

ECE 4530 - Parallel Programming  
Graduate Project  
Conway's Game of Life on a Tetrahedral Mesh

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# 1 Project Description

For my project, I implemented a 3D version of Conway's Game of Life on an unstructured, finite, tetrahedral mesh. This project builds on the ORB code of Lab 3, with some significant changes to facilitate the Game of Life.

For my project, I generated tetrahedral meshes using gmsh. A tetrahedral mesh is a partitioning of a physical volume into a set of non-intersecting tetrahedra whose union approximately fills the physical volume. Such a mesh can be described by a set of 4-tuples in 3D space – each of which describes the 4 corners of a tetrahedron. This is implemented in gmsh as a list of points in 3D space, and a list of integer 4-tuples which index list of points.

Conway's Game of Life is normally played on an infinite square grid. Such a structure is nicely ordered, and Conway's simple set of rules can produce very interesting emergent properties on the grid. For example, one can build a glider gun that continuously shoots out structures that travel indefinitely. Some people choose to draw meaningful conclusions about human life from Conway's game. I think that's ridiculous. Real life doesn't happen on a nice uniform grid. Not only that, we don't live in planes any more, everybody lives among and on top of one another. We now need three co-ordinates to describe our relationships. People today live like vertices in a mesh. We are suspended, tenuously, barely help up by our friends, yearning to avoid the abyss below. For a 3D tetrahedral Game of Life, I could have chosen to have either the tetrahedra or the vertices be the elements of interest. For reference, a simple, in Fig. 1, I have included a simple, coarse mesh. I chose to explore the Game of Life on vertices, for 2 reasons:

1. The degree of the vertices in a mesh is not uniform, whereas each tetrahedral element has 4 face-neighbours
2. In a tetrahedral setup, we would have to deal with the exterior faces. They would need to be treated as dead neighbours, and that's too morbid.

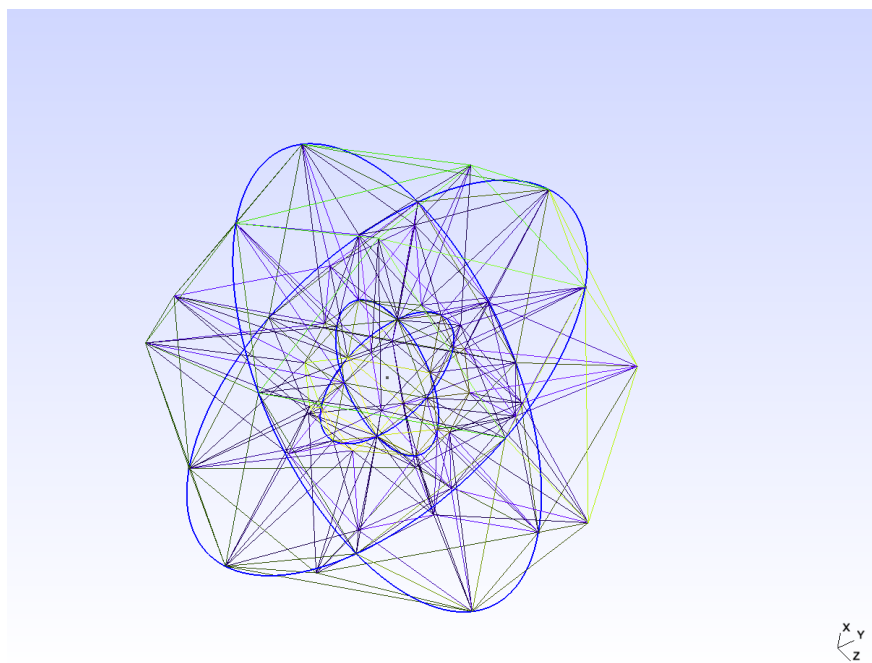


Figure 1: Sample Mesh

In Conway's Game of Life, the grid is assumed to be infinite. This is not the case on my vertex mesh. The mesh is finite. Despite this fact, we don't need to worry about treating fictitious boundary neighbours as 'dead'. Rather, the nature of the vertex-based mesh means that each of a vertex's neighbours exist in the playing area. This Game of Life is also inherently cyclic. There is a finite number of vertices, each of which

can either be alive or dead. If we have  $v$  vertices, then there are  $2^v$  possible states of the mesh. Therefore the game will repeat in as many as  $2^v$  steps. Bear in mind that (everybody is dead)  $\rightarrow$  (everybody is dead) is a valid cycle.

## 2 Implementation Details

My Game of Life code built off of the mesh partitioning code that was developed for Lab 3. In order to run a Game of Life simulation on an unstructured tetrahedral mesh, the following steps needed to be taken:

1. Modify certain mesh data types to include information about connectivity and life state.
2. Decide how to distribute vertices among the processors.
3. Decide on a method for initializing the mesh's life states.
4. Develop an efficient method to update the mesh's life states when they are shared among many processors.
5. Formulate a way to visualize the game.

### 2.1 Vertex Distribution

I chose to divide the vertices by using the ORB code that was developed for Lab 3. I figured that it would be wise to minimize the interface area between processors. ORB should do a good job of minimizing that interface area. If I had chosen to, say, apply `parallelRange` to the vertices x-position, then I would end up with many thin slices of my mesh, which would probably lead to a whole lot of communication overhead.

The ORB code from Lab 3 perform ORB on the centroids of the tetrahedral mesh elements. I left this behaviour intact, instead of modifying the code to work on vertices. This means that each processor hold a unique list of elements, but its vertices may also exist on other processors. Since some vertices are shared, it is necessary to pick one of the processors who shares the vertex to be the owner. I explored two methods for deciding who owns a shared vertex: making the lowest rank the owner, and choosing the owner randomly. Ultimately, I decided to go with minimum-rank ownership. Reasons for this decision will be discussed later.

### 2.2 Vertex Connectivity

In order to capture the connectivity of the vertices in the mesh, I modified contents of the `vertex_t` data type. The new data type is shown below:

```

1 typedef struct vertex_t
2 {
3     double r[3];           // Position in 3-space
4     int mid;               // Mesh ID
5     bool current_state;    // Alive or dead
6     bool next_state;      // Alive or dead
7     int owner;             // Rank who owns vertex
8     bool is_shared;        // Tell me whether this is shared
9     int alive_dead[2];     // Number of alive/dead neighbours
10    std::vector<int> family; // List of ranks which share vertex
11    std::vector<vertex_t*> neighbours; // List of pointers to local neighbouring vertices
12    std::vector<int> global_nbr_mids; // List of global connections
13    std::vector<bool> nbr_was_counted; // Used during vertex update
14 }
15 vertex_t;
```

The vector `neighbours` stores pointers to local neighbouring vertices, making tabulation of neighbours' alive/dead counts simple. The vector `family` is a list of the ranks which share the vertex. The determination of this connectivity information is non-trivial. This is handled by the function `Mesh::calculateVertexConnectivity`

The first step toward determining the connectivity of the mesh is for each processor to loop over its local elements, and make a list of which local vertices are connected to each other, indexed by their mesh ID. The code for this is shown below:

```

1     std::map<int, std::vector<int>> > mid_connections_by_mid;
2
3     for(int ie = 0; ie < elements_3d_.size(); ie++)
4     {
5         element_t * cur_ele = &(elements_3d_[ie]);
6         for(int iv = 0; iv < (cur_ele->nvert-1); iv++)
7         {
```

```

8         int midj = cur_ele->vertex_mids[jv];
9         for(int jv = iv+1; jv < (cur_ele->nvert); jv++)
10         {
11             int midj = cur_ele->vertex_mids[jv];
12             mid_connections_by_mid[midi].push_back(midj);
13             mid_connections_by_mid[midj].push_back(midi);
14         }
15     }
16 }

```

This leads to plenty of over-counting, so these lists are sorted and shrunk after all the elements are processed. At the same time, a map from vertex mesh ID to local linear index is generated. This map makes the update step flow smoothly.

```

1 // You probably double-counted a bunch. Make sure each list
2 // contains no copies.
3 int my_highest_mid = 0;
4 for(int iv = 0; iv < vertices_.size(); iv++)
5 {
6     int midj = vertices_[iv].mid;
7     mid2lindx_[midi] = iv;
8     if(midi > my_highest_mid) my_highest_mid = midi;
9     sort(mid_connections_by_mid[midi].begin(), mid_connections_by_mid[midi].end());
10    mid_connections_by_mid[midi].erase(unique(mid_connections_by_mid[midi].begin(), mid_connections_by_mid[midi].end()), mid_connections_by_mid[midi].end());
11 }

