Project INF5631- Biological model for infection

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Biological model

In this project I will look at a diffusion equation which will describe how an infection can be spread in a society.
The model:

$$u_t = \nabla \cdot \alpha(u)\nabla u + f(u) \tag{1}$$

This equation consist of two parts that controls the behavior. I will do a study of them both, to see how they affect the equation.

Time derivative

The first part that I want to investigate, is the time derivate part:

$$u_t = f(u) \tag{2}$$

When we talk about the time derivative, we are interesting in how the change in time affect the concentration at a specific point. This time derivative part can consist of several functions, so I will make a general solution of it first.

$$\begin{aligned} u_t &= f(u) \\ \frac{u_i^n - u_i^{n-1}}{\Delta t} &= f(u_i^n) \\ u_i^n - \Delta t f(u_i^n) &= u_i^{n-1} \end{aligned}$$

This gives us a linear equation $Au = b$

A given function

$$f(u) = ru(1 - \frac{u}{m}) \tag{3}$$

Now we have a function for $f(u)$ where r and m are constants.The solution will then be.

$$\begin{aligned} u_i^n - \Delta t r u_i^n (1 - \frac{u_i^n}{m}) &= u_i^{n-1} \\ u_i^n (1 - \Delta t r (1 - \frac{u_i^n}{m})) &= u_i^{n-1} \end{aligned}$$

Since this equation gives us a nonlinear equation, we can use Picard to solve it. The idea with Picard is to replace the u on the right side with u_{-}. This is to get rid of the nonlinearity in this equation. u_{-} will in the first iteration be sat to value from the step before $u_{-}1$.

$$u_{-} = u^{n-1}$$

We can check the correct value u against our pre produced u_{-} each round. If the difference between them are less than what we demand, it continue. If not, the new u_{-} will be a combination of u_{-} and u. How we weight the combination is called relaxation

$$u_{-} = \alpha u + (1-\alpha)u_{-}, 0 <= \alpha <= 1$$

Our new equation will then be

$$u_i^n(1 - \Delta tr(1 - \frac{u_{-i}^{\ n}}{m})) = u_i^{n-1}$$

Since we are using an approximation to u, we need to refine u_{-} until it fulfil our expectations.

Spatial diffusion

In this part I will take a dive into the last fraction of our equation.

$$u_t = \nabla \cdot \alpha(u)\nabla u \tag{4}$$

This part consist of a function $\alpha(u)$, which the user defines. To solve this numerically, we need to discretize the equation.

$$\left[D_t^- u = D_x(\alpha(u)D_x u)\right]$$

I use Backward Euler for the time discrete and Crank Nicolson for the spatial discrete. Since we only use CN one time for α, we need to use arithmetic mean.

$$\alpha_{i\pm\frac{1}{2}} = \frac{1}{2}(\alpha_i + \alpha_{i\pm1})$$

This can be inserted in our equation under.

$$\begin{aligned}
\frac{u_i^n - u_i^{n-1}}{\Delta t} =& \frac{1}{\Delta x^2}\left(\alpha_{i+\frac{1}{2}}(u_{i+1} - u_i) - \alpha_{i-\frac{1}{2}}(u_i - u_{i-1})\right) \\
\frac{u_i^n - u_i^{n-1}}{\Delta t} =& \frac{1}{2\Delta x^2}\left((\alpha_{i+1} + \alpha_i)(u_{i+1} - u_i) - (\alpha_i - \alpha_{i-1})(u_i - u_{i-1})\right) \\
u_i^{n-1} =& u_i^n - \frac{\Delta t}{2\Delta x^2}\left((\alpha_{i+1} + \alpha_i)(u_{i+1} - u_i) - (\alpha_i - \alpha_{i-1})(u_i - u_{i-1})\right)
\end{aligned}$$

Then we are able to put this into $Au = b$, where b is the previous u.

