Colony Collapse in a nutshell

01/26/2019

Abstract

This solution provides a numerical simulation of the collapse of the bacteria colony by evolving the Keller-Segel equations with modified boundary conditions for a shell in the center of the domain.

1 Introduction

The phenomenon of bacteria motion and colony evolution can be described using the Keller-Segel equations. The question predicts that given a small hollow shell with volume much less than the total volume of the environment, the colony of the bacteria will grow and, eventually, collapse into the shell. This computational experiment intends to use several numerical methods to approximate the result of the solution.

1.1 Keller-Segel equations

We simplify the Keller-Segel equations as shown below:

$$\partial_t b = D_b \nabla^2 b - k(\nabla b(\nabla c) + \alpha b = D_b \nabla^2 b - k(\nabla b \cdot \nabla c + b \nabla^2 c) + \alpha b \tag{1}$$

$$\partial_t c = D_c \nabla^2 c + \beta b f \tag{2}$$

$$\partial_t f = D_f \nabla^2 f - \gamma b \tag{3}$$

where b is the bacterial density, c is the attractant concentration, and f is food concentration. The parameters D_b , D_c and D_f are the diffusivity coefficients of the bacteria, the chemo attractant molecules and the food molecules. The parameter is the sensitivity of bacteria to the chemo concentration gradient, α is the bacterial growth rate, β is the chemo production rate, and γ is the food consumption rate.
This experiments are in two parts: in the first part, we use normal boundaries and a dropping point of bacteria in the center of the grid for the bacteria to evolve and collapse within the domain of the environment; in the second part, we introduce a small shell in the center of grid, and we change the drop points to the center of the four quadrant of the grid.

2 Procedure

2.1 Finite difference methods

To find the spatial derivatives and also hold the spatial symmetry for stability, we use second differential order, first order finite difference method to get the laplacian of a vector array[x,y]:

$$\begin{aligned} laplace[x,y] = & \frac{((array[x+1,y] - array[x,y]) - (array[x,y] - array[x-1,y]))}{dx^2} \\ & + \frac{((array[x,y+1] - array[x,y]) - (array[x,y] - array[x,y-1]))}{dy^2} \end{aligned}$$

We use first differential order, second order finite difference method to get the dot product of the gradient of two vectors array1[x,y], array2[x,y]:

$$graddotgrad[x,y] = \frac{(array1[x+1,y] - array1[x-1,y])(array2[x+1,y] - array2[x-1,y])}{4dx^2} + \frac{(array1[x,y+1] - array1[x,y-1])(array2[x,y+1] - array2[x,y-1])}{4dy^2}$$

2.2 Initial conditions

For initial conditions, we use a grid of 41 * 41 boxes with dx = 0.01, dy = 0.01. We use $D_b = 0.1$, $D_c = 0.1$, $D_f = 0.1$, $k = 10.0$, $\alpha = 0.1$, $\beta = 0.1$, $\gamma = 0.1$. We use $b_0 = 0.01$, $c_0 = 0.0$, $f_0 = 0.001$ for the initial values for every points on the grid, in which we also apply a perturbation of $1000 * b_0$ for dropping points of the bacteria.
In the first experiment, the drop point is at (x,y) = (21, 21). In the second experiment, the drop points are at (x,y) = (11,11), (11,31), (31,11), (31,31).

2.3 Boundary conditions

To install boundary conditions, we introduce ghost points for all b, c, f at the boundaries where x = 1, 41 and y = 1, 41. The ghost points image the value of the grid point neighboring the boundary to create the effect of an open boundary (i.e the imaginary ghost point at x=0, y=15 has the same value as the point at x=1, y = 15).

2.4 Shell boundary condition

In the second part of the experiment, we carefully analyze the partial derivative equations in sight of a comparison with the continuity equation for the bacteria.

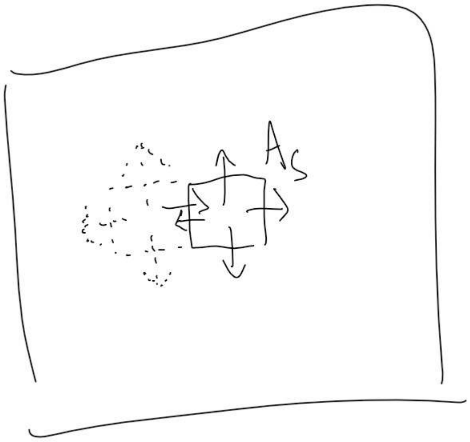


Figure 1: The diagram of the shell. The arrows are the flux that will be limited, whereas the dotted arrows are the flux that shouldn't be changed.