```

Once all the local connectivity information is determined, the processors need to figure out the connectivity of vertices between partitions. This is done in a loop over the global mesh IDs. For each global mesh ID, if a processor has that vertex locally, it attempts to attain ownership of the vertex. The lowest rank processor is granted ownership of the vertex. The owner vertex determines the global list of mesh IDs which are connected to this vertex. This list is useful during the update step, when the owner may need to process redundant messages about this vertex's neighbours.

```

1 // Determine ownership and families
2 for(int midi = 0; midi <= global_highest_mid; midi++)
3 {
4     // Do I have a vertex with this mid?
5     std::map<int,int>::iterator it;
6     it = mid2lindx_.find(midi);
7
8     bool vertex_exists_locally = (it != mid2lindx_.end());
9
10    std::vector<int> send_existence(nproc, vertex_exists_locally);
11    std::vector<int> recv_existence(nproc);
12    // Tell everyone else whether I have this mid locally.
13    // Find out who else has this mid locally.
14    MPI_Alltoall(
15        &(send_existence[0]),
16        1,
17        MPI_INT,
18        &(recv_existence[0]),
19        1,
20        MPI_INT,
21        MPI_COMM_WORLD
22    );
23
24    int vertex_owner = nproc;
25    // Pick the lowest rank with a local copy of this mid as then
26    // owner.
27    for(int iproc = 0; iproc < nproc; iproc++)
28    {
29        if(recv_existence[iproc])
30        {
31            vertex_owner = iproc;
32            break;
33        }
34    }
35
36    if(vertex_exists_locally)
37    {
38        int lindx = mid2lindx_[midi];
39        vertex_t * cur_v = &(vertices_[lindx]);
40        cur_v->owner = vertex_owner;
41        // Fill the family for this vertex
42        cur_v->family.resize(0);
43        for(int iproc = 0; iproc < nproc; iproc++)
44        {
45            if(recv_existence[iproc]) cur_v->family.push_back(iproc);
46        }
47    }
48    if(vertex_owner < nproc)
49    {
50        // If this mid was actually claimed by someone, then
51        // make sure the owner knows all of the global mids that
52        // are connected to this mid.
53        std::vector<std::vector<int>> send_mid_connections(nproc);
54        std::vector<std::vector<int>> recv_mid_connections(nproc);
55        if(vertex_exists_locally)
56        {
57            // Tell the owner about all the connections I am aware
58            // of.
59            send_mid_connections[vertex_owner] = mid_connections_by_mid[midi];
60        }
61        MPI_Alltoall_vecvecT(send_mid_connections, recv_mid_connections);
62        if(vertex_owner == rank)
63        {
64            for(int iproc = 0; iproc < nproc; iproc++)

```

```

65         {
66             for(int icon = 0; icon < recv_mid_connections[iproc].size(); icon++)
67             {
68                 // Add this connection to my list of global connections.
69                 vertices_[mid2lindx_[midi]].global_nbr_mids.push_back(recv_mid_connections[iproc][icon]);
70             }
71         }
72         // Delete any copies from the list of global connections.
73         sort(vertices_[mid2lindx_[midi]].global_nbr_mids.begin(), vertices_[mid2lindx_[midi]].global_nbr_mids.end());
74         vertices_[mid2lindx_[midi]].global_nbr_mids.erase(unique(vertices_[mid2lindx_[midi]].global_nbr_mids.begin(), vertices_[mid2lindx_[
75             midi]].global_nbr_mids.end()), vertices_[mid2lindx_[midi]].global_nbr_mids.end());
76         vertices_[mid2lindx_[midi]].nbr_was_counted.resize(vertices_[mid2lindx_[midi]].global_nbr_mids.size());
77     }
78 }

```

## 2.3 Initialization of the Mesh

In order to run a Game of Life simulation, the mesh needs to have some initial state. This is the responsibility of the function `Mesh::populateMeshVertices`. Basically, each processor loops over its vertices and assigns an initial state to each vertex according to some rule. If a vertex is shared among processors, then the owner decides its initial state and communicates that state to the other family members. Currently, my code assigns initial states in a deterministic way, depending on the vertices' mesh IDs. Communication among processors is not strictly necessary in this case, but if I wish to assign states randomly, then communication would become necessary.

## 2.4 Vertex State Update

The distributed update step is handled in the function `Mesh::updateVertexStates`. In this function, there are six loops which serve to efficiently communicate vertex states between processors, and calculate and broadcast new states to families. This function takes advantage of the non-blocking nature of `MPI.Send` to communicate vertex states quickly.

In the first loop, each processor looks at each of its vertices, trying to find vertices which it does not own. These vertices' owners will eventually be responsible for calculating their next state, so they need to know the current state of all of the vertices in their neighbourhoods. If a processor has a local vertex neighbouring someone else's vertex, it sends the owner the neighbour vertex's mesh ID, the host vertex's mesh ID, and the neighbour's state, wrapped up in a `helper_vertex_t` structure.

```

1 typedef struct helper_vertex_t
2 {
3     int host_mid;
4     int nbr_mid;
5     bool nbr_state;
6 }

```

Next, the processors collectively swap these helper vertices so that they have all they need to update their local vertices.

In the second loop, each processor tallies up the alive/dead counts for all of its local vertices which it owns. If any local vertices are owned by someone else, then they will be updated by someone else, so it is unnecessary to perform any work on them. When a vertex's neighbour's state is tallied, a flag is set in an accompanying array to indicate that the connection between the host and neighbour has already been considered.

In the third loop, the helper vertices are tabulated. This is where the map from mesh ID to local vertex index comes in handy. Each processor can look at its helper vertices' mesh IDs and quickly find out their corresponding local vertex. It is possible, at this point, that some of the helper vertices are supplying redundant information. The mesh IDs in each helper are checked against the `nbr_was_counted` array to prevent double-counting vertex states.

The fourth loop is where the vertex states actually get updated. The actual update calculation will be discussed later. A processor only updates the state of vertices which it owns. Once a vertex's state is updated, the processor uses `MPI.Send` to communicate the new state to the other members of the vertex's family. These messages are not immediately received – the corresponding `MPI.Recv` commands don't appear until the next loop. The fact the send command is non-blocking allows each processor to complete this loop without checking whether the message made it to its destination.

The fifth loop takes care of receiving all of the floating `MPI.Send` commands. Each processor loops through its vertices, looking for vertices which it does not own. If such a vertex is found, the processor grabs the

message from MPI and updates its local copy of that vertex with its new information. Finally, in the sixth loop, each processor loops through its vertices and moves the value from `next_state` into `current_state`. Additionally, the processor zeros out the counts in `alive_dead`, and clears all the `nbr_was_counted` flags to prevent contamination in the next update.

### 2.4.1 State Update Rules

In the 2D Game of Life, cells are updated as follows:

```

IF Cell is currently alive
    IF Cell has 2 or 3 live neighbours
        Cell stays alive
    ELSE
        Cell dies
ELSE Cell is currently dead
    IF Cell has 3 live neighbours
        Cell becomes alive
    ELSE
        Cell stays dead

```

These rules are meant to emulate the effect of community on organisms' health. Organisms can die of loneliness or overpopulation, and cells can become alive if the population density is correct. These rules could be directly applied to the vertex mesh, but that would fail to capture the intention of the rules. The rules focus on the population *density* in a cell's neighbourhood. The size of a cell's neighbourhood is highly variable on the vertex mesh. For example, consider the histogram shown in Fig. 2, which shows the degrees of all the vertices in a sample mesh. There is a wide spread of vertex degrees, thus the state update rules need to consider the *proportion* of neighbouring vertices which are alive or dead.

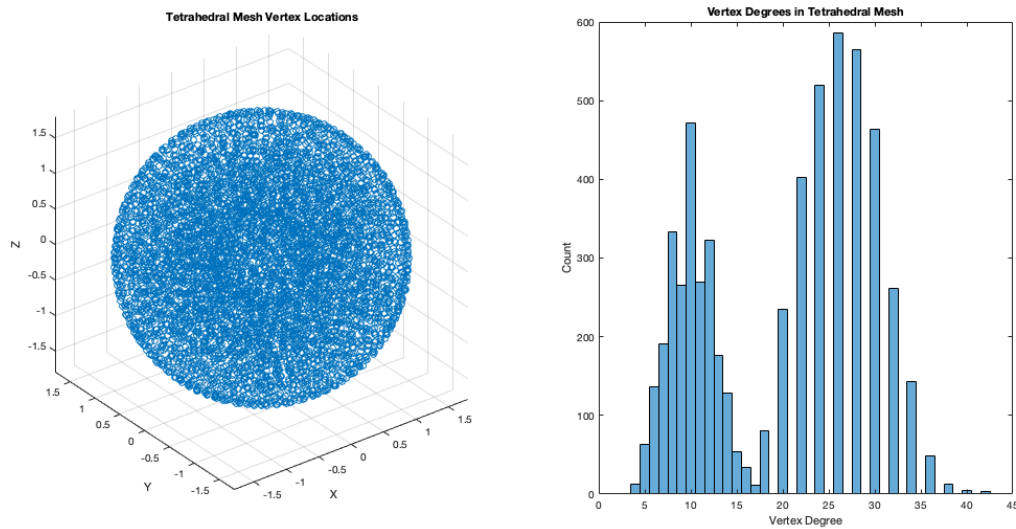


Figure 2: Vertex Degrees for a Fine Tetrahedral Mesh

My state update logic is found in `GOL_CalculateNextState`, shown below. These values seem to produce populations that don't immediately die out.

```

1 bool GOL_CalculateNextState(bool current_state, int n_alive, int n_dead)
2 {
3     double life_rate = (double)(n_alive + n_dead);
4     life_rate = 1/life_rate;
5     life_rate *= (double)(n_alive);
6     bool next_state = current_state;
7     if(current_state)
8     {
9         if(life_rate < 0.2999)
10        {
11            // Die of loneliness
12            next_state = false;
13        }
14        else if(life_rate < 0.5111)
15        {
16            // Keep living because you're in a good community.
17            next_state = true;
18        }
19        else
20        {
21            // Die from overpopulation
22            next_state = false;
23        }
24    }
25    else
26    {
27        if((0.2999 < life_rate) && (life_rate < 0.5111))
28        {
29            // Get born
30            next_state = true;
31        }
32        else
33        {
34            // Stay dead
35            next_state = false;
36        }
37    }
38    return(next_state);
39 }

```

## 2.5 Visualization

I decided to use Matlab for my visualization because I didn't want to figure out how to make 3D plots in openCV. My c++ code can append its mesh's state to a text file at each iteration. When the log file is created, each processor writes down a list of its vertices' positions. For each subsequent write, each processor just loops through its vertices and writes down a 0 or 1, to mark its vertices' states. I included a command-line parameter to turn off this file I/O, since it is an inherently slow, serial process. If logging is disabled, then only the vertices' positions and their final states are recorded.

