Reaction Diffusion Equation

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Our Project

Reaction diffusion Partial Differential Equations are used to model a variety of phenomena in biology, chemistry, and physics. We use a reaction diffusion equation to model bacteria in a thin tube that has antibiotics at both ends. The bacteria diffuse and replicate in the tube. When they reach the ends of the tube they die due to the antibiotics.

The diffusion PDE:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial t^2}$$

is a consequence of Fick's law which states that particles diffuse from higher to lower concentration.

We combine the diffusion equation with the differential equation for the logistic growth model for bacteria (the reaction term):

$$\frac{dc}{dt} = \frac{r_0}{K}c(K-c)$$

to get our reaction diffusion equation.

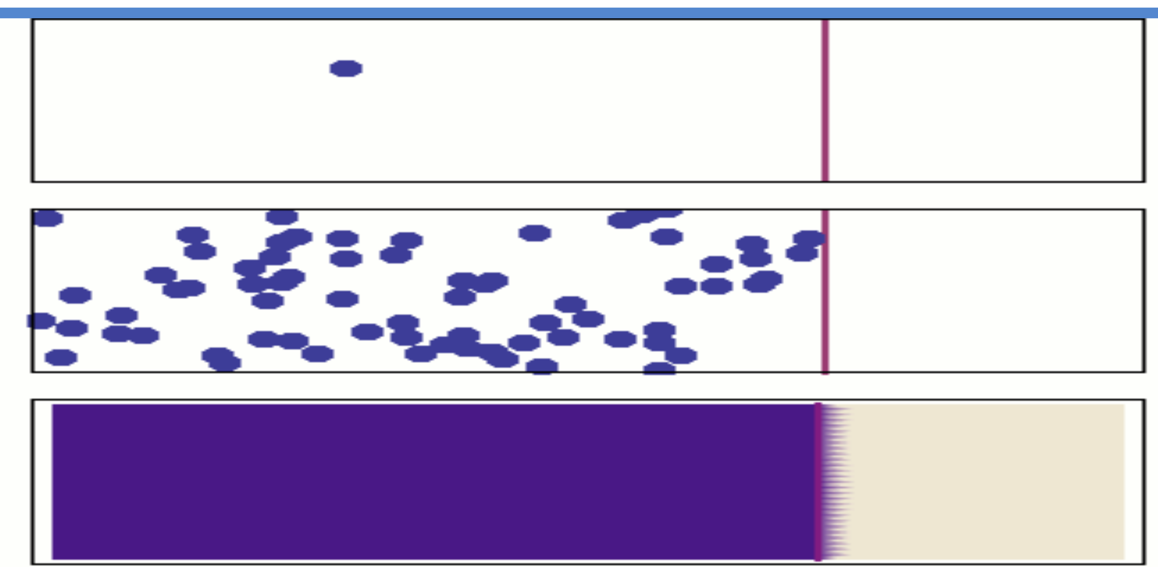
$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial t^2} + \frac{r_0}{K}c(K-c)$$

Boundary Conditions:
$u(0,t) = u(0,L) = 0$
bacteria are killed by antibiotics
at the ends of tube $x = 0$ and $x = L$

c = concentration
x = position
t = time
D = diffusivity constant
K = concentration carrying capacity
r_0 = instantaneous relative growth rate at low concentrations

We numerically solve this reaction diffusion equation and use it to analyze the diffusion and concentration of bacteria in a tube with antibiotics at both ends.