We impose the boundary condition for the shell as a passing-filter for the bacteria travelling through the four edges of the center block, where the filter coefficient η is defined as:

$$\eta = \frac{\text{area of the hole}}{\text{cross area of the small volume}} = \frac{A_s}{2(dx+dy)} \tag{4}$$

The coefficient denotes that all flux passing through the shell boundary should be lowered by multiplying the coefficient. We break down the laplacian and the dot product of the gradient and insert the coefficient

at the correct term in order to filter each bacteria crossing the ”shelled” area.
For the center grid point, all boundaries are simply multiplied by the coefficient η. For points neighboring the grid point, however, the derivatives are much more complicated.
For example, we take a look at the term (xs - 1, ys) left to the center point (xs, ys). This point has three edges with no travelling limitations, with the boundary to the center limited by the coefficient. We separate the terms in laplacian to get a new function specifically for these points:

$$laplace[xs-1,ys] = \frac{(\eta(array[xs,ys]-array[xs-1,ys])-(array[xs-1,ys]-array[xs-2,ys]))}{dx^2} + \frac{((array[xs-1,ys+1]-array[xs-1,ys])-(array[xs-1,ys]-array[xs-1,ys-1]))}{dy^2}$$

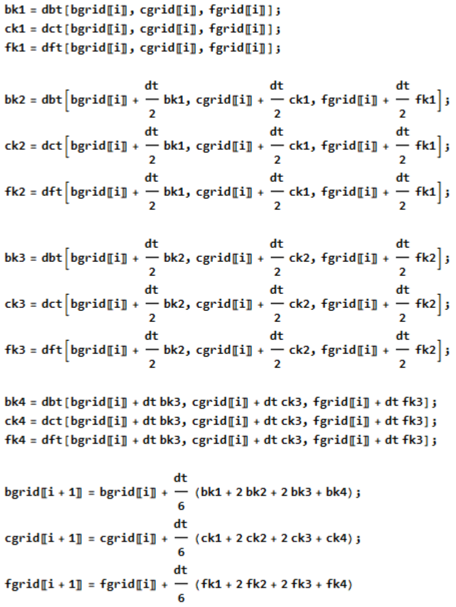
For the same grid point, we use the formula below as the dot product of the gradient function:

$$graddotgrad[xs-1,ys] = \frac{(\eta(array1[xs,ys]-array1[xs-1,ys])+(array1[xs-1,ys]-array1[xs-2,ys]))}{2dx} \times \frac{(\eta(array2[xs,ys]-array2[xs-1,ys])+(array2[xs-1,ys]-array2[xs-2,ys]))}{2dx} + \frac{((array1[xs-1,ys+1]-array1[xs-1,ys])+(array1[xs-1,ys]-array1[xs-1,ys-1]))}{2dy} \times \frac{((array2[xs-1,ys+1]-array2[xs-1,ys])+(array2[xs-1,ys]-array2[xs-1,ys-1]))}{2dy}$$

In the experiment, we use $\eta = 0.01$.

2.5 Time evolution

For better precision, we use 4th order Runge-Kutta method to evolve the system in time (as shown in fig:RK4).



```
bk1 = dbt[bgrid⟦i⟧, cgrid⟦i⟧, fgrid⟦i⟧];
ck1 = dct[bgrid⟦i⟧, cgrid⟦i⟧, fgrid⟦i⟧];
fk1 = dft[bgrid⟦i⟧, cgrid⟦i⟧, fgrid⟦i⟧];

bk2 = dbt[bgrid⟦i⟧ + dt/2 bk1, cgrid⟦i⟧ + dt/2 ck1, fgrid⟦i⟧ + dt/2 fk1];
ck2 = dct[bgrid⟦i⟧ + dt/2 bk1, cgrid⟦i⟧ + dt/2 ck1, fgrid⟦i⟧ + dt/2 fk1];
fk2 = dft[bgrid⟦i⟧ + dt/2 bk1, cgrid⟦i⟧ + dt/2 ck1, fgrid⟦i⟧ + dt/2 fk1];

bk3 = dbt[bgrid⟦i⟧ + dt/2 bk2, cgrid⟦i⟧ + dt/2 ck2, fgrid⟦i⟧ + dt/2 fk2];
ck3 = dct[bgrid⟦i⟧ + dt/2 bk2, cgrid⟦i⟧ + dt/2 ck2, fgrid⟦i⟧ + dt/2 fk2];
fk3 = dft[bgrid⟦i⟧ + dt/2 bk2, cgrid⟦i⟧ + dt/2 ck2, fgrid⟦i⟧ + dt/2 fk2];

bk4 = dbt[bgrid⟦i⟧ + dt bk3, cgrid⟦i⟧ + dt ck3, fgrid⟦i⟧ + dt fk3];
ck4 = dct[bgrid⟦i⟧ + dt bk3, cgrid⟦i⟧ + dt ck3, fgrid⟦i⟧ + dt fk3];
fk4 = dft[bgrid⟦i⟧ + dt bk3, cgrid⟦i⟧ + dt ck3, fgrid⟦i⟧ + dt fk3];

bgrid⟦i + 1⟧ = bgrid⟦i⟧ + dt/6 (bk1 + 2 bk2 + 2 bk3 + bk4);
cgrid⟦i + 1⟧ = cgrid⟦i⟧ + dt/6 (ck1 + 2 ck2 + 2 ck3 + ck4);
fgrid⟦i + 1⟧ = fgrid⟦i⟧ + dt/6 (fk1 + 2 fk2 + 2 fk3 + fk4)
```

Figure 2: The 4th Runge-Kutta method used for the simmulation

3 Result

The evolution is shown in the relative density plot with white being more bacteria or food and black being less bacteria or food in each plot. For different images the colors can't be compared since they only represent the relative difference in the data, which comes in useful since the data drops critically right after the starting value.