I then wrote a Matlab script which parses the log file and displays the vertices' states with a 3D scatter plot, pausing between each state. An animation of a game of life simulation can be found in the included ./Mod2HalfAliveAnimateGOL.mov file. In this example, the vertices with positive x-position were initially alive, and the ones with negative x-position were initially dead. Red vertices are dead and blue vertices are alive.

## 3 Results and Analysis

### 3.1 Speedup Analysis

Processing speed was tested by running games of life on four different meshes of a sphere. There various meshes are summarized in Table. 1.

Table 1: Mesh Statistics

|                        | Nodes | Elements |
|------------------------|-------|----------|
| <b>Coarse Mesh</b>     | 62    | 270      |
| <b>Medium Mesh</b>     | 217   | 734      |
| <b>Fine Mesh</b>       | 1113  | 4745     |
| <b>Super Fine Mesh</b> | 5797  | 28874    |

Looking at the Tables 2, 4, and 3, it seems like all this work was for naught. For most of the meshes, the number of vertices processed per second decreases when more processors are added. The memory footprint does not seem to have any better results. For the meshes, parallelizing the problem generally leads to slower performance with meagre memory savings.

Table 2: Iterations Per Second

|                        | Number of Processors |      |      |      |      |      |
|------------------------|----------------------|------|------|------|------|------|
|                        | 1                    | 2    | 3    | 4    | 5    | 6    |
| <b>Coarse Mesh</b>     | 20900                | 8630 | 9060 | 6120 | 6020 | 5120 |
| <b>Medium Mesh</b>     | 6280                 | 3960 | 4210 | 3030 | 3310 | 3160 |
| <b>Fine Mesh</b>       | 1080                 | 940  | 987  | 847  | 1020 | 978  |
| <b>Super Fine Mesh</b> | 168                  | 198  | 216  | 200  | 247  | 247  |

Table 3: Vertices Updated Per Second [ $\times 10^6$ ]

|                        | Number of Processors |       |       |       |       |       |
|------------------------|----------------------|-------|-------|-------|-------|-------|
|                        | 1                    | 2     | 3     | 4     | 5     | 6     |
| <b>Coarse Mesh</b>     | 1.3                  | 0.535 | 0.562 | 0.379 | 0.373 | 0.317 |
| <b>Medium Mesh</b>     | 1.37                 | 0.856 | 0.914 | 0.658 | 0.718 | 0.686 |
| <b>Fine Mesh</b>       | 1.2                  | 1.05  | 1.01  | 1.14  | 1.14  | 1.09  |
| <b>Super Fine Mesh</b> | 0.974                | 1.15  | 1.25  | 1.16  | 1.43  | 1.43  |

The fine mesh, unlike the other, smaller meshes, does benefit from parallel computation with several processors. This suggests to me that the behaviour expressed in these tables is not the asymptotic behaviour of this algorithm. It is probably true that in order to see good speedup, it would be necessary to process a very, very large mesh file. I do not have the means to process such a file on my computer, but there bigger computers which would be capable of handling such a task. A bigger problem would see better speedup because the volume a mesh grows much faster than its surface area. During the update step, the processors need to communicate with each other to determine the states of vertices which are shared between processors. These shared vertices are only found on the edge of the mesh partitions on interface surfaces. As the problem size increase, the volume of a problem grows as a cubic function, while the interface surface only grows as a quadratic function. Therefore, for sufficiently large problems, the interface vertices would make up a vanishingly small portion of a processor's work. To illustrate this point, consider the impact of turning off the ORB partition. Without the ORB partition, the mesh's elements are distributed among the processors almost randomly. This leads to much more sharing of vertices, and much larger interface areas. Table 5 shows the number of iterations completed per second with and without ORB enabled. With 4 processors running, ORB leads to a 5x speedup.

## 4 Conclusion

For this report, a parallel program was developed which is capable of running a simulation in the style of Conway's Game of Life, on the vertices of a three-dimensional, unstructured mesh of arbitrary geometry. The geometrical differences between a standard grid and an unstructured mesh meant that it became necessary to determine complex connectivity information in order to iterate the Game of Life on a mesh. The notion of a single Game of Life update also had to be re-worked, in order to fit with this new problem. Furthermore, the act of parallelizing the problem introduced the problem of redundant neighbourhood calculations. In order to solve this problem, the parallel code had to not only tally up the states of a vertex's neighbours,

Table 4: Memory Per Processor in Megabytes

|                        | Number of Processors |      |      |      |     |      |
|------------------------|----------------------|------|------|------|-----|------|
|                        | 1                    | 2    | 3    | 4    | 5   | 6    |
| <b>Coarse Mesh</b>     | 2.2                  | 2.4  | 2.4  | 2.4  | 2.5 | 2.5  |
| <b>Medium Mesh</b>     | 2.4                  | 2.7  | 2.6  | 2.6  | 2.8 | 2.8  |
| <b>Fine Mesh</b>       | 4.0                  | 5.0  | 4.6  | 4.6  | 4.4 | 4.3  |
| <b>Super Fine Mesh</b> | 14.8                 | 15.1 | 13.7 | 11.1 | 9.8 | 10.6 |



Table 5: Impact of ORB on Iteration Rate

|                              | <b>Number of Processors</b> |      |     |     |      |     |
|------------------------------|-----------------------------|------|-----|-----|------|-----|
|                              | 1                           | 2    | 3   | 4   | 5    | 6   |
| <b>Fine Mesh with ORB</b>    | 1080                        | 940  | 987 | 847 | 1020 | 978 |
| <b>Fine Mesh without ORB</b> | 1080                        | 1040 | 223 | 170 | 173  | 170 |

but also ensure that every state is counted exactly once. This redundancy-checking ultimately adds a large amount of overhead to the parallel code, meaning that this Game of Life implementation is best suited to run on big computers and with huge meshes.

# A Code

## A.1 Main

```
1 #include <iostream>
2 #include <mpi.h>
3 #include <vector>
4 #include <stdlib.h>
5 #include <sstream>
6 #include "Mesh.h"
7
8
9
10
11 int main(int argc, char** argv)
12 {
13     int rank,nproc;
14     MPI_Init(&argc, &argv);
15     MPI_Comm_rank(MPI_COMM_WORLD, &rank);
16     MPI_Comm_size(MPI_COMM_WORLD, &nproc);
17     srand(MPI_Wtime() + rank);
18
19     std::stringstream mesh_name;
20     std::stringstream cell_filename;
21     cell_filename << "CellMatrix_P" << nproc << ".txt";
22     mesh_name << argv[1] << ".msh";
23
24     int n_iter = atoi(argv[2]);
25     double pop_percent = atof(argv[3]);
26     double pop_rate = (pop_percent)/100.0;
27     bool log_each_iteration = (atoi(argv[4])>0);
28     std::cout << "pop rate = " << pop_rate << std::endl;
29     Mesh BallMesh(mesh_name.str());
30
31     BallMesh.partitionMesh();
32     BallMesh.calculateVertexConnectivity();
33     BallMesh.populateMeshVertices(pop_rate);
34     BallMesh.writeCellMatrixFile(cell_filename.str(),false);
35     //BallMesh.outputStatistics();
36     BallMesh.updateVertexStates();
37     double tstart = MPI_Wtime();
38     double tnow;
39     double iter_per_s;
40     MPI_Barrier(MPI_COMM_WORLD);
41     int disp_counter = 0;
42     for(int iter = 0; iter < n_iter; iter++)
43     {
44         if(log_each_iteration)
45         {
46             BallMesh.writeCellMatrixFile(cell_filename.str(),true);
47         }
48         BallMesh.updateVertexStates();
49         if((disp_counter++ > 200))
50         {
51             if(rank == 0)
52             {
53                 disp_counter = 0;
54                 tnow = MPI_Wtime();
55                 iter_per_s = iter/(tnow-tstart);
56                 std::cout << "\r" << iter << " / " << n_iter << ", " << iter_per_s << std::flush;
57             }
58         }
59     }
60     if(rank == 0) std::cout << std::endl;
61     BallMesh.writeCellMatrixFile(cell_filename.str(),true);
62     MPI_Finalize();
63
64     return (0);
65 }
```