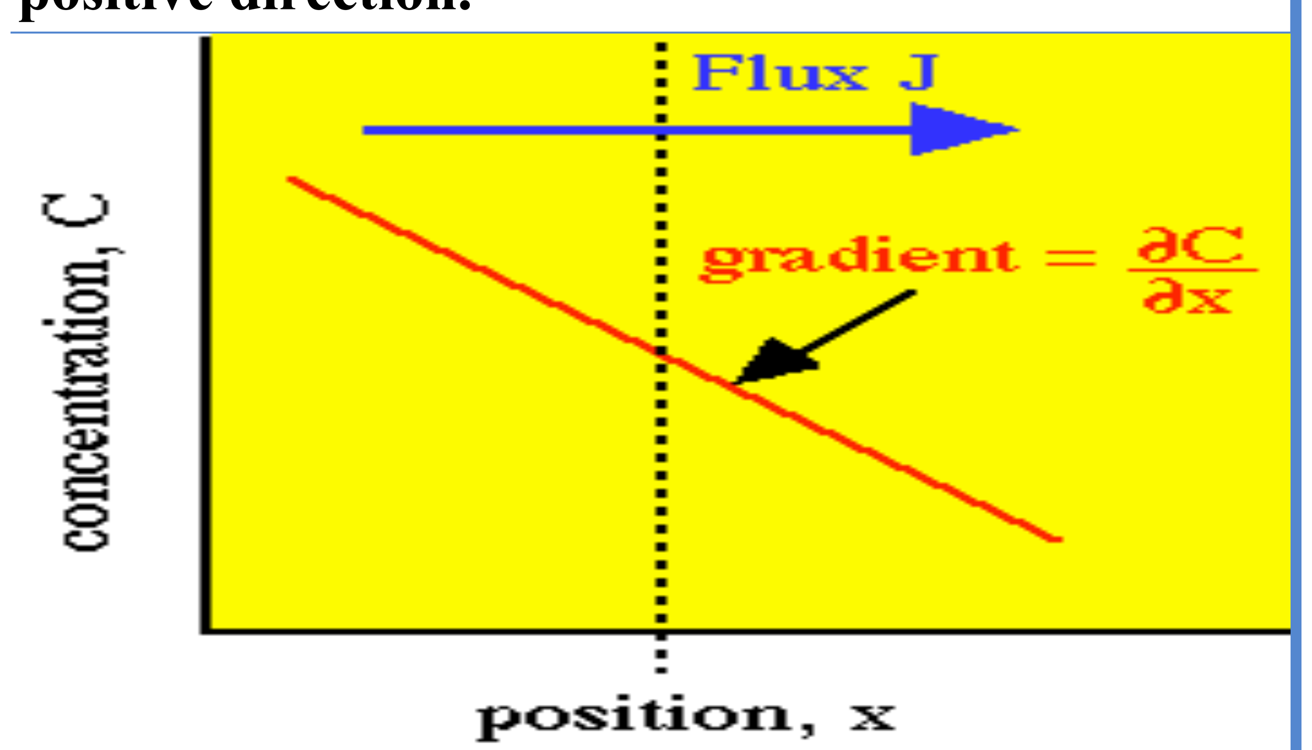
Background



The animation above shows random motion leads to diffusion

Diffusion is the movement of particles from a region of higher concentration to lower concentration. Mathematically diffusion occurs in response to a concentration gradient.

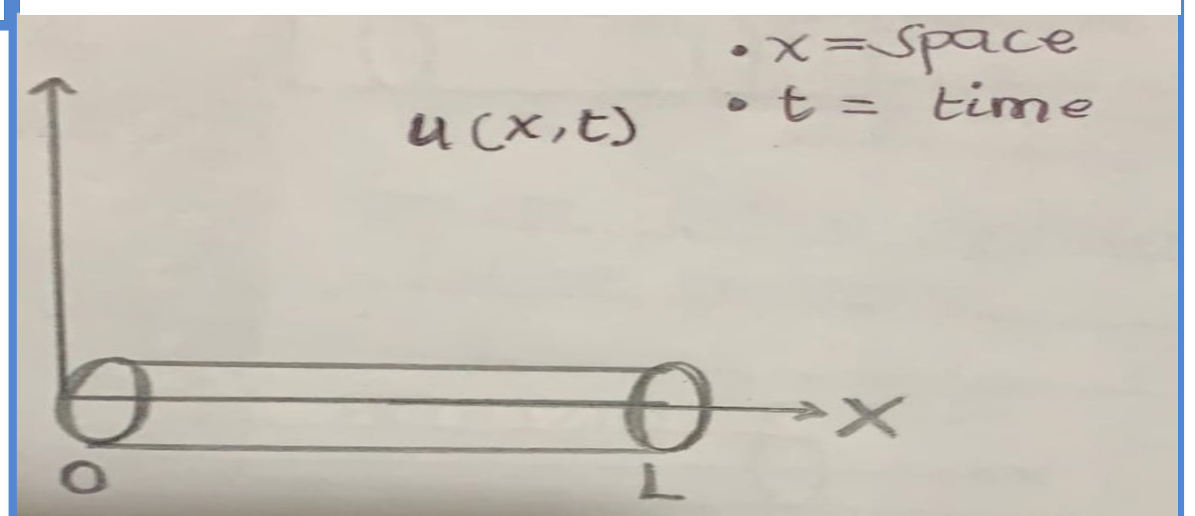
The figure below shows Fick's first law of diffusion: that the net flux (or flow of particles) is proportional to the negative gradient. The gradient is the slope of the concentration function. In this figure the slope (gradient) is negative. So, the net flow of particles is in the positive direction.



