameter_string {
5      local -n array=$1
6
7      str=""
8
9      str+="GOL-${array[version_name]}"
10     str+=" .nomp-${array[n_omp]}"
11     str+=" .ngrid-${array[grid_height]}x${array[grid_width]}"
12     str+=" .nsteps-${array[num_steps]}"
13     str+=" .ic_type-${array[initial_conditions_type]}"
14     str+=" .vis_type-${array[visualisation_type]}"
15     str+=" .rule_type-${array[rule_type]}"
16     str+=" .nghbr_type-${array[neighbour_type]}"
17     str+=" .bndry_type-${array[boundary_type]}"
18
19     echo ${str}
20 }
21
22 # parameter sets
23 version_names_serial="01_gol_cpu_serial_fort 02_gol_cpu_serial_fort"
24 version_names_parallel="02_gol_cpu_openmp_loop_fort"
25 version_names="${version_names_serial} ${version_names_parallel}"
26 grid_lengths="2 4 8 16 32 64 128 256 512 1024 2048 4096 8192 16384"
27 n_oms="1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16"
28
29 # parameter associative array with default values
30 declare -A parameters
31
32 parameters[version_name]=" "
33 parameters[n_omp]=4
34 parameters[grid_height]=1
35 parameters[grid_width]=1
36 parameters[num_steps]=1
37 parameters[initial_conditions_type]=0
38 parameters[visualisation_type]=3
39 parameters[rule_type]=0
40 parameters[neighbour_type]=0
41 parameters[boundary_type]=0
42
43 # GOL scaling batch
44 parameters[num_steps]=100
45 parameters[visualisation_type]=3
46
47 mkdir -p data/scaling
48
49 for version_name in ${version_names} ; do
50     parameters[version_name]=${version_name}
51
52     data_file="data/scaling/${version_name}.csv"
53
54     if [ -f ${data_file} ] ; then
55
56         echo "${data_file} already exists"

```

```

57
58     else
59
60         for grid_length in ${grid_lengths}; do
61             parameters[grid_height]=${grid_length}
62             parameters[grid_width]=${grid_length}
63
64             str=$(parameter_string parameters)
65
66             echo ${str}
67
68             last_line=$(tail -n 1 output/${str}/log.txt)
69
70             echo ${last_line}
71             time_pattern="([0-9].+)s"
72             if [[ $last_line =~ $time_pattern ]] ; then
73                 time=${BASH_REMATCH[1]}
74                 echo $time
75
76                 printf "${grid_length} , ${time}\n" >> ${data_file}
77             else
78                 echo "failed to find time"
79             fi
80         done
81     fi
82 done
83 echo
84
85 # GOL thread scaling
86 parameters[num_steps]=100
87 parameters[visualisation_type]=3
88
89 mkdir -p data/parallel_thread_scaling
90
91 for version_name in ${version_names_parallel} ; do
92     parameters[version_name]=${version_name}
93
94     for n_omp in ${n_omps}; do
95         parameters[n_omp]=${n_omp}
96
97         data_file="data/parallel_thread_scaling/${version_name}-${n_omp}.csv"
98
99         if [ -f ${data_file} ] ; then
100
101             echo "${data_file} already exists"
102
103         else
104
105             for grid_length in ${grid_lengths}; do
106                 parameters[grid_height]=${grid_length}
107                 parameters[grid_width]=${grid_length}
108
109                 str=$(parameter_string parameters)
110
111                 echo ${str}
112
113                 last_line=$(tail -n 1 output/${str}/log.txt)
114

```

```
115         echo ${last_line}
116         time_pattern="([0-9].+)s"
117         if [[ $last_line =~ $time_pattern ]] ; then
118             time=${BASH_REMATCH[1]}
119             echo $time
120
121             printf "${grid_length} , ${time}\n" >> ${data_file}
122         else
123             echo "failed to find time"
124         fi
125     done
126 fi
127 done
128 done
129 echo
```