Fundamentals of Numerical Thermo-Fluid Dynamics
322.061
Team Project

Numerical Modelling of Zombie epidemy

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Mathematical formulation

Our aim is to model an outbreak of zombie epidemy. In particular, we want to resolve the spatio-temporal evolution of the population of humans and zombies to investigate the ability of humans to survive. Following the arguments of Woolley et. al. [1], we formulate the mathematical problem with the transport equations of two reacting species - humans (H) and zombies (Z):

$$\frac{\partial H}{\partial t} = D_H \triangle H - \vec{v} \cdot (\vec{\nabla} H) - H(\vec{\nabla} \cdot \vec{v}) - \alpha H Z \qquad \text{on } \Omega \tag{1}$$

$$\frac{\partial Z}{\partial t} = D_Z \triangle Z + \beta H Z \qquad \text{on } \Omega \tag{2}$$

$$\frac{\partial H}{\partial \vec{n}} = 0 \qquad \text{on } \partial\Omega \tag{3}$$

$$\frac{\partial Z}{\partial \vec{n}} = 0 \qquad \text{on } \partial\Omega \tag{4}$$

where the *diffusive* terms $D_H \triangle H$, $D_Z \triangle Z$ model the chaotic, disorganized motion of individuals, the *convective* terms $-\vec{v} \cdot (\vec{\nabla} H) - H(\vec{\nabla} \cdot \vec{v})$ model the collective migration and the *reaction* terms $-\alpha HZ$, βHZ represent the interaction between the two species. Adopting the reasoning of Woolley et. al. [1] we use the following assumptions:

- Humans are more organized than zombies, and the diffusivity of zombies is therefore higher than that of humans. We neglect the variation of diffusivity of both species in space and time.
- We assume that zombies suffer a significant decay of intellect and thus they move completely randomly without any collective migration. There is therefore no convective term in the transport equation for zombies (2).
- We neglect the diffusive flux of humans and zombies through domain boundaries $\partial\Omega$ by imposing homogeneous Neumann conditions (3, 4). Although such conditions do not hold in general, it allows us to investigate the interaction of the species in an isolated environment.

The coupling terms $-\alpha HZ$ and βHZ represent interaction between Humans and Zombies. The interaction is modelled as a system of chemical reactions where the speed of reaction is proportional to the product of reactants. We consider the same interaction as Wooley et. al [1], i.e.:

- $H + Z \xrightarrow{a} H$ (humans kill zombies at the average rate a)
- $H + Z \xrightarrow{b} Z$ (zombies kill humans at the average rate b)
- $H + Z \xrightarrow{c} Z + Z$ (zombies infect humans by biting or scratching at the average rate c)

which defines the net removal rate of humans $\alpha = b + c$ and the net creation rate of zombies $\beta = c - a$. For the estimate of these parameters we further assume that

- The time-scale of the epidemy is so short that the natality of humans is negligible.

- The deadliness of zombies b is higher than that of humans a.
- Humans can run faster than zombies, so they can survive the interaction. However, there is a high likelihood that zombie injures human by biting or scratching before the human manages to escape. The injury then leads to infection and subsequent zombification. The infectiousness of zombies c is therefore similar to the deadliness of zombies.
- There exists a **safety zone** where humans collect all available vapons. Inside this safety zone the deadliness of humans is higher than the infectiousness and deadliness of zombies.

1 Classification of the problem

Assuming only one spatial coordinate x and a constant migration velocity $v =$ const., convert the problem into an equivalent system of first order equations. Show that this system is parabolic

[5 Points]

2 Discretization

2.1 Discretize equation (1a) with Crank-Nicholson method in time and second-order centered finite differences in one spatial dimension on a grid with uniform spacing Δx. Assume that $v, div(v), \alpha, \beta$ are known values at every grid point. Using von Neumann stability analysis, show that the local amplification factor of the dicretization is given by

$$G_H = \frac{1 - \frac{\Delta t D_H}{\Delta x^2}(1 - \cos\theta) - \frac{\Delta t\ v}{2\Delta x} i \sin\theta - div(v) - \alpha Z^n}{1 + \frac{\Delta t D_H}{\Delta x^2}(1 - cos\theta) + \frac{\Delta t\ v}{2\Delta x} i \sin\theta + div(v) + \alpha Z^{n+1}} \quad (5)$$

[3 Points]

2.2 Compute the order of accuracy of this discretization in space and time using Taylor expansion. Does the spatial discretization create artificial diffusivity?