3.1 Free evolution

3.1.1 The evolution of the bacteria

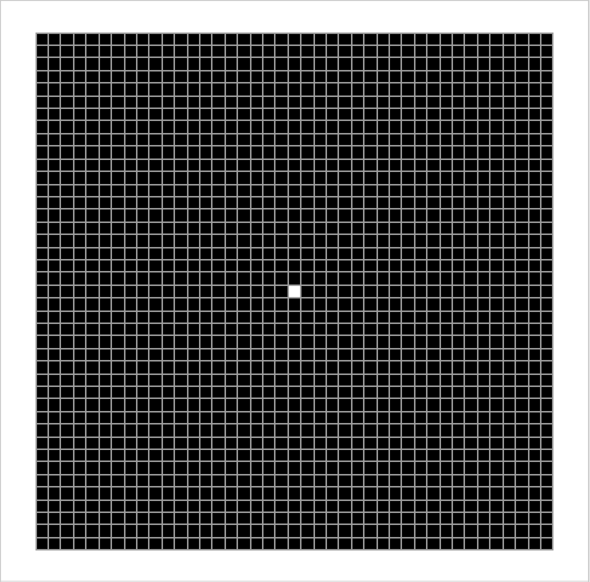


Figure 3: At the start the evolution, the bacteria starts the center.

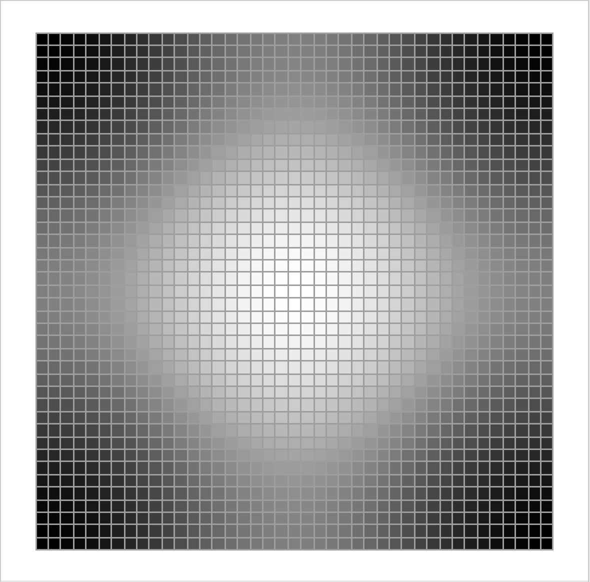


Figure 4: The bacteria spreads over the space except the edges.

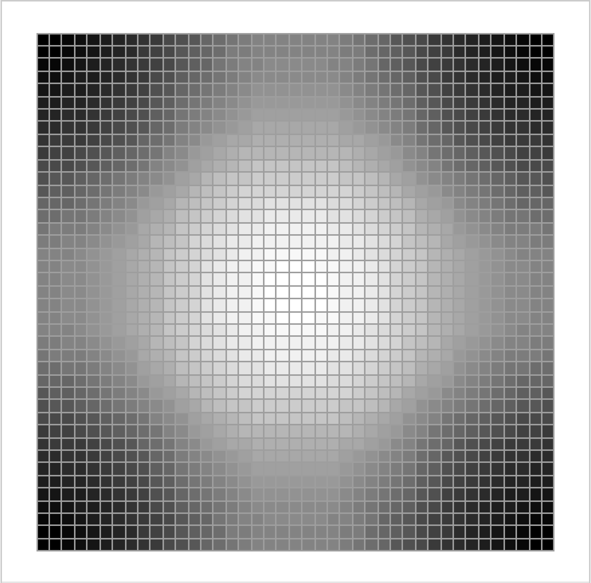


Figure 5: The state stays equilibrium relatively for a moment, and it suddenly becomes unstable.

