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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 O1\_gol\_cpu\_serial\_fort and O2\_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 bash 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
- intial\_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.

- 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 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, ..., 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,  $n_{\rm omp}=1,\ldots,16$ , on a  $10\times10$  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,  $n_{\rm omp}=1,\ldots,16$ , and for a range of grid sizes,  $2^n\times 2^n$  for  $n=1,\ldots 14$  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.
- 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: a bug in the game\_of\_life\_stats() subroutine has been

## 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 Bash Scripts

#### 2.2 Serial Code

```
integer, dimension(0:NUMSTATES-1) :: num_in_state
real*4, dimension(0:NUMSTATES-1) :: frac

do i = 0, NUMSTATES-1
    write(10,fmt, advance="no") "Frac in state ", i, " = ", frac(i), " "
end do
```

- 2.2.1 Original Serial Code
- 2.2.2 Improved Serial Code
- 2.2.3 Profiling Comparison
- 2.3 Parallel Loop Code

- 3 Results
- 3.1 Uniform Behaviour Verification
- 3.2 Scaling Behaviour
- 3.3 Thread Independence Verification
- 3.4 Thread Scaling Behaviour

## A Appendix

#### A.1 src/common\_fort.f90

```
1 !> Conway's Game of Life - Common
  !> This module provides a common set of functionality which is used across all
  !> serial and parallel versions of the GOL code.
  !> The only modification to this module has been adjusting the length of the
  !> 'arg' variable in getinput() from 32 to 2000, to accommodate long statsfile
  !> filenames.
  module gol_common
  1----<del>-</del>
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
      integer, parameter :: CellState_DYING = 2
19
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
      integer, parameter :: ICType_IC_RAND = 0
29
30
      integer, parameter :: ICType_IC_FILE = 1
31
      integer, parameter :: NUMRULES = 3
32
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
          integer :: n, m, nsteps
49
          integer :: iictype
50
          integer :: ivisualisetype
51
          integer :: iruletype
52
          integer :: ineighbourtype
          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
            integer, intent(in) :: step, n, m
 62
 63
            integer, dimension(:,:), intent(in) :: grid
 64
            character :: cell
            integer :: i, j
 65
 66
 67
            write(*,*) "Game of Life"
            write(*,*) "Step ", step
 68
 69
            do i = 1, n
                do j = 1, m
 70
 71
                    cell = ''
 72
                    ! could use where
 73
                    if (grid(i,j) .eq. CellState_ALIVE) cell = '*'
 74
                    write(*,"(A)", advance="no") cell
 75
                end do
                write(*,*) ""
 76
 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
        subroutine visualise_none(step)
 89
 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
             \textbf{else if (ivisualisechoice .eq. VisualiseType\_VISUAL\_PNG) then } \\
104
                call visualise_png(step, grid, n, m)
105
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
            do i = 1, n
118
                do j = 1, m
119
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
                        grid(i,j) = CellState_ALIVE
128
129
                    end if
130
                end do
131
            end do
132
133
        end subroutine
134
135
        ! generate IC
136
        subroutine generate_IC(ic_choice, grid, n, m)
           implicit none
137
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
        ! UT
152
        subroutine getinput(opt)
153
            implicit none
154
            type(Options), intent(inout) :: opt
155