$$A = \begin{pmatrix} A_{0,0} & A_{0,1} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ A_{1,0} & A_{1,1} & A_{1,2} & \ddots & & & & & \vdots \\ 0 & A_{2,1} & A_{2,2} & A_{2,3} & \ddots & & & & \vdots \\ \vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & 0 & A_{i,i-1} & A_{i,i} & A_{i,i+1} & \ddots & \vdots \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & & \ddots & \ddots & \ddots & A_{N_x-1,N_x} \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & A_{N_x,N_x-1} & A_{N_x,N_x} \end{pmatrix} \tag{14}$$

Our matrix A will then be tridiagonal with the values.

$$\begin{aligned} A_{i,i} =& 1 + \frac{\Delta t}{2\Delta x^2}(\alpha(u_{i+1}) + 2\alpha(u_i) + \alpha(u_{i-1})) \\ A_{i,i-1} =& -\frac{\Delta t}{2\Delta x^2}(\alpha(u_i) + \alpha(u_{i-1})) \\ A_{i,i+1} =& -\frac{\Delta t}{2\Delta x^2}(\alpha(u_{i+1}) + \alpha(u_i)) \end{aligned} \tag{5}$$

If we look at this matrix above,we can see that in the cases where we replace $\alpha(u)$ with a value defined by u, we will get a nonlinear equation.

Linear equation

The only solution if we want this to be linear, is to replace the function by a constant.

$$\alpha(u) = k \tag{6}$$

We can then use our matrix from(5) and insert the function. This gives us the matrix:

$$\begin{aligned} A_{i,i} =& 1 + \frac{\Delta t}{2\Delta x^2}(4k) = 1 + \frac{2k\Delta t}{\Delta x^2} \\ A_{i,i-1} =& -\frac{\Delta t}{2\Delta x^2}(2k) = -\frac{k\Delta t}{\Delta x^2} \\ A_{i,i+1} =& -\frac{\Delta t}{2\Delta x^2}(2k) = -\frac{k\Delta t}{\Delta x^2} \end{aligned}$$

Nonlinear equation

For all solutions that include u, we will get a nonlinear solution. There different techniques to handle them. I will try Picard as my first method.

Picard

Ordinary u

$$\alpha(u) = u \tag{7}$$

Then we can insert this in the matrix(5).

$$\begin{aligned}
A_{i,i} =& 1 + \frac{\Delta t}{2\Delta x^2}(u_{i+1} + 2u_i + u_{i-1}) \\
A_{i,i-1} =& -\frac{\Delta t}{2\Delta x^2}(u_i + u_{i-1}) \\
A_{i,i+1} =& -\frac{\Delta t}{2\Delta x^2}(u_{i+1} + u_i)
\end{aligned}$$

This gives also gives us a nonlinear problem, we can here replace u by u_- as explained in the section *Time Derivative*.

$$\begin{aligned}
A_{i,i} =& 1 + \frac{\Delta t}{2\Delta x^2}(u_{-i+1} + 2u_{-i} + u_{-i-1}) \\
A_{i,i-1} =& -\frac{\Delta t}{2\Delta x^2}(u_{-i} + u_{-i-1}) \\
A_{i,i+1} =& -\frac{\Delta t}{2\Delta x^2}(u_{-i+1} + u_{-i})
\end{aligned}$$

Spatial derivation wrapped with an absolute value

$$\alpha(u) = |\nabla(u)| \tag{8}$$

This gives us a little bit more complicated equation than the constant in our subsection over. We can also see that we will get a non linear equation. This I will handle with a Picard iteration.

$$\begin{aligned}
A_{i,i} =& 1 + \frac{\Delta t}{2\Delta x^2}(|\nabla(u_{i+1})| + 2|\nabla(u_i)| + |\nabla(u_{i-1})|) \\
A_{i,i-1} =& -\frac{\Delta t}{2\Delta x^2}(|\nabla(u_i)| + |\nabla(u_{i-1})|) \\
A_{i,i+1} =& -\frac{\Delta t}{2\Delta x^2}(|\nabla(u_{i+1})| + |\nabla(u_i)|)
\end{aligned}$$