[2 Points]

2.3 Discretize the system (1a, 1b) with the same methods, now assuming a two-dimensional Cartesian grid of $I \times J$ nodes with uniform spacings $\Delta y, \Delta x$. The position of a grid node is described by two indices i, j such that

$$\phi_{i,j} := \phi(x_i, y_j) \quad \text{for } i = 1 \dots I,\ j = 1 \dots J$$

where

$$x_i := x_0 + (j-1)\Delta x \quad \text{and} \quad y_i := y_N - (i-1)\Delta y$$

[4 Points]

2.4 Define a mapping from two-index notation to single-index notation

$$u_{i,j} \rightarrow u_k \quad \text{for } k = 1 \dots K \equiv I\ J$$

such that the discrete problem is written in single-index notation as

$$
\begin{aligned}
H_k^{n+1} - \frac{\Delta t}{2} \Bigg(& D_H \left(\frac{H_{k+I}^{n+1} - 2H_k^{n+1} + H_{k-I}^{n+1}}{\Delta x^2} + \frac{H_{k+1}^{n+1} - 2H_k^{n+1} + H_{k-1}^{n+1}}{\Delta y^2} \right) \\
& - v_k^x \frac{H_{k+I}^{n+1} - H_{k-I}^{n+1}}{2\Delta x} - v_k^y \frac{H_{k-1}^{n+1} - H_{k+1}^{n+1}}{2\Delta y} \\
& - div(v)_k H_k^{n+1} - \alpha_k H_k^{n+1} Z_k^{n+1} \Bigg) \\
= H_k^n + \frac{\Delta t}{2} \Bigg(& D_H \left(\frac{H_{k+I}^{n} - 2H_k^{n} + H_{k-I}^{n}}{\Delta x^2} + \frac{H_{k+1}^{n} - 2H_k^{n} + H_{k-1}^{n}}{\Delta y^2} \right) \\
& - v_k^x \frac{H_{k+I}^{n} - H_{k-I}^{n}}{2\Delta x} - v_k^y \frac{H_{k-1}^{n} - H_{k+1}^{n}}{2\Delta y} \\
& - div(v)_k H_k^{n} - \alpha_k H_k^{n} Z_k^{n} \Bigg)
\end{aligned}
\tag{6}
$$

$$
\begin{aligned}
Z_k^{n+1} - \frac{\Delta t}{2} \Bigg(& D_Z \left(\frac{Z_{k+I}^{n+1} - 2Z_k^{n+1} + Z_{k-I}^{n+1}}{\Delta x^2} + \frac{Z_{k+1}^{n+1} - 2Z_k^{n+1} + Z_{k-1}^{n+1}}{\Delta y^2} \right) \\
& + \beta_k H_k^{n+1} Z_k^{n+1} \Bigg) \\
= Z_k^n + \frac{\Delta t}{2} \Bigg(& D_Z \left(\frac{Z_{k+I}^{n} - 2Z_k^{n} + Z_{k-I}^{n}}{\Delta x^2} + \frac{Z_{k+1}^{n} - 2Z_k^{n} + Z_{k-1}^{n}}{\Delta y^2} \right) \\
& + \beta_k H_k^{n} Z_k^{n} \Bigg)
\end{aligned}
\tag{7}
$$

[1 Point]

3 Implementation

3.1 Write a MatLab function to create discretization matrices $\mathbf{D}_{x1}, \mathbf{D}_{y1}$ approximating first derivatives, and $\mathbf{D}_{x2}, \mathbf{D}_{y2}$ approximating second derivatives of a discrete function ϕ_k with second order centered finite differences. Apply the ghost-point method to enforce the homogeneous Neumann boundary conditions (3, 4) and to approximate the second normal derivatives on boundary nodes. Use the template `FDMatrices.m`.

[5 Points]

3.2 The discretized equations (6, 7) can be written in matrix-vector form as

$$\mathbf{A}_{HH} \cdot \vec{H^{n+1}} + \mathbf{A}_{HZ} \cdot \vec{Z^{n+1}} = \mathbf{B}_{HH} \cdot \vec{H^n} + \mathbf{B}_{HZ} \cdot \vec{Z^n} \tag{8}$$

$$\mathbf{A}_{ZZ} \cdot \vec{Z^{n+1}} + \mathbf{A}_{ZH} \cdot \vec{Z^{n+1}} = \mathbf{B}_{ZZ} \cdot \vec{Z^n} + \mathbf{B}_{ZH} \cdot \vec{H^n} \tag{9}$$