## A.2 Mesh

```
1 #include <iostream>
2 #include <vector>
3 #include <fstream>
4 #include <math.h>
5 #include <cassert>
6 #include <mpi.h>
7 #include <sstream>
8 #include <map>
9 #include <iostream>
10 #include <iomanip>
11 #include "Mesh.h"
12 #include "MeshUtilities.h"
13
14 using namespace std;
15
16 //-----
17 // Constructor
18 //-----
19 Mesh::Mesh(string filename)
20 {
21     vertices_.resize(0);
22     elements_3d_.resize(0);
23     MPI_Comm_size(MPI_COMM_WORLD,&nproc);
24     MPI_Comm_rank(MPI_COMM_WORLD,&rank_);
25     readMesh(filename);
26     getElementVertices(); //complete the vertices we have for local elements
27     createElementCentroidsList(); //create the list of centroids as private member
28 }
29
30 //-----
```

```

31 // Destructor - free dynamically allocated
32 // memory here
33 //-----
34 Mesh::~Mesh()
35 {
36 }
37 }
38
39 //-----
40 // Get a pointer to a vertex from the
41 // mesh id (mid). Returns NULL if not
42 // found.
43 //-----
44 const vertex_t* Mesh::getVertexFromMID(int vertex_mid) const
45 {
46     vertex_t search_vertex;
47     search_vertex.mid = vertex_mid;
48     void* result = bsearch(&search_vertex, &vertices[0], vertices.size(), sizeof(vertex_t), searchVertexByMIDPredicate);
49     if (result != NULL) // found vertex
50     {
51         const vertex_t* found_vertex = (const vertex_t*)result;
52         return found_vertex;
53     }
54     else
55     {
56         return NULL;
57     }
58 }
59
60 //-----
61 // Read a Gmsh formatted (version 2+)
62 // mesh. Creates list of vertices and
63 // elements. Not guaranteed to have
64 // vertices for local elements.
65 //-----
66 void Mesh::readMesh(string filename)
67 {
68     ifstream in_from_file(filename.c_str(), std::ios::in);
69
70     if (!in_from_file.is_open())
71     {
72         if (rank_ == 0) std::cerr << "Mesh File " << filename << " Could Not Be Opened!" << std::endl;
73         MPI_Finalize();
74         exit(1);
75     }
76
77     std::string parser = "";
78     in_from_file >> parser;
79
80     if (parser != "$MeshFormat")
81     {
82         if (rank_ == 0) std::cerr << "Invalid Mesh Format/File" << std::endl;
83         MPI_Finalize();
84         exit(1);
85     }
86
87     double dummy;
88     in_from_file >> dummy >> dummy >> dummy;
89     in_from_file >> parser; //skip $EndMeshFormat and $Nodes
90
91     //Vertex Read
92     int n_vertices_in_file;
93     in_from_file >> n_vertices_in_file;
94     int local_vert_start;
95     int local_vert_stop;
96     int local_vert_count;
97     parallelRange(0, n_vertices_in_file - 1, rank_, nproc_, local_vert_start, local_vert_stop, local_vert_count);
98
99     vertices_.resize(0);
100     vertex_t vertex;
101
102
103
104     for (int ivert = 0; ivert < n_vertices_in_file; ivert++)
105     {
106         if (ivert >= local_vert_start && ivert <= local_vert_stop)
107         {
108             in_from_file >> vertex.mid >> vertex.r[0] >> vertex.r[1] >> vertex.r[2];
109             vertices_.push_back(vertex);
110         }
111         else //skip over the line
112         {
113             int dummy;
114             in_from_file >> dummy;
115             in_from_file.ignore(1000, '\n');
116         }
117     }
118
119     //3D Tetrahedral Element Read
120
121     elements_3d_.resize(0);
122
123     in_from_file >> parser >> parser; //skip $EndNodes and $Elements
124
125     if (parser != "$Elements")
126     {
127         std::cerr << "Something has gone very wrong" << std::endl;
128         assert(0==1);
129     }
130
131     int n_elements_in_file = 0;
132     in_from_file >> n_elements_in_file;
133
134     int local_ele_start;
135     int local_ele_stop;
136     int local_ele_count;
137     parallelRange(0, n_elements_in_file - 1, rank_, nproc_, local_ele_start, local_ele_stop, local_ele_count);

```

```

138
139 int element_num_tags;
140 element_t element;
141
142 int n_global_3d_elements = 0;
143
144 for (int i_ele = 0; i_ele < n_elements_in_file; i_ele++)
145 {
146     int ele_in_range = (i_ele >= local_ele_start && i_ele <= local_ele_stop);
147
148     in_from_file >> element.mid >> element.type >> element_num_tags >> dummy >> dummy;
149     for (int itag = 0; itag < element_num_tags - 2; itag++)
150     {
151         in_from_file >> dummy;
152     }
153
154     //we are going to skip over anything that isn't a tetrahedral element so we just peel off the vertex mids
155     if (element.type == FV_MESH_GMESH_ELEMENT_POINT)
156     {
157         in_from_file >> dummy;
158     }
159     else if (element.type == FV_MESH_GMESH_ELEMENT_FIRST_ORDER_LINE)
160     {
161         in_from_file >> dummy >> dummy;
162     }
163     else if (element.type == FV_MESH_GMESH_ELEMENT_FIRST_ORDER_TRIANGLE)
164     {
165         in_from_file >> dummy >> dummy >> dummy;
166     }
167     else if (element.type == FV_MESH_GMESH_ELEMENT_FIRST_ORDER_QUADRANGLE)
168     {
169         in_from_file >> dummy >> dummy >> dummy >> dummy;
170     }
171     else if (element.type == FV_MESH_GMESH_ELEMENT_FIRST_ORDER_TETRAHEDRAL)
172     {
173         in_from_file >> element.vertex_mids[0];
174         in_from_file >> element.vertex_mids[1];
175         in_from_file >> element.vertex_mids[2];
176         in_from_file >> element.vertex_mids[3];
177         element.nvert = 4;
178         if (ele_in_range) elements_3d_.push_back(element);
179     }
180     else if (element.type == FV_MESH_GMESH_ELEMENT_FIRST_ORDER_HEXAHEDRAL)
181     {
182         in_from_file >> dummy >> dummy >> dummy >> dummy >> dummy >> dummy >> dummy;
183     }
184     else
185     {
186         std::cerr << "Hit an unsupported element type" << std::endl;
187         assert(0==1);
188     }
189 } //for each element
190 in_from_file.close();
191 }
192
193
194 //-----
195 // Construct the list of element centroids.
196 //-----
197
198 void Mesh::createElementCentroidsList()
199 {
200     element_3d_centroids_.resize(elements_3d_.size());
201     const vertex_t* vertex_pointer;
202
203     for (unsigned int iele = 0; iele < elements_3d_.size(); iele++)
204     {
205         element_3d_centroids_[iele].r[0] = 0.0;
206         element_3d_centroids_[iele].r[1] = 0.0;
207         element_3d_centroids_[iele].r[2] = 0.0;
208
209         //The centroid of a simplex is just the average of the vertex coordinates
210         for (unsigned int ivert = 0; ivert < elements_3d_[iele].nvert; ivert++)
211         {
212             vertex_pointer = getVertexFromMID(elements_3d_[iele].vertex_mids[ivert]);
213             element_3d_centroids_[iele].r[0] += vertex_pointer->r[0];
214             element_3d_centroids_[iele].r[1] += vertex_pointer->r[1];
215             element_3d_centroids_[iele].r[2] += vertex_pointer->r[2];
216         }
217
218         element_3d_centroids_[iele].r[0] /= (double)elements_3d_[iele].nvert;
219         element_3d_centroids_[iele].r[1] /= (double)elements_3d_[iele].nvert;
220         element_3d_centroids_[iele].r[2] /= (double)elements_3d_[iele].nvert;
221     }
222
223     //Sanity check - the average of the centroids should be the "center" of the mesh.
224
225     double3_t centroid_sum;
226     centroid_sum.r[0] = 0.0;
227     centroid_sum.r[1] = 0.0;
228     centroid_sum.r[2] = 0.0;
229
230     for (unsigned int iele = 0; iele < element_3d_centroids_.size(); iele++)
231     {
232         centroid_sum.r[0] += element_3d_centroids_[iele].r[0];
233         centroid_sum.r[1] += element_3d_centroids_[iele].r[1];
234         centroid_sum.r[2] += element_3d_centroids_[iele].r[2];
235     }
236
237     double3_t total_centroid_sum;
238     MPI_Reduce(&centroid_sum.r[0], &total_centroid_sum.r[0], 3, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
239
240     int centroid_count = element_3d_centroids_.size();
241     int total_centroid_count;
242
243     MPI_Reduce(&centroid_count, &total_centroid_count, 1, MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD);
244