            character(len=2000) :: cmd
156
            character(len=2000) :: arg
            character(len=2000) :: statsfilename
157
158
            integer :: count
159
            integer*8 :: nbytes
160
            real*4 :: memfootprint
161
            ! get the commands passed and the number of args passed
162
            call get_command(cmd)
163
            count = command_argument_count()
164
            if (count .1t. 2) then
165
                write(*,*) "Usage: <grid height> <grid width> "
                write(*,*) "[<nsteps> <IC type> <Visualisation type> <Rule type> <</pre>
166
        Neighbour type> "
167
                write(*,*) "<Boundary type> <stats filename> ]"
168
                call exit();
```

```
169
            end if
170
171
            statsfilename = "GOL-stats.txt"
172
            call get_command_argument(1, arg)
173
            read(arg,*) opt%n
174
            call get_command_argument(2, arg)
175
            read(arg,*) opt%m
176
            opt%nsteps = -1
            opt%ivisualisetype = VisualiseType_VISUAL_ASCII
177
178
            opt%iruletype = RuleType_RULE_STANDARD
179
            opt%iictype = ICType_IC_RAND
            opt%ineighbourtype = NeighbourType_NEIGHBOUR_STANDARD
180
            opt%iboundarytype = BoundaryType_BOUNDARY_HARD
181
            if (count .ge. 3) then
182
183
                call get_command_argument(3, arg)
184
                read(arg,*) opt%nsteps
185
            end if
186
            if (count .ge. 4) then
187
                call get_command_argument(4, arg)
                read(arg,*) opt%iictype
188
189
            end if
190
            if (count .ge. 5) then
191
                call get_command_argument(5, arg)
192
                read(arg,*) opt%ivisualisetype
193
194
            if (count .ge. 6) then
195
                call get_command_argument(6, arg)
196
                read(arg,*) opt%iruletype
197
            end if
198
            if (count .ge. 7) then
199
                call get_command_argument(7, arg)
200
                read(arg,*) opt%ineighbourtype
            end if
201
202
            if (count .ge. 8) then
203
                call get_command_argument(8, arg)
204
                read(arg,*) opt%iboundarytype
205
206
            if (count .ge. 9) then
207
                call get_command_argument(9, arg)
208
                read(arg,*) statsfilename
209
            end if
210
            if (opt%n .le. 0 .or. opt%m .le. 0) then
                write(*,*) "Invalid grid size."
211
212
                call exit(1)
213
            end if
214
            opt%statsfile = statsfilename
            nbytes = sizeof(opt%n) * opt%n * opt%m
215
216
            memfootprint = real(nbytes)/1024.0/1024.0/1024.0
217
            write(*,*) "Requesting grid size of ", opt%n, opt%m
218
            write(*,*) " which requires", memfootprint, " GB "
219 #ifndef USEPNG
220
            if (opt%ivisualisetype .eq. VisualiseType_VISUAL_PNG) then
                write(*, *) "PNG visualisation not enabled at compile time,"
221
                write(*, *) "turning off visualisation from now on."
222
223
            end if
224 #endif
225
        end subroutine
226
```

```
227
        ! get some basic timing info
228
        real*8 function init_time()
229
            integer, dimension(8) :: value
230
            call date_and_time(VALUES=value)
231
           init_time = value(5)*3600.0+value(6)*60.0+value(7)+value(8)/1000.0
232
           return
233
        end function
234
        ! get the elapsed time relative to start
235
        subroutine get_elapsed_time(start)
236
           real *8, intent(in) :: start
237
            real*8 :: finish, delta
238
           integer, dimension(8) :: value
239
            call date_and_time(VALUES=value)
240
           finish = value(5) *3600.0+value(6) *60.0+value(7) +value(8) /1000.0
            delta = finish - start
241
242
            write(*,*) "Elapsed time is ", delta, "s"
243
        end subroutine
244
245 end module
```