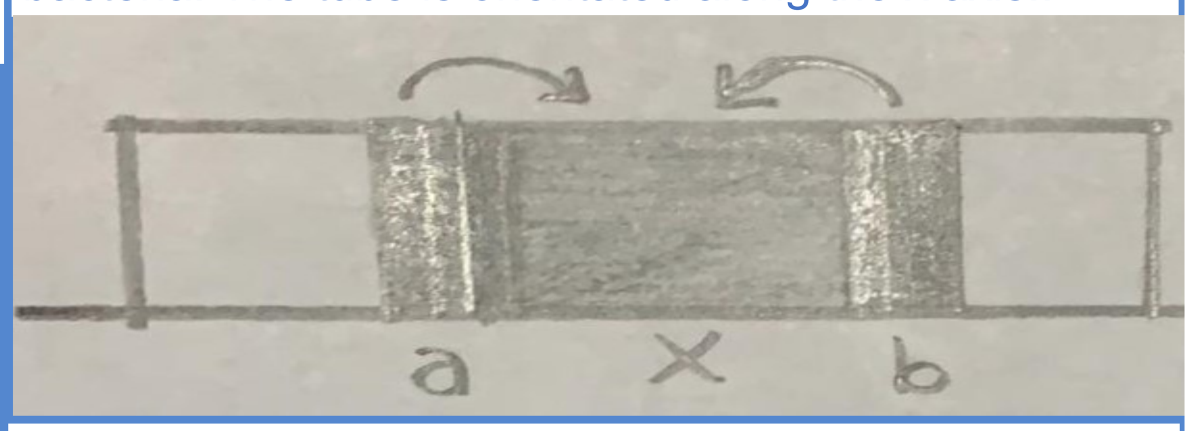
The logistic growth model for bacteria assumes that bacteria are less successful at reproducing as the concentration (density) of bacteria increases due to overcrowding and competition for resources. If the bacteria concentration exceeds the carrying capacity *K,* the bacteria will start to die off more quickly than they reproduce. As a result, in the logistic growth model, the carrying capacity is a stable equilibrium: the concentration of bacteria will tend to the carrying capacity.

Photo of e coli bacteria

Method and Results



The figure above represents the tube with the bacteria. The tube is orientated along the x axis..