As we can see here, demands this equation a lot more work. This will give us a nonlinear equation and we need to take care of the absolute value. I will discretize $|\nabla(u)|$, and insert this in our matrix above. Here we have three different options BW,FW or CN. I choose to use CN, and then use an arithmetic mean.

$$\begin{aligned}
|\nabla(u_i)| =& \left| \frac{u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}}{\Delta x} \right| \\
=& \frac{1}{2} \left| \frac{(u_{i+1} + u_i) - (u_i + u_{i-1})}{\Delta x} \right| \\
=& \frac{1}{2\Delta x} |u_{i+1} - u_{i-1}|
\end{aligned}$$

If we insert this, our equation will be

$$
\begin{aligned}
A_{i,i} =& 1 + \frac{\Delta t}{4\Delta x^3}(|u_{i+2} - u_i| + 2|u_{i+1} - u_{i-1}| + |u_i - u_{i-2}|) \\
A_{i,i-1} =& - \frac{\Delta t}{4\Delta x^3}(|u_{i+1} - u_{i-1}| + |u_i - u_{i-2}|) \\
A_{i,i+1} =& - \frac{\Delta t}{4\Delta x^3}(|u_{i+2} - u_i| + |u_{i+1} - u_{i-1}|)
\end{aligned}
$$

Since this will give us a nonlinear equation, we need to use Picard. The matrix will then be

$$
\begin{aligned}
A_{i,i} =& 1 + \frac{\Delta t}{4\Delta x^3}(|u_{-i+2} - u_{-i}| + 2|u_{-i+1} - u_{-i-1}| + |u_{-i} - u_{-i-2}|) \\
A_{i,i-1} =& - \frac{\Delta t}{4\Delta x^3}(|u_{-i+1} - u_{-i-1}| + |u_{-i} - u_{-i-2}|) \\
A_{i,i+1} =& - \frac{\Delta t}{4\Delta x^3}(|u_{-i+2} - u_{-i}| + |u_{-i+1} - u_{-i-1}|)
\end{aligned}
$$

Absolute value powered by m

$$
\alpha(u) = |\nabla(u)|^m \tag{9}
$$

Here I have tried to use the same technique as for the *Spatial derivation wrapped with an absolute value.* The values will be:

$$
\begin{aligned}
|\nabla(u_i)|^m =& \left| \frac{u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}}{\Delta x} \right|^m \\
=& \frac{1}{2} \left| \frac{(u_{i+1} + u_i) - (u_i + u_{i-1})}{\Delta x} \right|^m \\
=& \frac{1}{2\Delta x} |u_{i+1} - u_{i-1}|^m
\end{aligned}
$$

Then we just use Picard, and our matrix will be

$$
\begin{aligned}
A_{i,i} =& 1 + \frac{\Delta t}{4\Delta x^3}(|u_{-i+2} - u_{-i}|^m + 2|u_{-i+1} - u_{-i-1}|^m + |u_{-i} - u_{-i-2}|^m) \\
A_{i,i-1} =& - \frac{\Delta t}{4\Delta x^3}(|u_{-i+1} - u_{-i-1}|^m + |u_{-i} - u_{-i-2}|^m) \\
A_{i,i+1} =& - \frac{\Delta t}{4\Delta x^3}(|u_{-i+2} - u_{-i}|^m + |u_{-i+1} - u_{-i-1}|^m)
\end{aligned}
$$

Newton

Newtons method is another way to handle nonlinear equations.

$$
F(u) = 0 \tag{10}
$$

This method linearizes the equation by using Taylor series expansion around u_-. This only keeping only the linear part.

$$
\begin{aligned}
F(u) &= F(u_-) + F'(u_-)(u-u_-) + \frac{1}{2}F''(u_-)(u-u_-)^2 + \cdots \\
&\approx F(u_-) + F'(u_-)(u-u_-) = \hat{F}(u)
\end{aligned}
$$