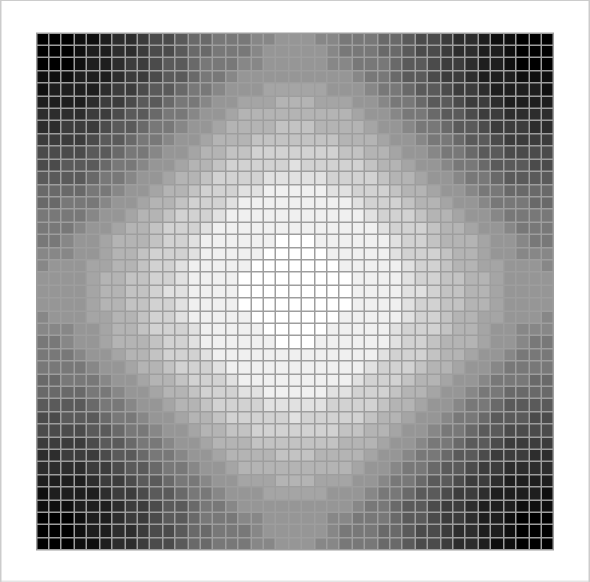


Figure 6: The bacteria collapses to the center of the grid.

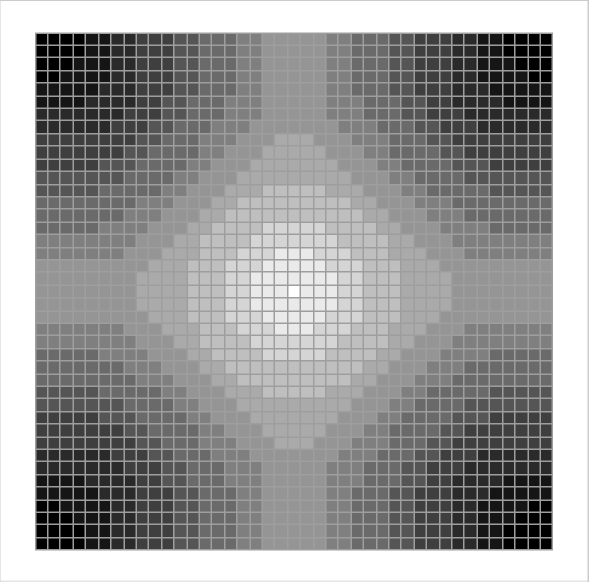


Figure 7: The bacteria continues collapsing to the center of the grid.

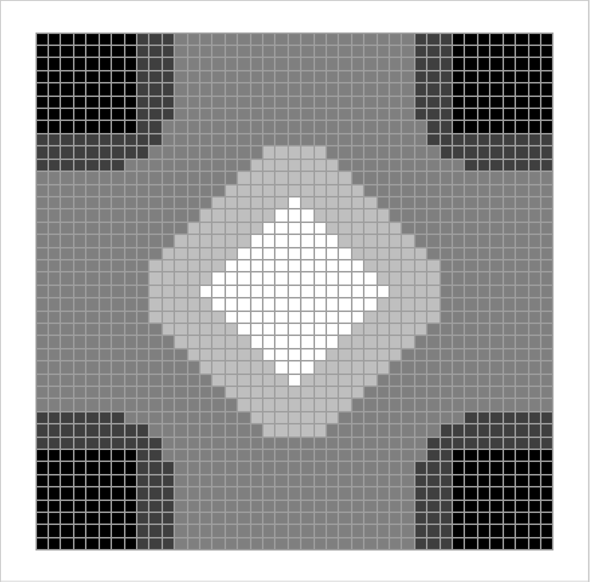


Figure 8: The bacteria right before converging to the center.

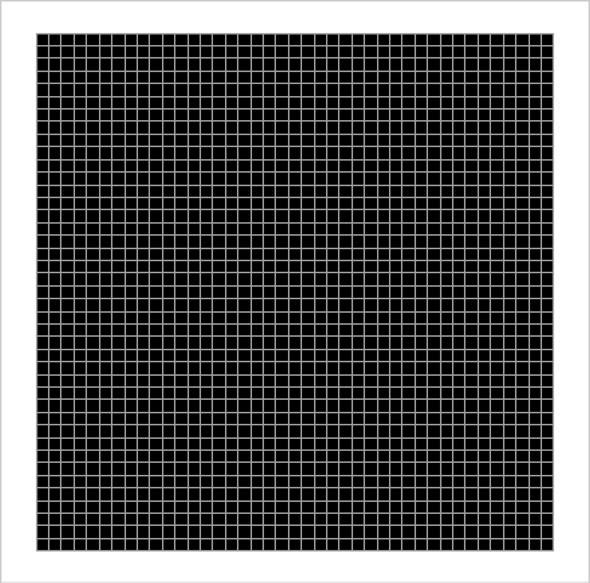


Figure 9: The bacteria remains small amount throughout the area, leaving zero laplacian everywhere.