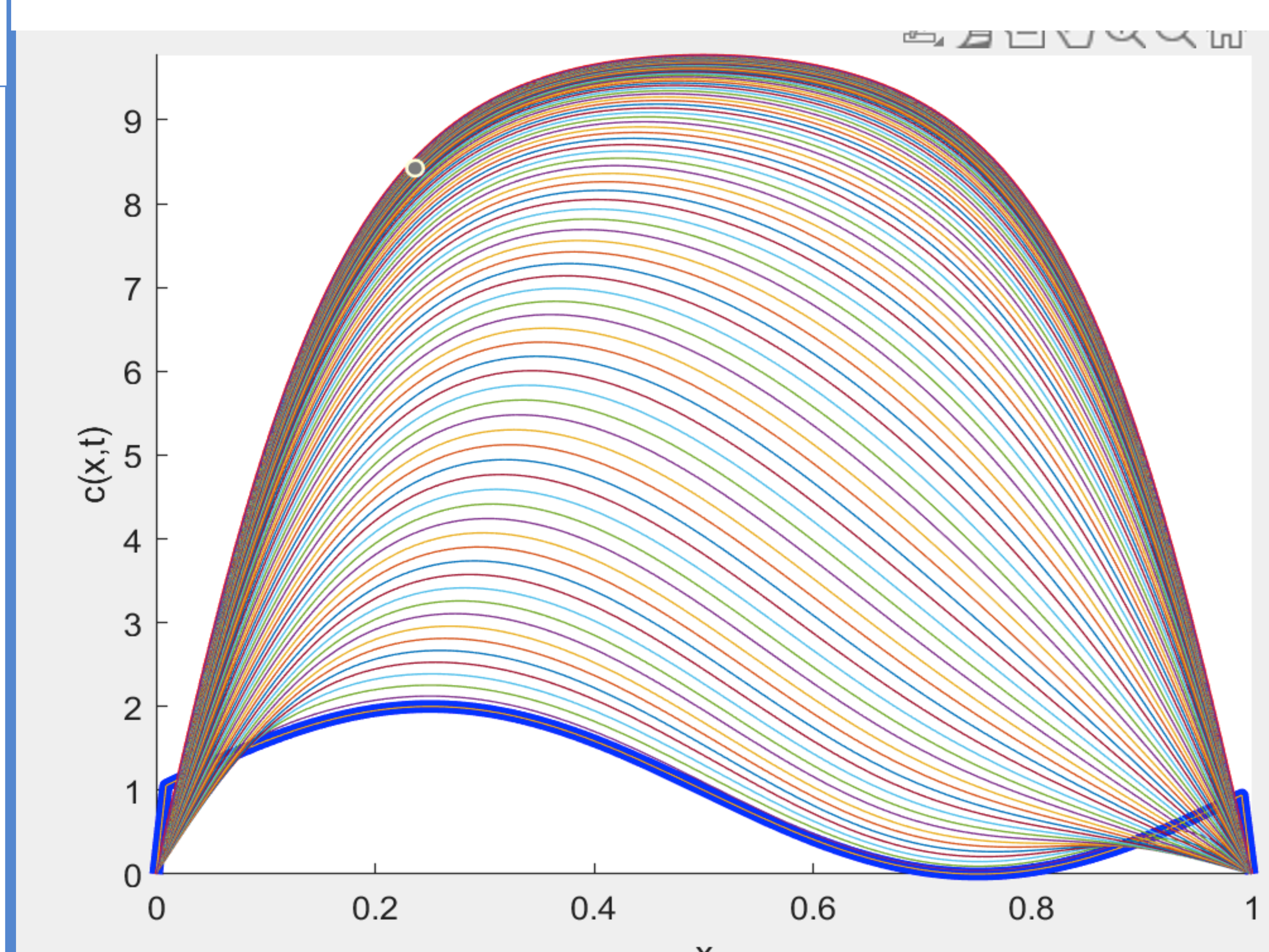


The figure above represents a section of the tube with diffusing bacteria.

Below is the Mat lab code we developed to numerically solve the reaction diffusion equation. It makes use of the Euler (Finite Difference) method. On the right is the final frame from the animation produced by the code. An initial concentration is shown in dark blue. Eventually the distribution takes an upside-down U shape.

```
numx = 111;
numt =  20000;
dx = 1/(numx - 1);
dt = 0.0000005;
dt/dx^2
x = 0:dx:1;
C = zeros(numx,numt);
t(1) = 0;
C(1,1) = 0;
C(1,numx) = 0;
mu = 0.5;
sigma = 0.05;
for i=2:numx-1
   C(i,1) = exp(-(x(i)-mu)^2/
(2*sigma^2)) / sqrt(2*pi*sigma^2);
end

for i=2:numx-1
   C(i,1) = 1+ 1*sin(x(i)*2*pi);
end
k=10; r = 100;
for j=1:numt
   t(j+1) = t(j) + dt;
   for i=2:numx-1
      C(i,j+1) = C(i,j) + 10*(dt/
dx^2)*(C(i+1,j) - 2*C(i,j) + C(i-1,j)) +
r*C(i,j)*(k - C(i,j))*dt;
   end
End
plotNum = 20000;
C(:,plotNum);
max(C(:,plotNum));
min(C(:,plotNum));
figure(1);
hold on;
plot(x,C(:,1),'b', 'LineWidth',4);
plot(x,C(:,plotNum),'r' ,'LineWidth',1);
xlabel('x');
ylabel('c(x,t)');
axis tight manual
set(gca,'nextplot','replacechildren');
V=VideoWriter('RD1.avi');
open(v);
for k = 1:200:plotNum
    hold on
    plot(x,C(:,k))
    frame = getframe(gcf);
    writeVideo(v,frame);
    M(k) = getframe;
end
```



Discussion And Conclusion

We were able to solve the reaction diffusion equation numerically and create an animation showing the concentration of bacteria over time. Regardless of the initial conditions we chose (dark blue curve), in the end, the bacteria concentration would take the form of an upside-down U shape. In the above figure L = 1 and most of the bacteria are concentrated between x=0.2 to x=0.8. This is due to the bacteria at the ends of the tube being killed by the antibiotics.

ACKNOWLEDGEMENTS

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