```

```

245
246     if (rank_ == 0)
247     {
248         double3_t average_centroid = total_centroid_sum;
249         average_centroid.r[0] /= (double)total_centroid_count;
250         average_centroid.r[1] /= (double)total_centroid_count;
251         average_centroid.r[2] /= (double)total_centroid_count;
252
253         //std::cout << "The average centroid across all processors is (" << average_centroid.r[0] << ", " << average_centroid.r[1] << ", " <<
         average_centroid.r[2] << ")" << std::endl;
254     }
255 }
256
257 //-----
258 // Obtain the list of unique vertices that completes our elements on
259 // every processor.
260 //-----
261 void Mesh::getElementVertices()
262 {
263     if (nproc_ == 1) return;
264
265     //determine the vertices that we need to complete our local elements
266     std::vector<int> vertex_mid_requests(0);
267     for (unsigned int iele = 0; iele < elements_3d_.size(); iele++)
268     {
269         for (unsigned int ivert = 0; ivert < elements_3d_[iele].nvert; ivert++)
270         {
271             vertex_mid_requests.push_back(elements_3d_[iele].vertex_mids[ivert]);
272         }
273     }
274
275     //make the list unique
276     sort(vertex_mid_requests.begin(), vertex_mid_requests.end());
277     vertex_mid_requests.erase(unique(vertex_mid_requests.begin(), vertex_mid_requests.end()), vertex_mid_requests.end());
278
279     //now we know all the vertices we need to actually complete our elements
280
281     //should already be sorted based on sequential read from mesh - but just to be safe
282     sort(vertices_.begin(), vertices_.end(), sortVertexByMIDPredicate);
283
284
285     //having collected the vertex set, we can now obtain the vertices we require
286     //we send the vertices we need to every process (we could do better here)
287
288     std::vector<std::vector<int>> > outgoing_vertex_requests(0);
289     for (unsigned int iproc = 0; iproc < nproc_; iproc++) outgoing_vertex_requests.push_back(vertex_mid_requests);
290
291     std::vector<std::vector<int>> > incoming_vertex_requests(0);
292     MPI_Alltoall_vecvecT(outgoing_vertex_requests, incoming_vertex_requests);
293
294     std::vector<std::vector<vertex_t>> > outgoing_vertices(nproc_);
295     vertex_t search_vertex;
296     for (unsigned int iproc = 0; iproc < nproc_; iproc++)
297     {
298         outgoing_vertices[iproc].resize(0);
299         for (unsigned int ivert = 0; ivert < incoming_vertex_requests[iproc].size(); ivert++)
300         {
301             int vertex_mid = incoming_vertex_requests[iproc][ivert];
302             search_vertex.mid = vertex_mid;
303             void* result = bsearch(&search_vertex, &vertices_[0], vertices_.size(), sizeof(vertex_t), searchVertexByMIDPredicate);
304             if (result != NULL) // found vertex
305             {
306                 const vertex_t* found_vertex = (const vertex_t*)result;
307                 search_vertex.r[0] = found_vertex->r[0];
308                 search_vertex.r[1] = found_vertex->r[1];
309                 search_vertex.r[2] = found_vertex->r[2];
310                 outgoing_vertices[iproc].push_back(search_vertex);
311             }
312         }
313     }
314
315     std::vector<std::vector<vertex_t>> > incoming_vertices;
316     MPI_Alltoall_vecvecT(outgoing_vertices, incoming_vertices);
317
318     vertices_.resize(0);
319     std::map<int,int> vertex_map;
320     for (unsigned int iproc = 0; iproc < nproc_; iproc++)
321     {
322         for (unsigned int ivert = 0; ivert < incoming_vertices[iproc].size(); ivert++)
323         {
324             if (vertex_map.find(incoming_vertices[iproc][ivert].mid) == vertex_map.end())
325             {
326                 vertices_.push_back(incoming_vertices[iproc][ivert]);
327                 vertex_map[incoming_vertices[iproc][ivert].mid] = 1;
328             }
329         }
330     }
331
332     sort(vertices_.begin(), vertices_.end(), sortVertexByMIDPredicate);
333
334     //now we should be able to find the vertices for any element we have locally.
335     //sanity check.
336     for (unsigned int iele = 0; iele < elements_3d_.size(); iele++)
337     {
338         for (unsigned int ivert = 0; ivert < elements_3d_[iele].nvert; ivert++)
339         {
340             const vertex_t* vertex = getVertexFromMID(elements_3d_[iele].vertex_mids[ivert]);
341             assert(vertex != NULL);
342         }
343     }
344 }
345
346 // This routine will run ORB on all of the mesh's element centroids
347 // to determine a block partition of the elements. Then, this function
348 // will swap global element.mids so that each processor owns one of
349 // the ORB partitions. Then, each processor will call a routine to

```

```

351 // get all the vertices associated with that list of elements.
352 void Mesh::partitionMesh()
353 {
354     if(nproc_ == 1) return; // Partition is already complete.
355
356     // Perform ORB on element centroids
357     std::vector<std::vector<int>> > local_idcs_per_dom(nproc_);
358     ORB(
359         nproc_,
360         element_3d_centroids_,
361         local_idcs_per_dom
362     );
363     // Now you know which of your elements to send to the other procs,
364     // by your local index. It would be more helpful to just give the
365     // whole element to the other processor. Do that.
366     std::vector<std::vector<element_t>> > global_elements_per_dom(nproc_);
367     for(int idom = 0; idom < local_idcs_per_dom.size(); idom++)
368     {
369         global_elements_per_dom[idom].resize(local_idcs_per_dom[idom].size());
370         for(int iloc = 0; iloc < local_idcs_per_dom[idom].size(); iloc++)
371         {
372             global_elements_per_dom[idom][iloc] = elements_3d_[local_idcs_per_dom[idom][iloc]];
373         }
374     }
375     // Do the big group swap of global elements.
376     std::vector<std::vector<element_t>> > recv_elements_per_dom(nproc_);
377     MPI_Alltoall_vecvecT(global_elements_per_dom, recv_elements_per_dom);
378     // Rewrite my elements_3d_ with what I just received.
379     int new_ele_3d_count = 0;
380     for(int iproc = 0; iproc < nproc_; iproc++) new_ele_3d_count += recv_elements_per_dom[iproc].size();
381     elements_3d_.resize(new_ele_3d_count);
382     int ele_3d_idx = 0;
383     for(int iproc = 0; iproc < nproc_; iproc++)
384     {
385         for(int ipt = 0; ipt < recv_elements_per_dom[iproc].size(); ipt++)
386         {
387             elements_3d_[ele_3d_idx++] = recv_elements_per_dom[iproc][ipt];
388         }
389     }
390     // Get the vertices and centroids associated with my elements.
391     getElementVertices();
392     createElementCentroidsList();
393 }
394
395
396
397 //-----
398 // Write unstructured mesh to Paraview XML format. This will create P+1 files
399 // on P processors. The .vtu files are pieces of the mesh. The .pvtu file is a
400 // single wrapper file that can be loaded in paraview such that every .vtu file with
401 // the corresponding names will be opened simultaneously.
402 //
403 // Inputs:
404 //
405 // The filename should be a complete path with NO extension (.vtu and .pvtu
406 // will be added.
407 //
408 // Value label is a string that will be written to the vtu file labeling the values
409 // that you are writing for each element (e.g. "rank").
410 //
411 // Values is a vector with length elements_3d_.size() corresponding to a single
412 // scalar value to be associated with each element in the mesh.
413 //-----
414 void Mesh::writeMesh(string filename, std::string value_label, const vector<double>& values) const
415 {
416     ofstream vtu_out, pvtu_out;
417
418     std::ostringstream converter;
419     converter << filename << "_P" << nproc_ << "_R" << rank_;
420     std::string vtu_filename = converter.str() + ".vtu";
421
422     //-----
423     // Open the VTU file (All ranks)
424     //-----
425
426     vtu_out.open(vtu_filename.c_str());
427     if (!vtu_out.is_open())
428     {
429         std::cerr << "Could not open vtu file" << std::endl;
430         assert(0==1);
431     }
432
433     vtu_out << "<?xml version='1.0'?'>" << std::endl;
434     vtu_out << "<VTKFile type='UnstructuredGrid' version='0.1' byte_order='LittleEndian'>" << std::endl;
435
436     //-----
437     // Open the PVTU file (Rank 0)
438     //-----
439
440     if (rank_==0)
441     {
442         std::ostringstream pconverter;
443         pconverter << filename << "_P" << nproc_;
444         std::string pvtu_filename = pconverter.str() + ".pvtu";
445         pvtu_out.open(pvtu_filename.c_str());
446         if (!pvtu_out.is_open())
447         {
448             std::cerr << "Could not open pvtu file" << std::endl;
449             assert(0==1);
450         }
451
452         pvtu_out << "<?xml version='1.0'?'>" << std::endl;
453         pvtu_out << "<VTKFile type='PUUnstructuredGrid' version='0.1' byte_order='LittleEndian'>" << std::endl;
454     }
455
456     //-----
457     // Write the 3D Mesh Elements to File