3.1.2 The evolution of the food

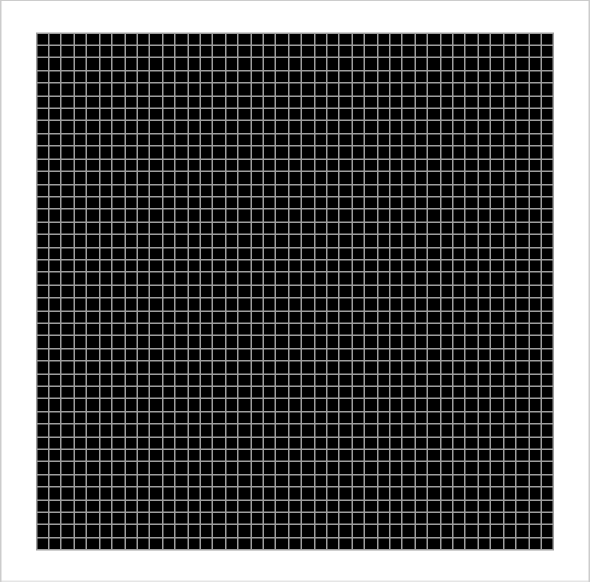


Figure 10: The food is the same everywhere initially.

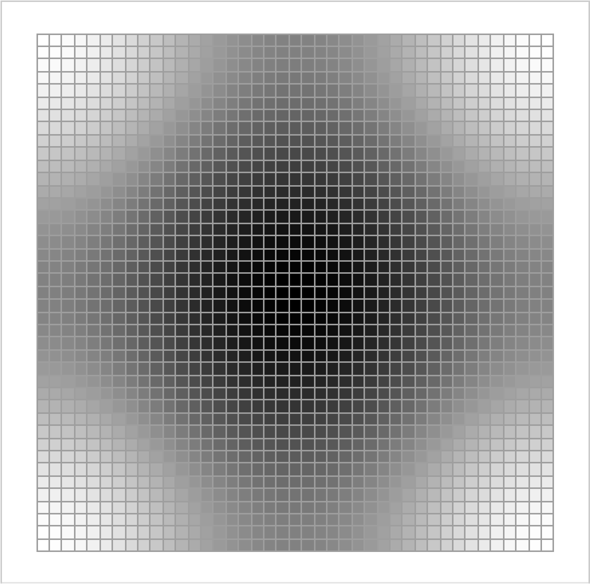


Figure 11: The food decreases accordingly to the distribution of bacteria.

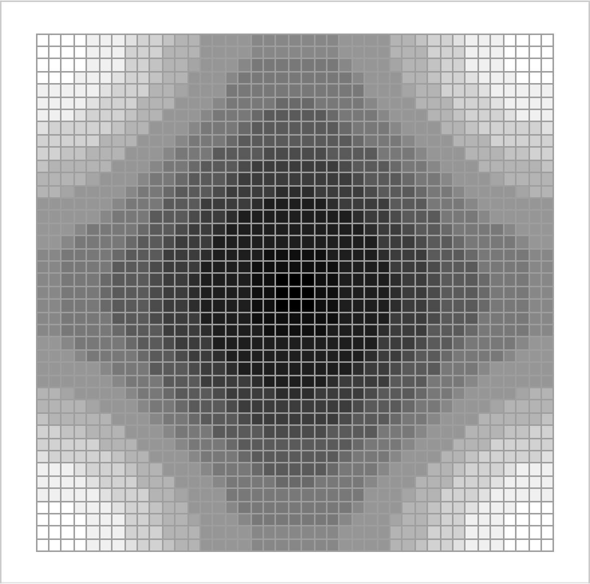


Figure 12: The food decreases accordingly to the distribution of bacteria.

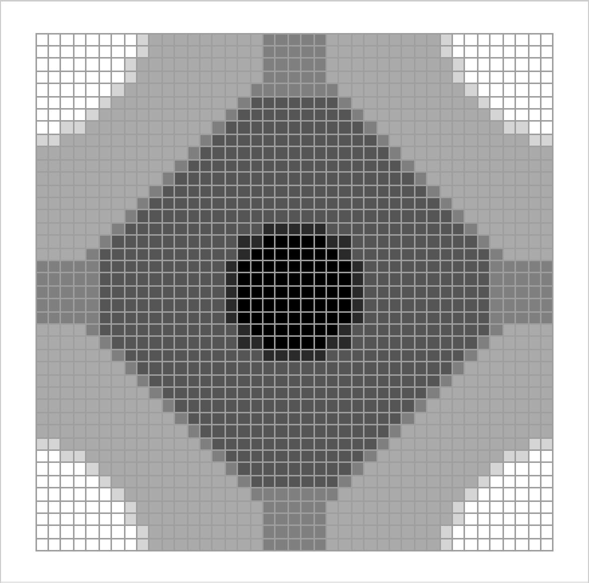


Figure 13: The food decreases accordingly to the distribution of bacteria.