The linear equation will be

$$
u = u_- - \frac{F(u_-)}{F'(u_-)} \tag{11}
$$

This method require a Jacobian matrix. This means that we need to differentiate $F(u) = A(u)u - b(u)$ for all the values of u. Our F will be

$$
F_i = A_{i,i-1}(u_{i-1},u_i)u_{i-1} + A_{i,i}(u_{i-1},u_i,u_{i+1})u_i + A_{i,i+1}(u_i,u_{i+1})u_{i+1} - b_i(u_i^{n-1})
$$

$$
\begin{aligned}
J_{i,i} =& \frac{\partial F_i}{\partial u_i} = \frac{\partial A_{i,i-1}}{\partial u_i}u_{i-1} + \frac{\partial A_{i,i}}{\partial u_i}u_i + A_{i,i} + \frac{\partial A_{i,i+1}}{\partial u_i}u_{i+1} - \frac{\partial b_i}{\partial u_i} \\
J_{i,i-1} =& \frac{\partial F_i}{\partial u_{i-1}} = \frac{\partial A_{i,i-1}}{\partial u_{i-1}}u_{i-1} + A_{i,i-1} + \frac{\partial A_{i,i}}{\partial u_{i-1}}u_i - \frac{\partial b_i}{\partial u_{i-1}} \\
J_{i,i+1} =& \frac{\partial F_i}{\partial u_{i+1}} = \frac{\partial A_{i,i}}{\partial u_{i+1}}u_i + \frac{\partial A_{i,i+1}}{\partial u_{i+1}}u_{i+1} + A_{i,i+1} - \frac{\partial b_i}{\partial u_{i+1}}
\end{aligned}
$$

Since this demands a lot of calculating, I will show how to do it for the first $J_{i,i}$. I calculate each subsection in one line

$$
\begin{aligned}
\frac{\partial A_{i,i-1}}{\partial u_i}u_{i-1} =& -\frac{\Delta t}{2\Delta x^2}(\alpha'(u_i)u_{i-1}) \\
\frac{\partial A_{i,i}}{\partial u_i}u_i =& \frac{\Delta t}{2\Delta x^2}(2\alpha'(u_i)u_i) \\
A_{i,i} =& 1 + \frac{\Delta t}{2\Delta x^2}(\alpha(u_{i+1}) + 2\alpha(u_i) + \alpha(u_{i-1})) \\
\frac{\partial A_{i,i+1}}{\partial u_i}u_{i+1} =& -\frac{\Delta t}{\Delta x^2}(\alpha'(u_i)u_{i+1}) \\
-\frac{\partial b_i}{\partial u_i} =& -b'(u_i)
\end{aligned}
$$

This gives us the matrix

$$
\begin{aligned}
J_{i,i} =& -\frac{\Delta t}{2\Delta x^2}(\alpha'(u_i)u_{i-1}) + \frac{\Delta t}{2\Delta x^2}(2\alpha'(u_i)u_i) \\
&+1 + \frac{\Delta t}{2\Delta x^2}(\alpha(u_{i+1}) + 2\alpha(u_i) + \alpha(u_{i-1})) - \frac{\Delta t}{2\Delta x^2}(\alpha'(u_i)u_{i+1}) - b'(u_i) \\
J_{i,i-1} =& -\frac{\Delta t}{2\Delta x^2}(\alpha'(u_{i-1})u_{i-1}) - \frac{\Delta t}{2\Delta x^2}(\alpha(u_{i-1}) + \alpha(u_i)) + \frac{\Delta t}{2\Delta x^2}(\alpha'(u_{i-1})u_i) \\
J_{i,i+1} =& \frac{\Delta t}{2\Delta x^2}(\alpha'(u_{i+1})u_i) - \frac{\Delta t}{2\Delta x^2}(\alpha'(u_{i+1})u_{i+1}) - \frac{\Delta t}{2\Delta x^2}(\alpha(u_i) + \alpha(u_{i+1}))
\end{aligned}
$$

This matrix can be used to compute the Newton's method. We just need to replace $\alpha(u)$ by the function.

Ordinary u

Spatial derivation...

Spatial derviation power by m

Solution for the biological equation