### A.2 src/01\_gol\_cpu\_serial\_fort.f90

```
program GameOfLife
2
3
4
5
      This program runs Conway's Game of Life
6
7
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
               integer, dimension(:,:), intent(in) :: current_grid
integer, dimension(:,:), intent(out) :: next_grid
19
20
21
           end subroutine
22
           ! GOL stats protoype
23
           subroutine game_of_life_stats(opt, steps, current_grid)
24
               use gol_common
25
               implicit none
26
               type(Options), intent(in) :: opt
               integer, intent(in) :: steps
27
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
       nsteps = opt%nsteps
39
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)
           time2 = init_time()
55
```

```
write(*,*) "Finnished GOL"
57
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
        integer, intent(in) :: n, m
 68
        integer, dimension(:,:), intent(in) :: current_grid
integer, dimension(:,:), intent(out) :: next_grid
 69
 70
        integer :: neighbours, i, j, k
 71
 72
        integer, dimension(8) :: n_i, n_j
 73
 74
        ! loop over current grid and determine next grid
        do i = 1, n
 75
            do j = 1, m
 76
 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
                 n_i(6) = i + 1
 89
                 n_j(6) = j
 90
 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)
        ) .le. m) then
99
                          if (current_grid(n_i(k), n_j(k)) .eq. CellState_ALIVE) then
100
                              neighbours = neighbours + 1
101
                          end if
102
                     end if
103
                 end do
104
105
                 ! set the next grid
106
                 if(current_grid(i,j) .eq. CellState_ALIVE .and. (neighbours .eq. 2 .or.
        neighbours .eq. 3)) then
107
                     next_grid(i,j) = CellState_ALIVE
108
                 else if (current_grid(i,j) .eq. CellState_DEAD .and. neighbours .eq. 3)
        then
109
                     next_grid(i,j) = CellState_ALIVE
110
                 else
111
                     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
       integer, dimension(:,:), intent(in) :: current_grid
123
124
        integer :: i, j, state
125
       integer*8 :: ntot
126
       integer, dimension(0:NUMSTATES-1) :: num_in_state
127
        real*4, dimension(0:NUMSTATES-1) :: frac
128
       character(len=30) :: fmt
129
       fmt = "(A15,I1,A3,F10.4,A4)"
130
131
       ntot = opt%n * opt%m
132
        num_in_state = 0;
        do i = 1, opt%n
133
134
            do j = 1, opt%m
135
                state = current_grid(i,j)
136
                num_in_state(state) = num_in_state(state) + 1
137
            end do
138
        end do
139
        frac = num_in_state/real(ntot)
140
        if (step .eq. 0) then
           open(10, file=opt%statsfile, access="sequential")
141
142
        else
143 #if defined(_CRAYFTN) || defined(_INTELFTN)
144
            open(10, file=opt%statsfile, position="append")
145 #else
146
            open(10, file=opt%statsfile, access="append")
147 #endif
148
        end if
        write(10,*) "step ", step
149
150
        do i = 0, NUMSTATES-1
151
           write(10,fmt, advance="no") "Frac in state ", i, " = ", frac(i), " "
152
        end do
153
        write(10,*) ""
154
        close(10)
155 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:
   !> - a 2D grid with hard, torodial or a hybrid boundary,
   !> - possible cell states S = \{0, 1\}; that is, dead or alive,
   ! - a Moore neighbourhood; that is, where for a given cell, the cells directly
      and diagonally adjacent are considered its neighbours,
8 !> - Conway's update rule, which updates the state of a cell in accordance with
       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,
       - 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, O1_gol_cpu_serial_fort, in the
16 !> following ways:
17 !> - Inner and outer loops over grid(i, j) have been swapped to ensure more
       efficient array caching (noting that Fortran is column-major).
19 !> - Fixed error in game_of_life_stats() which was indexing states from
       [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 protoype.
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.
```

```
call getinput(opt)
 57
 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
     integer, dimension(:,:), intent(in) :: current_grid
116
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
         n_j(2) = j
133
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.
         do k = 1, 8
155
           156
157
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
166
           next_grid(i,j) = CellState_ALIVE
167
168
         else if (current_grid(i,j) .eq. CellState_DEAD .and. neighbours .eq. 3) then
169
           next_grid(i,j) = CellState_ALIVE
170
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
     integer, dimension(:,:), intent(in) :: current_grid
184
      integer :: i, j, state
185
186
     integer*8 :: ntot
187
     integer, dimension(0:NUMSTATES-1) :: num_in_state
188
     real*8, dimension(0:NUMSTATES-1) :: frac
189
     character(len=30) :: fmt
190
191
     fmt = "(A15, I1, A3, F10.4, A4)"
192
     ntot = opt%n * opt%m
193
194
      ! Calculated the number of cells in each state across the entire grid.
195
     ! Inner and outer loops have been swapped due to Fortran storing arrays in
196
     ! column-major order.
197
     num_in_state(:) = 0;
198
     do j = 1, opt%m
199
       do i = 1, opt%n
200
         state = current_grid(i,j)
201
         num_in_state(state) = num_in_state(state) + 1
202
       end do
203
      end do
204
205
      ! Converted the state occupation from absolute terms to fractional terms.
206
     frac(:) = num_in_state(:)/real(ntot)
207
208
     if (step .eq. 0) then
209
       open(10, file=opt%statsfile, access="sequential")
210
      else
211 #if defined(_CRAYFTN) || defined(_INTELFTN)
212
        open(10, file=opt%statsfile, position="append")
213 #else