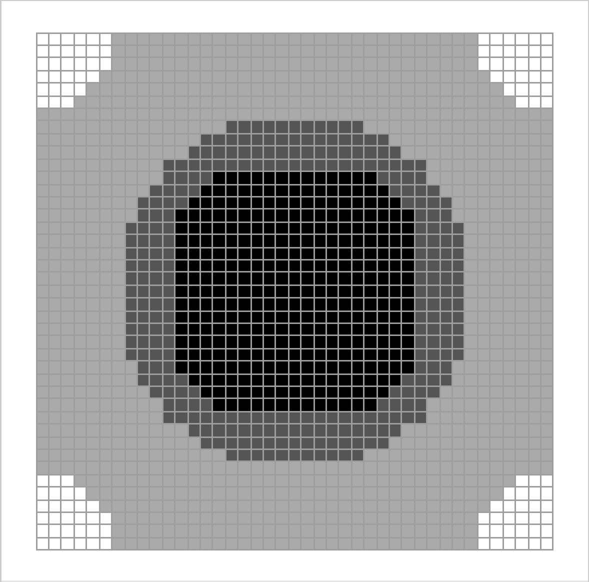


Figure 14: The food decreases accordingly to the distribution of bacteria.

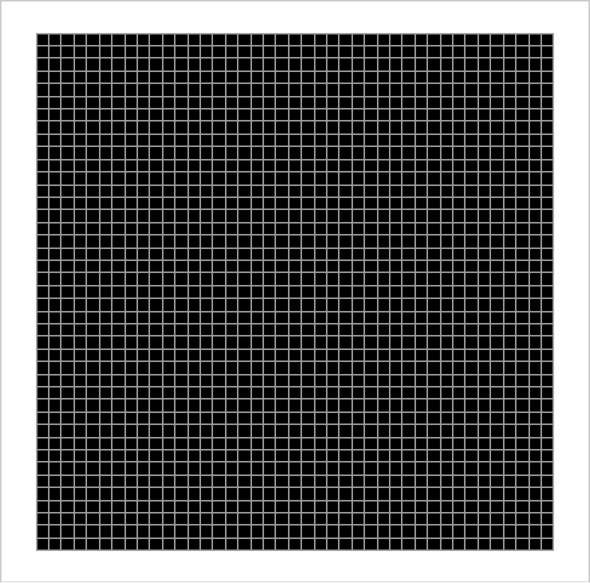


Figure 15: The food drops to a low level everywhere throughout the grid, similar to the bacteria.

3.2 Shell collapse

3.2.1 The evolution of bacteria

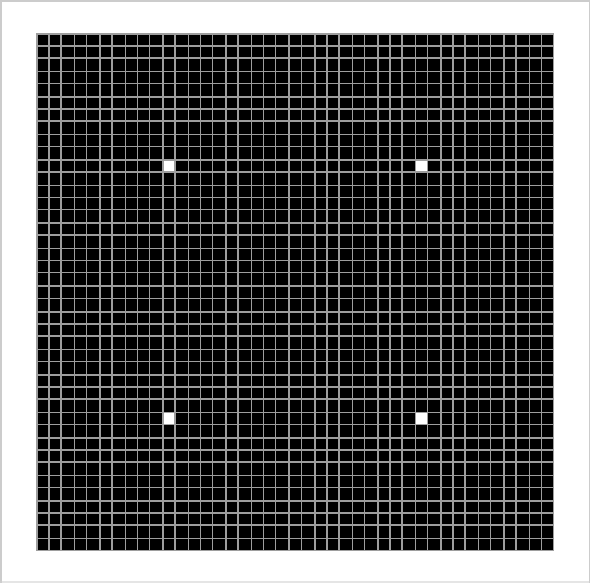


Figure 16: The bacteria starts at the center of the four quadrants.

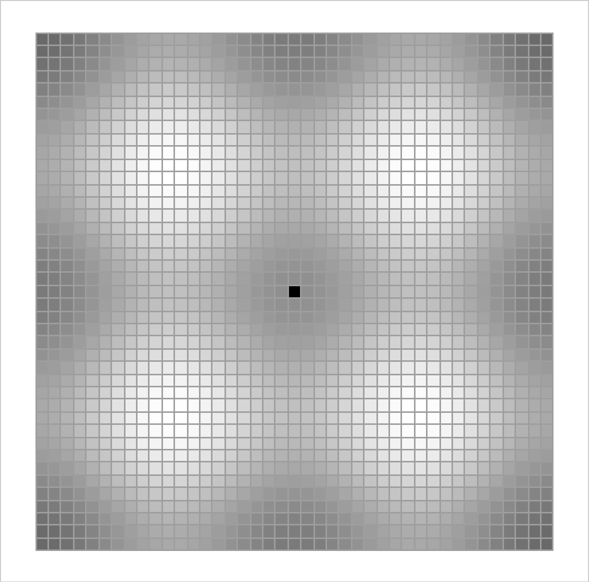


Figure 17: The bacteria starts spreading out in a circle, leaving the shell relatively empty.