```

```

458 //-----
459
460 int n_elements = elements_3d_.size();
461
462 //-----
463 // VTU Mesh
464 //-----
465
466 //Preamble
467 vtu_out << "<UnstructuredGrid>" << std::endl;
468 vtu_out << "<Piece NumberOfPoints=\"" << vertices_.size() << "\" NumberOfCells=\"" << n_elements << "\">" << std::endl;
469
470 //Vertices
471 vtu_out << "<Points>" << std::endl;
472 vtu_out << "<DataArray type=\"Float32\" NumberOfComponents=\"3\" format=\"ascii\">" << std::endl;
473 for (unsigned int ivert = 0; ivert < (int)vertices_.size(); ivert++)
474 {
475     vtu_out << vertices_[ivert].r[0] << " " << vertices_[ivert].r[1] << " " << vertices_[ivert].r[2] << " ";
476 }
477 vtu_out << std::endl;
478 vtu_out << "</DataArray>" << std::endl;
479 vtu_out << "</Points>" << std::endl;
480
481 vtu_out << "<Cells>" << std::endl;
482
483 //Element Connectivity
484 vtu_out << "<DataArray type=\"Int32\" Name=\"connectivity\">" << std::endl;
485 for (unsigned int iele = 0; iele < (int)elements_3d_.size(); iele++)
486 {
487     for (unsigned int ivert = 0; ivert < elements_3d_[iele].nvert; ivert++)
488     {
489         const vertex_t* vertex = getVertexFromMID(elements_3d_[iele].vertex_mids[ivert]);
490         assert(vertex != NULL);
491         int vertex_lid = (vertex - &vertices_[0]);
492         assert(vertices_[vertex_lid].mid == elements_3d_[iele].vertex_mids[ivert]);
493         assert(vertex_lid >= 0 && vertex_lid < vertices_.size());
494         vtu_out << vertex_lid << " ";
495     }
496 }
497 vtu_out << std::endl;
498 vtu_out << "</DataArray>" << std::endl;
499
500 //Offsets
501 vtu_out << "<DataArray type=\"Int32\" Name=\"offsets\">" << std::endl;
502 int vert_sum = 0;
503 for (unsigned int iele = 0; iele < elements_3d_.size(); iele++)
504 {
505     vert_sum += elements_3d_[iele].nvert;
506     vtu_out << vert_sum << " ";
507 }
508 vtu_out << std::endl;
509 vtu_out << "</DataArray>" << std::endl;
510
511 //Types
512 vtu_out << "<DataArray type=\"UInt8\" Name=\"types\">" << std::endl;
513 for (unsigned int iele = 0; iele < (int)elements_3d_.size(); iele++)
514 {
515     vtu_out << "10 ";
516 }
517 vtu_out << std::endl;
518
519 vtu_out << "</DataArray>" << std::endl;
520 vtu_out << "</Cells>" << std::endl;
521
522 //-----
523 // PVTU Mesh
524 //-----
525
526 if (rank_ == 0)
527 {
528     pvtu_out << "<PUnstructuredGrid GhostLevel=\"0\">" << std::endl;
529
530     pvtu_out << "<PPoints>" << std::endl;
531     pvtu_out << "<PDataArray type=\"Float32\" NumberOfComponents=\"3\" format=\"ascii\">" << std::endl;
532
533     pvtu_out << "</PDataArray>" << std::endl;
534     pvtu_out << "</PPoints>" << std::endl;
535
536     pvtu_out << "<PCells>" << std::endl;
537
538     //Connectivity
539     pvtu_out << "<PDataArray type=\"Int32\" Name=\"connectivity\">" << std::endl;
540     pvtu_out << "</PDataArray>" << std::endl;
541
542     //Offsets
543     pvtu_out << "<PDataArray type=\"Int32\" Name=\"offsets\">" << std::endl;
544     pvtu_out << "</PDataArray>" << std::endl;
545
546     //Types
547     pvtu_out << "<PDataArray type=\"UInt8\" Name=\"types\">" << std::endl;
548     pvtu_out << "</PDataArray>" << std::endl;
549     pvtu_out << "</PCells>" << std::endl;
550 }
551
552 //-----
553 // VTU Cell Data Open
554 //-----
555
556 vtu_out << "<CellData>" << std::endl;
557
558 vtu_out << "<DataArray type=\"Float32\" format=\"ascii\" Name=\"" << value_label << "\">" << std::endl;
559 assert(values.size() == elements_3d_.size());
560 for (int iele = 0; iele < (int)elements_3d_.size(); iele++)
561 {
562     vtu_out << values[iele] << " ";
563 }
564

```

```

565 vtu_out << "</DataArray>" << std::endl;
566 vtu_out << "</CellData>" << std::endl;
567
568 //-----
569 // PVTU Cell Data Open
570 //-----
571
572 if (rank_ == 0)
573 {
574     pvtu_out << "<PCellData>" << std::endl;
575     pvtu_out << "<PDataArray type=\"Float32\" format=\"ascii\" Name=\"" << value_label << "\">" << std::endl;
576     pvtu_out << "</PDataArray>" << std::endl;
577     pvtu_out << "</PCellData>" << std::endl;
578 }
579
580 //-----
581 // VTU Close
582 //-----
583
584 vtu_out << "</Piece>" << std::endl;
585 vtu_out << "</UnstructuredGrid>" << std::endl;
586 vtu_out << "</VTKFile>" << std::endl;
587 vtu_out.close();
588
589 //-----
590 // PVTU Close
591 //-----
592
593 if (rank_ == 0)
594 {
595     for (int iproc = 0; iproc < nproc_; iproc++)
596     {
597         std::ostringstream vtu_converter;
598         //vtu_converter << vtkfilename << "_Run" << iRun << "_N" << num_proc_ << "_P" << iproc << ".vtu";
599         //We always assume the pvtu file exists in the same directory as the other files so here vtkfilename must only be the relative name
600         vtu_converter << filename << "_P" << nproc_ << "_R" << iproc << ".vtu";
601         pvtu_out << "<Piece Source=\"" << vtu_converter.str() << "\">" << std::endl;
602     }
603
604     pvtu_out << "</PUnstructuredGrid>" << std::endl;
605     pvtu_out << "</VTKFile>" << std::endl;
606     pvtu_out.close();
607 }
608 }
609 }
610
611 //-----
612 // Output some statistics including
613 // number of elements/vertices on each
614 // processor and global number of
615 // elements/vertices. Nicely formatted.
616 //-----
617 void Mesh::outputStatistics() const
618 {
619     MPI_Barrier(MPI_COMM_WORLD);
620     int local_n_eles = elements3d_.size();
621     int global_n_eles = 0;
622     int local_n_vert = vertices_.size();
623     int global_n_vert = 0;
624     // Figure out number of global elements and vertices
625     MPI_Reduce(
626         &local_n_eles,
627         &global_n_eles,
628         1,
629         MPI_INT,
630         MPI_SUM,
631         0,
632         MPI_COMM_WORLD
633     );
634
635     MPI_Reduce(
636         &local_n_vert,
637         &global_n_vert,
638         1,
639         MPI_INT,
640         MPI_SUM,
641         0,
642         MPI_COMM_WORLD
643     );
644
645     if(rank_ == 0)
646     {
647         std::cout << "\nGlobal Mesh Statistics:" << std::endl;
648         std::cout << "\tGlobal Element Count: " << global_n_eles << std::endl;
649         std::cout << "\tGlobal Vertex Count: " << global_n_vert << "\n" << std::endl;
650         std::cout << "Element/Vertex Counts By Processor:\n" << std::endl;
651         std::cout << "\tProc\t";
652         std::cout << "\tEles\t";
653         std::cout << "\tVrts\t";
654         std::cout << "\tX Min\t";
655         std::cout << "\tX Max\t";
656         std::cout << "\tY Min\t";
657         std::cout << "\tY Max\t";
658         std::cout << "\tZ Min\t";
659         std::cout << "\tZ Max\t";
660         std::cout << " " << std::endl;
661         std::cout << "=====" << std::endl;
662         std::cout << "=====" << std::endl;
663         std::cout << "=====" << std::endl;
664         std::cout << "=====" << std::endl;
665         std::cout << "=====" << std::endl;
666         std::cout << "=====" << std::endl;
667         std::cout << "=====" << std::endl;
668         std::cout << "=====" << std::endl;
669         std::cout << "=====" << std::endl;
670         std::cout << "=====" << std::endl;
671     }

```



```

672
673 // Calculate your local extent
674 std::vector<std::vector<double> > extents(3, std::vector<double>(2, 1));
675 extents[0][0] = DBL_MAX;
676 extents[1][0] = DBL_MAX;
677 extents[2][0] = DBL_MAX;
678 extents[0][1] = DBL_MIN;
679 extents[1][1] = DBL_MIN;
680 extents[2][1] = DBL_MIN;
681 for(int ivert = 0; ivert < vertices_.size(); ivert++)
682 {
683     for (int idim = 0; idim < 3; idim++)
684     {
685         if(vertices_[ivert].r[idim] < extents[idim][0]) extents[idim][0] = vertices_[ivert].r[idim];
686         if(vertices_[ivert].r[idim] > extents[idim][1]) extents[idim][1] = vertices_[ivert].r[idim];
687     }
688 }
689
690 for(int irank = 0; irank < nproc_; irank++)
691 {
692     MPI_Barrier(MPI_COMM_WORLD);
693     if(irank == rank_)
694     {
695         std::cout << "\t" << rank_ << "\t";
696         std::cout << "\t" << elements_3d_.size() << "\t";
697         std::cout << "\t" << vertices_.size() << "\t";
698         std::cout << "\t" << std::setw(15) << extents[0][0];
699         std::cout << "\t" << std::setw(15) << extents[0][1];
700         std::cout << "\t" << std::setw(15) << extents[1][0];
701         std::cout << "\t" << std::setw(15) << extents[1][1];
702         std::cout << "\t" << std::setw(15) << extents[2][0];
703         std::cout << "\t" << std::setw(15) << extents[2][1];
704         std::cout << "\t" << std::endl;
705         std::cout << "-----"
706         std::cout << "-----"
707         std::cout << "-----"
708         std::cout << "-----"
709         std::cout << "-----"
710         std::cout << "-----"
711         std::cout << "-----"
712         std::cout << "-----"
713         std::cout << "-----"
714         std::cout << "\t" << std::endl;
715     }
716 }
717 }
718
719 void Mesh::calculateVertexConnectivity()
720 {
721     // Run through all of my elements and see which vertex mids are
722     // connected to each other. This makes an mid -> mid list
723
724     int rank, nproc;
725     MPI_Status status;
726     MPI_Comm_rank(MPI_COMM_WORLD, &rank);
727     MPI_Comm_size(MPI_COMM_WORLD, &nproc);
728     std::stringstream msg;
729
730     for(int iv = 0; iv < vertices_.size(); iv++)
731     {
732         vertices_[iv].neighbours.resize(0);
733     }
734
735     std::map<int, std::vector<int> > mid_connections_by_mid;
736
737     for(int ie = 0; ie < elements_3d_.size(); ie++)
738     {
739         element_t * cur_ele = &(elements_3d_[ie]);
740         for(int iv = 0; iv < (cur_ele->nvert-1); iv++)
741         {
742             int midi = cur_ele->vertex_mids[iv];
743             for(int jv = iv+1; jv < (cur_ele->nvert); jv++)
744             {
745                 int midj = cur_ele->vertex_mids[jv];
746                 mid_connections_by_mid[midi].push_back(midj);
747                 mid_connections_by_mid[midj].push_back(midi);
748             }
749         }
750     }
751
752     // You probably double-counted a bunch. Make sure each list
753     // contains no copies.
754     int my_highest_mid = 0;
755     for(int iv = 0; iv < vertices_.size(); iv++)
756     {
757         int midi = vertices_[iv].mid;
758         mid2lindx_[midi] = iv;
759         if(midi > my_highest_mid) my_highest_mid = midi;
760         sort(mid_connections_by_mid[midi].begin(), mid_connections_by_mid[midi].end());
761         mid_connections_by_mid[midi].erase(unique(mid_connections_by_mid[midi].begin(), mid_connections_by_mid[midi].end()), mid_connections_by_mid[midi].end());
762     }
763
764     int global_highest_mid = my_highest_mid;
765
766     MPI_Allreduce(
767         &my_highest_mid,
768         &global_highest_mid,
769         1,
770         MPI_INT,
771         MPI_MAX,
772         MPI_COMM_WORLD
773     );
774
775     // Determine ownership and families
776     for(int midi = 0; midi <= global_highest_mid; midi++)
777     {