214
        open(10, file=opt%statsfile, access="append")
215 #endif
216
     end if
217
218
     write(10,*) "step ", step
219
220
     do i = 0. NUMSTATES-1
221
       write(10,fmt, advance="no") "Frac in state ", i, " = ", frac(i), " "
222
      end do
223
     write(10,*) ""
224
225
     close(10)
226 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:
   !> - a 2D grid with hard, torodial or a hybrid boundary,
   !> - possible cell states S = \{0, 1\}; that is, dead or alive,
   !> - a Moore neighbourhood; that is, where for a given cell, the cells directly
      and diagonally adjacent are considered its neighbours,
8 !> - Conway's update rule, which updates the state of a cell in accordance with
       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,
       - all other live cells die, and all other dead cells stay dead.
12 !>
13 ! >
14 !> This version of the program, 02_gol_cpu_openmp_loop_fort, is a parallel code,
   !> 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
      state can be performed independently of any other state.
19 !> - In game_of_life_stats(..), over the (i, j) indexes in calculating the
       number of cells in a given state.
21 program GameOfLife
22
23
     use omp_lib
24
    use gol_common
25
     implicit none
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 protoype.
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
     ! GOL initialisation.
```

```
call getinput(opt)
 57
 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
      integer, dimension(:,:), intent(in) :: current_grid
116
117
      integer, dimension(:,:), intent(out) :: next_grid
118
      integer :: neighbours, i, j, k
119
     integer, dimension(8) :: n_i, n_j
120
     ! Loop over current grid and determine next grid.
121
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,
         while minimising overhead is of particular concern - making a static
128
         scheduler the optimal choice.
129
130
      ! - The nested loops are not collapsed as testing revealed that including a
          'collapse(2)' clause leads to a ~10% slower execution time.
131
      1
132
133
      !$omp parallel do &
134
      !$omp schedule (static) &
135
              shared (n, m, current_grid, next_grid) &
      !$omp
136
      !$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. &
              (neighbours .eq. 2 .or. neighbours .eq. 3)) then
179
180
           next_grid(i,j) = CellState_ALIVE
          else if (current_grid(i,j) .eq. CellState_DEAD .and. neighbours .eq. 3) then
181
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
     !$omp end parallel do
189
   end subroutine game_of_life
190
191 !> GOL stats
192 subroutine game_of_life_stats(opt, step, current_grid)
193
     use gol_common
194
     implicit none
195
196
     type(Options), intent(in) :: opt
197
     integer, intent(in) :: step
198
     integer, dimension(:,:), intent(in) :: current_grid
199
      integer :: i, j, state
200
      integer*8 :: ntot
201
     integer, dimension(0:NUMSTATES-1) :: num_in_state
202
      real *8, dimension (0: NUMSTATES-1) :: frac
203
     character(len=30) :: fmt
204
205
     fmt = "(A15, I1, A3, F10.4, A4)"
206
     ntot = opt%n * opt%m
207
208
     num_in_state(:) = 0;
209
210
      ! Calculated the number of cells in each state across the entire grid.
211
      ! Inner and outer loops have been swapped due to Fortran storing arrays in
212
     ! column-major order.
213
214
     ! OMP parallel do
215
      ! - A static scheduler is chosen as the expected work per iteration should be
216
         approximately constant. Thus load balancing is unlikely to be an issue,
217
         while minimising overhead is of particular concern - making a static
218
         scheduler the optimal choice.
219
      ! - The nested loops are not collapsed as testing revealed that including a
220
          'collapse(2)' clause leads to a ~10% slower execution time.
221
      ! - A reduction clause is included for the num_in_state(:) variable as it can
222
         be reduced across all iterations. Without this clause, the parallel do is
223
         actually slower than the non-parallel do, however including it leads to
224
         performance benefits.
225
226
      !$omp parallel do &
227
      !$omp
              schedule (static) &
228
              shared (opt, current_grid) &
      !$omp
229
      !$omp
             private (i, j, state) &
      !$omp
            reduction(+:num_in_state)
```

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

#### A.5 gol-job-submission.slurm

```
1 #!/bin/bash -1
2
3 # SLURM details
#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
|\mathbf{14}| # Redundant when using gol-job-set-submission.sh to export parameter sets into
16 # version_name="01_gol_cpu_serial_fort"
17 \mid \# 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
27 # filenames
28 base_name="\
29 GOL-${version_name}.\
30 \mid nomp - \{n_omp\}.
31 ngrid-${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 - ${boundary_type}"
39 output_dir="output/${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 \mid \$\{num\_steps\} \setminus
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
       echo "GOL output directory will be created"
75
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 -1
2
3 # kv_string
  # utility function for converting parameter associative array into an export
  # string suitable for the command
6 # > parameter_string=$(kv_string parameters)
  # > "sbatch gol-job-submission.slurm --export=${parameter_string}"
8 function kv_string {
9
       local -n array=$1
10
       str=""
11
12
13
       declare -i counter=1
14
       length=${#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
       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
        parameters[version_name] = ${version_name}
120
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
        parameters[version_name] = ${version_name}
149
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
164
        done
165
    done
166
    echo
```