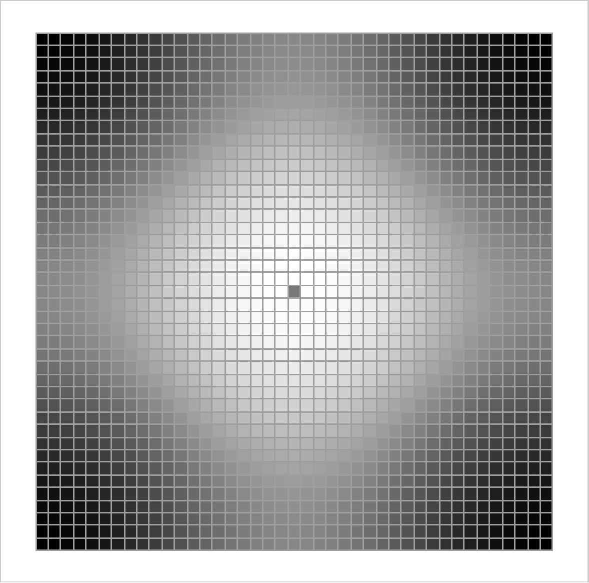


Figure 18: The bacteria outside the shell reaches the equilibrium state, whereas it is still relatively empty in the shell.

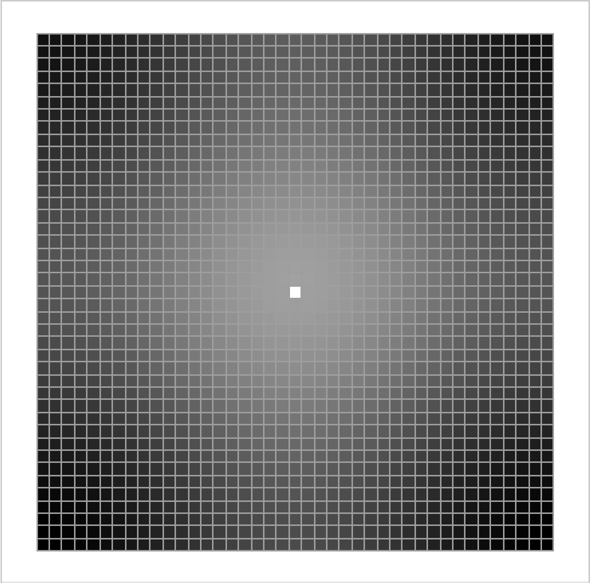


Figure 19: **The bacteria outside the shell decays as the bacteria in the shell grows. The state stays for a long while until the eventual decay of the bacteria inside the shell, leaving numerical errors dominating the density distribution.

3.2.2 The evolution of the food

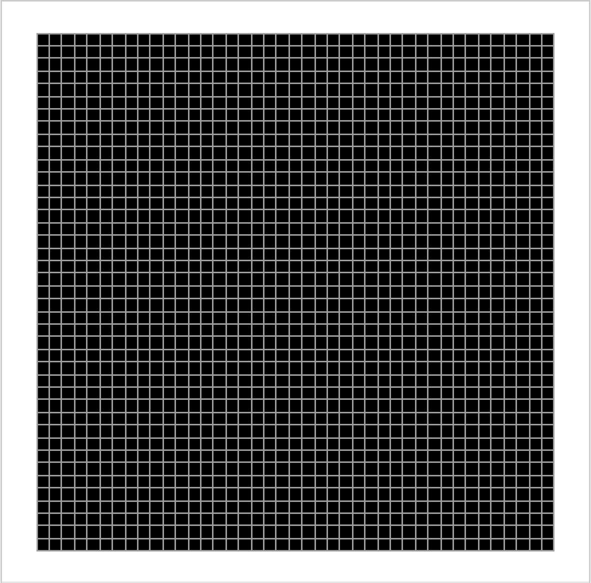


Figure 20: The food is the same everywhere initially.

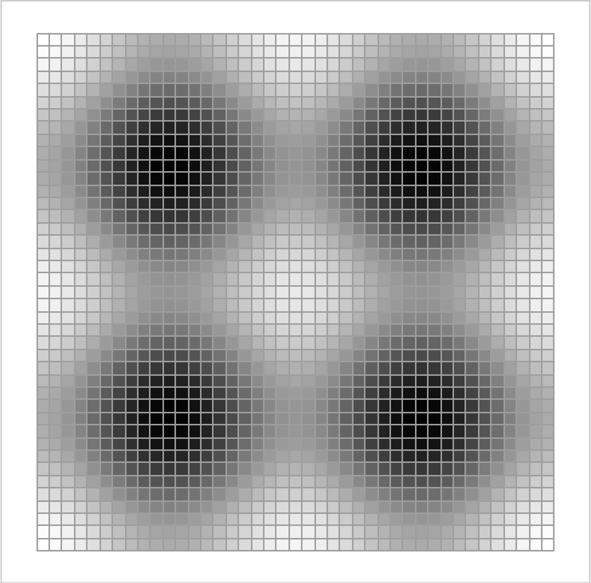


Figure 21: The food decreases accordingly to the distribution of bacteria. The shell doesn't seem to have much effect on the food distribution.