```

```

778 // Do I have a vertex with this mid?
779 std::map<int,int>::iterator it;
780 it = mid2lindx_.find(midi);
781
782 bool vertex_exists_locally = (it != mid2lindx_.end());
783
784 std::vector<int> send_existence(nproc, vertex_exists_locally);
785 std::vector<int> rcv_existence(nproc);
786 // Tell everyone else whether I have this mid locally.
787 // Find out who else has this mid locally.
788 MPI_Alltoall(
789     &(send_existence[0]),
790     1,
791     MPI_INT,
792     &(rcv_existence[0]),
793     1,
794     MPI_INT,
795     MPI_COMM_WORLD
796 );
797
798 int vertex_owner = nproc;
799 // Pick the lowest rank with a local copy of this mid as then
800 // owner.
801 for(int iproc = 0; iproc < nproc; iproc++)
802 {
803     if(rcv_existence[iproc])
804     {
805         vertex_owner = iproc;
806         break;
807     }
808 }
809
810 if(vertex_exists_locally)
811 {
812     int lindx = mid2lindx_[midi];
813     vertex_t * cur_v = &(vertices_[lindx]);
814     cur_v->owner = vertex_owner;
815     // Fill the family for this vertex
816     cur_v->family.resize(0);
817     for(int iproc = 0; iproc < nproc; iproc++)
818     {
819         if(rcv_existence[iproc]) cur_v->family.push_back(iproc);
820     }
821 }
822 if(vertex_owner < nproc)
823 {
824     // If this mid was actually claimed by someone, then
825     // make sure the owner knows all of the global mids that
826     // are connected to this mid.
827     std::vector<std::vector<int> > send_mid_connections(nproc);
828     std::vector<std::vector<int> > rcv_mid_connections(nproc);
829     if(vertex_exists_locally)
830     {
831         // Tell the owner about all the connections I am aware
832         // of.
833         send_mid_connections[vertex_owner] = mid_connections_by_mid[midi];
834     }
835     MPI_Alltoall_vecvecT(send_mid_connections,rcv_mid_connections);
836     if(vertex_owner == rank)
837     {
838         for(int iproc = 0; iproc < nproc; iproc++)
839         {
840             for(int icon = 0; icon < rcv_mid_connections[iproc].size(); icon++)
841             {
842                 // Add this connection to my list of global connections.
843                 vertices_[mid2lindx_[midi]].global_nbr_mids.push_back(rcv_mid_connections[iproc][icon]);
844             }
845             // Delete any copies from the list of global connections.
846             sort(vertices_[mid2lindx_[midi]].global_nbr_mids.begin(), vertices_[mid2lindx_[midi]].global_nbr_mids.end());
847             vertices_[mid2lindx_[midi]].global_nbr_mids.erase(unique(vertices_[mid2lindx_[midi]].global_nbr_mids.begin(), vertices_[mid2lindx_[
848 midi]].global_nbr_mids.end()), vertices_[mid2lindx_[midi]].global_nbr_mids.end());
849             vertices_[mid2lindx_[midi]].nbr_was_counted.resize(vertices_[mid2lindx_[midi]].global_nbr_mids.size());
850         }
851     }
852 }
853 // Fill neighbour pointers
854 for(int iv = 0; iv < vertices_.size(); iv++)
855 {
856     vertex_t * cur_v = &(vertices_[iv]);
857     int midi = cur_v->mid;
858     cur_v->neighbours.resize(0);
859     for(int jj = 0; jj < mid_connections_by_mid[midi].size(); jj++)
860     {
861         int midj = mid_connections_by_mid[midi][jj];
862         vertex_t * nbr_v = &(vertices_[mid2lindx_[midj]]);
863         cur_v->neighbours.push_back(nbr_v);
864     }
865 }
866
867 }
868
869
870
871
872 void Mesh::populateMeshVertices(double alive_probability)
873 {
874     int rank,nproc;
875     MPI_Status status;
876     MPI_Comm_rank(MPI_COMM_WORLD,&rank);
877     MPI_Comm_size(MPI_COMM_WORLD,&nproc);
878
879     if(alive_probability > 1) alive_probability = 1;
880     if(alive_probability < 0) alive_probability = 0;
881     int n_vert = vertices_.size();
882     int n_alive_verts = 0;
883     unsigned int alive_checker = (unsigned int)((double)RAND_MAX)*alive_probability);

```

```

884 bool initial_state;
885 for(int ivert = 0; ivert<n_vert;ivert++)
886 {
887     if(vertices_[ivert].owner == rank)
888     {
889         initial_state = (rand() < alive_checker);
890         //initial_state = (vertices_[ivert].mid%2);
891         //initial_state = (vertices_[ivert].r[0] > 0);
892         for(int ifam = 0; ifam < vertices_[ivert].family.size(); ifam++)
893         {
894             if(vertices_[ivert].family[ifam] != rank)
895             {
896                 MPI_Send(
897                     &(initial_state),
898                     1,
899                     MPI_LOGICAL,
900                     vertices_[ivert].family[ifam],
901                     vertices_[ivert].mid,
902                     MPI_COMM_WORLD
903                 );
904             }
905         }
906     }
907     else
908     {
909         // Receive initial state from owner.
910         MPI_Recv(
911             &initial_state,
912             1,
913             MPI_LOGICAL,
914             vertices_[ivert].owner,
915             vertices_[ivert].mid,
916             MPI_COMM_WORLD,
917             &status
918         );
919     }
920     vertices_[ivert].current_state = initial_state;
921     if(initial_state)n_alive_verts++;
922 }
923 }
924
925 bool GOL_CalculateNextState(bool current_state,int n_alive, int n_dead)
926 {
927     double life_rate = (double)(n_alive + n_dead);
928     life_rate = 1/128*life_rate;
929     life_rate *= (double)(n_alive);
930     bool next_state = current_state;
931     if(current_state)
932     {
933         if(life_rate < 0.2999)
934         {
935             // Die of loneliness
936             next_state = false;
937         }
938         else if(life_rate < 0.5111)
939         {
940             // Keep living because you're in a good community.
941             next_state = true;
942         }
943         else
944         {
945             // Die from overpopulation
946             next_state = false;
947         }
948     }
949     else
950     {
951         if((0.2999 < life_rate) && (life_rate < 0.5111))
952         {
953             // Get born
954             next_state = true;
955         }
956         else
957         {
958             // Stay dead
959             next_state = false;
960         }
961     }
962     return(next_state);
963 }
964
965 void Mesh::updateVertexStates()
966 {
967     int rank,nproc;
968     MPI_Status status;
969     MPI_Comm_rank(MPI_COMM_WORLD,&rank);
970     MPI_Comm_size(MPI_COMM_WORLD,&nproc);
971     int n_vert = vertices_.size();
972     int n_come_alive = 0;
973     int n_come_dead = 0;
974     int total_n_alive = 0;
975     std::stringstream msg;
976
977     std::vector<std::vector<helper_vertex_t>> send_helpers(nproc);
978     std::vector<std::vector<helper_vertex_t>> rcv_helpers(nproc);
979
980     // Loop over my vertices:
981     // For each vertex where I'm not the owner, send a collection of
982     // helper vertices.
983     int n_helpers_sent = 0;
984     for(int iv = 0; iv < n_vert; iv++)
985     {
986         vertex_t * cur_v = &(vertices_[iv]);
987         if((cur_v->owner != rank) && (cur_v->family.size()>0))
988         {
989             for(int inb = 0; inb < cur_v->neighbours.size(); inb++)
990             {

```

```

991         vertex_t * nbr_v = cur_v->neighbours[inb];
992         helper.vertex_t helper;
993         helper.host_mid = cur_v->mid;
994         helper.nbr_mid = nbr_v->mid;
995         helper.nbr_state = nbr_v->current_state;
996         send_helpers[cur_v->owner].push_back(helper);
997         n_helpers_sent++;
998     }
999 }
1000 }
1001 MPI_Alltoall_vecvecT(send_helpers, recv_helpers);
1002
1003 // For each of my vertices:
1004 // If you don't own this vertex, don't bother. You sent its
1005 // neighbours to its owner. You'll get its next state later on.
1006 // If you own it, then:
1007 // For each neighbour:
1008 //     add its state to alive_dead
1009 //     check off that that connection was counted
1010 for(int iv = 0; iv < vertices_.size(); iv++)
1011 {
1012     vertex_t * cur_v = &(vertices_[iv]);
1013     vertices_[iv].alive_dead[0] = 0;
1014     vertices_[iv].alive_dead[1] = 0;
1015     if(cur_v->owner != rank) continue;
1016     for(int inb = 0; inb < cur_v->neighbours.size(); inb++)
1017     {
1018         vertex_t * nbr_v = cur_v->neighbours[inb];
1019         // Has this connection been counted already?
1020         int gm_idx=-1;
1021         for(int igm = 0; igm < cur_v->global_nbr_mids.size(); igm++)
1022         {
1023             if(nbr_v->mid == cur_v->global_nbr_mids[igm])
1024             {
1025                 gm_idx = igm;
1026                 break;
1027             }
1028         }
1029         bool connection_already_counted = cur_v->nbr_was_counted[gm_idx];
1030         if(!connection_already_counted)
1031         {
1032             if(nbr_v->current_state)
1033             {
1034                 cur_v->alive_dead[0]++;
1035             }
1036             else
1037             {
1038                 cur_v->alive_dead[1]++;
1039             }
1040         }
1041         cur_v->nbr_was_counted[gm_idx] = true;
1042     }
1043 }
1044 }
1045
1046 // For each helper_vertex I received:
1047 // I received it because I AM THE OWNER
1048 // Find its host's index in my list using mid2lindx_
1049 // Update that host's alive_dead using the helper's state.
1050 for(int iproc = 0; iproc < nproc; iproc++)
1051 {
1052     for(int ih = 0; ih < recv_helpers[iproc].size(); ih++)
1053     {
1054         helper_vertex_t * helper = &(recv_helpers[iproc][ih]);
1055         // This helper is telling me that the host at host_mid
1056         // needs to know that its neighbour at nbr_mid has state
1057         // nbr_state.
1058         // Do I already know about this connection?
1059         vertex_t * host_v = &(vertices_[mid2lindx_[helper->host_mid]]);
1060         bool connection_was_counted = false;
1061         int gm_idx=-1;
1062         for(int igm = 0; igm < host_v->global_nbr_mids.size(); igm++)
1063         {
1064             if(helper->nbr_mid == host_v->global_nbr_mids[igm])
1065             {
1066                 gm_idx = igm;
1067                 connection_was_counted = host_v->nbr_was_counted[igm];
1068                 break;
1069             }
1070         }
1071         if(!connection_was_counted)
1072         {
1073             if(helper->nbr_state)
1074             {
1075                 host_v->alive_dead[0]++;
1076             }
1077             else
1078             {
1079                 host_v->alive_dead[1]++;
1080             }
1081             host_v->nbr_was_counted[gm_idx] = true;
1082         }
1083     }
1084 }
1085
1086 // For each of my vertices
1087 // If you own this vertex, update its state and communicate the
1088 // new state.
1089 for(int iv = 0; iv < vertices_.size(); iv++)
1090 {
1091     vertex_t * cur_v = &(vertices_[iv]);
1092     if(cur_v->owner == rank)
1093     {
1094         cur_v->next_state = GOL_CalculateNextState(
1095             cur_v->current_state,
1096             cur_v->alive_dead[0],
1097             cur_v->alive_dead[1]

```

```

1098     });
1099     for(int ifam = 0; ifam < cur_v->family.size(); ifam++)
1100     {
1101         // No need to talk to yourself, you already know the
1102         // next state
1103         if(cur_v->family[ifam] == rank) continue;
1104         // I am the owner. Only owners get to send out the
1105         // next_state of a vertex. Therefore, nobody else
1106         // will be trying to send this message.
1107         MPI_Send(
1108             &(cur_v->next_state),
1109             1,
1110             MPI_LOGICAL,
1111             cur_v->family[ifam],
1112             cur_v->mid,
1113             MPI_COMM_WORLD
1114         );
1115     }
1116 }
1117 }
1118 // For each of my vertices
1119 // If someone else owns it, then there should be a message waiting
1120 // for me telling me its new state.
1121 for(int iv = 0; iv < vertices_.size(); iv++)
1122 {
1123     vertex_t * cur_v = &(vertices_[iv]);
1124     if(cur_v->owner != rank)
1125     {
1126         MPI_Recv(
1127             &(cur_v->next_state),
1128             1,
1129             MPI_LOGICAL,
1130             cur_v->owner,
1131             cur_v->mid,
1132             MPI_COMM_WORLD,
1133             &status
1134         );
1135     }
1136 }
1137 // Finally, loop through all your vertices and make current state
1138 // become next state.
1139 for(int iv = 0; iv < vertices_.size(); iv++)
1140 {
1141     vertex_t * cur_v = &(vertices_[iv]);
1142     cur_v->current_state = cur_v->next_state;
1143     // Zero out alive_dead, just to be safe.
1144     cur_v->alive_dead[0] = 0;
1145     cur_v->alive_dead[1] = 0;
1146     for(int ig = 0; ig < cur_v->global_nbr_mids.size(); ig++)
1147     {
1148         cur_v->nbr_was_counted[ig] = false;
1149     }
1150 }
1151 }
1152
1153
1154
1155 void Mesh::writeCellMatrixFile(
1156     std::string filename,
1157     bool append=false
1158 )
1159 {
1160     {
1161         int rank, nproc;
1162         MPI_Comm_rank(MPI_COMM_WORLD, &rank);
1163         MPI_Comm_size(MPI_COMM_WORLD, &nproc);
1164         std::ofstream matfilestream;
1165         if(append)
1166         {
1167             for(int irank = 0; irank < nproc; irank++)
1168             {
1169                 if(irank == rank)
1170                 {
1171                     matfilestream.open(filename, std::ofstream::out | std::ofstream::app);
1172                     if(rank == 0) matfilestream << std::endl;
1173                     for(int iv = 0; iv < vertices_.size(); iv++)
1174                     {
1175                         if(vertices_[iv].owner == rank)
1176                         {
1177                             matfilestream << vertices_[iv].current_state << " ";
1178                         }
1179                         if(rank == (nproc-1)) matfilestream << std::endl;
1180                     }
1181                     matfilestream.close();
1182                 }
1183                 MPI_Barrier(MPI_COMM_WORLD);
1184             }
1185         }
1186         else
1187         {
1188             for(int irank = 0; irank < nproc; irank++)
1189             {
1190                 if(irank == rank)
1191                 {
1192                     if(rank == 0)
1193                     {
1194                         matfilestream.open(filename, std::ofstream::out);
1195                         // matfilestream << global_n_vertices << std::endl;
1196                     }
1197                     else
1198                     {
1199                         matfilestream.open(filename, std::ofstream::out | std::ofstream::app);
1200                     }
1201                     for(int iv = 0; iv < vertices_.size(); iv++)
1202                     {
1203                         //If you are the owner, output the mid and position
1204                         if(vertices_[iv].owner == rank)

```

```

1205         {
1206             matfilestream << vertices_[iv].mid << " " << vertices_[iv].r[0] << " " << vertices_[iv].r[1] << " " << vertices_[iv].r[2]
<< std::endl;
1207         }
1208     }
1209     matfilestream.close();
1210 }
1211 MPI_Barrier(MPI_COMM_WORLD);
1212 }
1213 for(int irank = 0; irank < nproc; irank++)
1214 {
1215     if(irank == rank)
1216     {
1217         matfilestream.open(filename, std::ofstream::out | std::ofstream::app);
1218         if(rank == 0) matfilestream << std::endl;
1219         for(int iv = 0; iv < vertices_.size(); iv++)
1220         {
1221             if(vertices_[iv].owner == rank)
1222             {
1223                 matfilestream << vertices_[iv].current_state << " ";
1224             }
1225         }
1226         if(rank == (nproc-1)) matfilestream << std::endl;
1227         matfilestream.close();
1228     }
1229     MPI_Barrier(MPI_COMM_WORLD);
1230 }
1231 }
1232 }
1233
1234 double Mesh::calculateVertexLifeRate()
1235 {
1236     int rank, nproc;
1237     MPI_Status status;
1238     MPI_Comm_rank(MPI_COMM_WORLD, &rank);
1239     MPI_Comm_size(MPI_COMM_WORLD, &nproc);
1240
1241     int total_owned_alive;
1242     int total_owned_dead;
1243     for(int iv = 0; iv < vertices_.size(); iv++)
1244     {
1245         vertex_t * cur_v = &(vertices_[iv]);
1246         if(cur_v->owner == rank)
1247         {
1248             if(cur_v->current_state)
1249             {
1250                 total_owned_alive++;
1251             }
1252             else
1253             {
1254                 total_owned_dead++;
1255             }
1256         }
1257     }
1258     int global_n_alive;
1259     int global_n_dead;
1260     MPI_Allreduce(
1261         &total_owned_alive,
1262         &global_n_alive,
1263         1,
1264         MPI_INT,
1265         MPI_SUM,
1266         MPI_COMM_WORLD
1267     );
1268     MPI_Allreduce(
1269         &total_owned_dead,
1270         &global_n_dead,
1271         1,
1272         MPI_INT,
1273         MPI_SUM,
1274         MPI_COMM_WORLD
1275     );
1276     double life_rate = (double)(global_n_alive+global_n_dead);
1277     if((global_n_alive + global_n_dead)>0)
1278     {
1279         life_rate = 1/life_rate;
1280         life_rate *= (double)(global_n_alive);
1281     }
1282     else
1283     {
1284         life_rate = 0;
1285     }
1286     return(life_rate);
1287 }

```