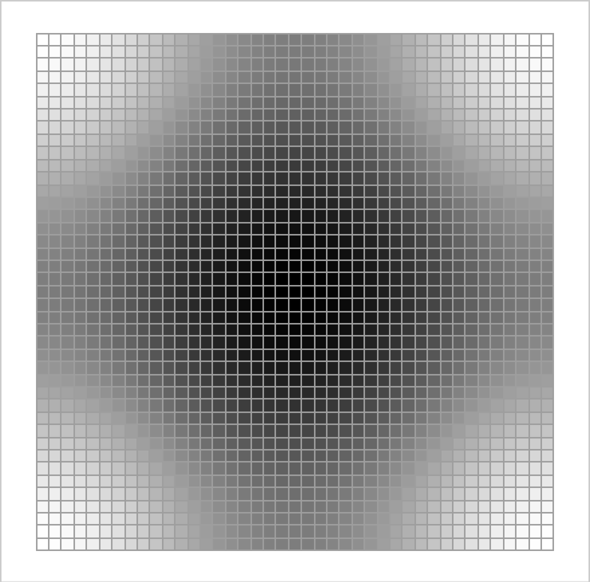


Figure 22: The food decreases accordingly to the distribution of bacteria. The shell doesn't seem to have much effect on the food distribution.

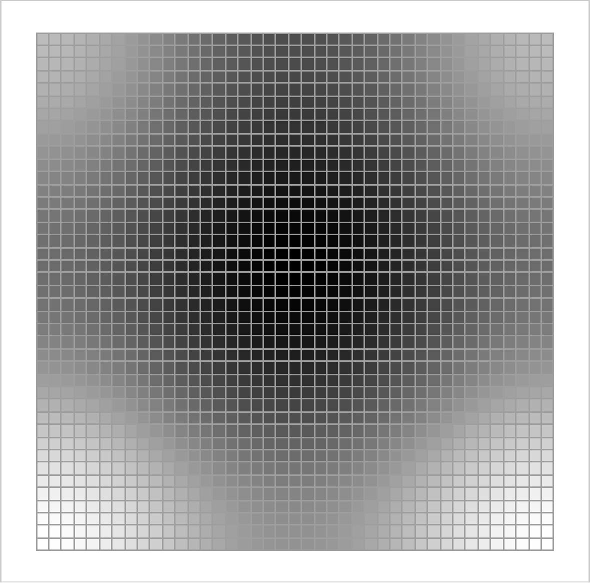


Figure 23: The food decreases accordingly to the distribution of bacteria. The shell doesn't seem to have much effect on the food distribution.

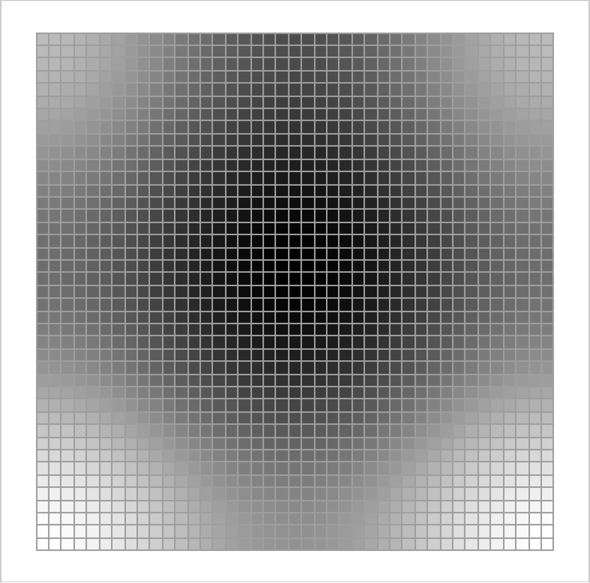


Figure 24: The food decreases accordingly to the distribution of bacteria. The shell doesn't seem to have much effect on the food distribution.

4 Conclusion

In this experiment, we can clearly observe the effect of the collapse of the bacteria (as shown in Figure 10 to 12), as well as the preserving effect of the shell that controls the flux going in and out (as shown in Figure 17). Similar to the result of the heat equation, the bacteria, chemo, and food distributes gradually. However, due to the consumption of food and the shortage of food, bacteria is seen to collapse and escape back to the center. They repel the edges simply due to the lack of chemo attractiveness at the area.
Given an empty shell in the center of the grid, we block the enormous flow coming from the outside once

the shortage occurs and causes it to collapse. Therefore, the bacteria inside is safe to grow and eventually outnumber the bacteria outside the shell.
These are the assumptions that we make from observing the effect from the simulation. We can conclude that with the modified boundary conditions and the Keller-Segel equations, we can successfully recreate the surprising phenomenon that the question inquires.