Each matrix ($\mathbf{A_{HH}}, \mathbf{A_{HZ}}, \mathbf{B_{HH}}, \mathbf{B_{HZ}}$, ...) can be written in terms of an identity matrix **Id**, the solution vectors $\vec{H^n}, \vec{Z^n}, \vec{H^{n+1}}, \vec{Z^{n+1}}$, the discretization matrices $\mathbf{D}_{x1}, \mathbf{D}_{y1}, \mathbf{D}_{x2}, \mathbf{D}_{y2}$ and the parameters of the problem. For example,

$$\mathbf{A}_{HH} := \mathbf{I} - \frac{\Delta t}{2}\Big(D_H\left(\mathbf{D}_{x2} + \mathbf{D}_{y2}\right) - \vec{v_x} \odot \mathbf{D}_{x1} - \vec{v_y} \odot \mathbf{D}_{y1} - \vec{div}(v) \odot \mathbf{Id}\Big)$$

$$\mathbf{A}_{HZ}(\vec{H^{n+1}}) := \frac{\Delta t}{2}\alpha \odot \vec{H^{n+1}} \odot \mathbf{Id}$$

where $\odot$ is the element-wise product (`.*` in MatLab). Express the matrices $\mathbf{A_{ZZ}}, \mathbf{A_{ZH}}, \mathbf{B_{HH}}, \mathbf{B_{HZ}}, \mathbf{B_{ZZ}}, \mathbf{B_{ZH}}$ in the same way.

[2 Points]

3.3 Since our mathematical formulation is a system of equations, let us define a global solution vector by appending our vectors of unknowns one after the other

$$\vec{U} := \begin{pmatrix} \vec{H} \\ \vec{Z} \end{pmatrix}$$

One can then express the discrete problem (6, 7) as

$$\mathbf{M}_1(\vec{U^{n+1}}) \cdot \vec{U^{n+1}} = \mathbf{M}_2(\vec{U^n}) \cdot \vec{U^n} \tag{10}$$

where

$$\mathbf{M}_1(\vec{U^{n+1}}) := \begin{pmatrix} \mathbf{A_{HH}} & \mathbf{A_{HZ}}(\vec{H^{n+1}}) \\ \mathbf{A_{ZH}}(\vec{Z^{n+1}}) & \mathbf{A_{ZZ}} \end{pmatrix}$$

$$\mathbf{M}_2(\vec{U^n}) := \begin{pmatrix} \mathbf{B_{HH}} & \mathbf{B_{HZ}}(\vec{H^n}) \\ \mathbf{B_{ZH}}(\vec{Z^n}) & \mathbf{B_{ZZ}} \end{pmatrix} \tag{11}$$

Write two MatLab functions, one to compute the matrix $\mathbf{M}_2$ from the known solution $\vec{U^n}$, and the other to compute the matrix $\mathbf{M}_1$ from some estimate of $\vec{U^{n+1}}$. Use the templates `DiscreteRHS.m, DiscreteLHS.m`.

[3 Points]

4 Newton-Raphson iteration

4.1 We choose to solve the non-linear problem (10) with Newton-Raphson method. We define a non-linear function

$$\vec{F}(\vec{V}) := \mathbf{M_1}\vec{V} - \mathbf{M_2}\vec{U^n} \stackrel{!}{=} 0 \tag{12}$$

where

$$\vec{V} := \vec{U^{n+1}}$$

One iteration of the Newton algorithm is then given by

$$\vec{V^{m+1}} = \vec{V^m} - \mathbf{J}^{-1}(\vec{V^m}) \cdot \vec{F^m}(\vec{V^m}) \tag{13}$$

where $\mathbf{J}$ is the Jacobian matrix of the function $\vec{F}(\vec{V})$

$$J_{i,j} := \frac{\partial F_i}{\partial V_j}$$

Implement a code to compute the Jacobian matrix using the template `ComputeJac.m`.

[5 Points]

4.2 Implement the Newton algorithm in the template function `Newton.m`.

[5 Points]

4.3 Run the script `epidemy.m` to check your implementation. How much time do you have to reach the safety zone before zombies spread over the rest of the domain (i.e. there is more than 1 zombie per km^2 everywhere except the neighbourhood of the safety zone)? Vary the parameters of the problem and describe which of them mostly affect the ability of humans to survive. You may define the ability to survive as the time after which the maximum concentration of humans drops below a certain threshold.

[5 Points]

5 Bonus

5.1 Note that the code at every time-step re-computes some matrices which are not changing if the migration velocity and diffusivity are constant in time. Optimize the code to only re-compute matrices which depend on the solution and measure the time savings per time step. You might want to increase the number of grid points and skip plotting of graphs to see the effect.

[0 Points]

5.2 The code becomes unstable when the reaction term forces the density of human population to negative values. The time step Δt must then be decreased, although the von Neumann's growth factor G is in the stable region. Try to adjust the Newton-Raphson algorithm such that it does not force populations to negative values.

[0 Points]

5.3 Compute the total number of humans and zombies in the domain by numerical integration and plot the evolution of the system in a phase-space of these two parameters. Implement a criterion to stop the time-stepping loop if one of the populations dies out.

[0 Points]

5.4 Compute the von Neumann growth rate (5) at every P-th time step to check that the discretization is in stable region. Use some educated guess for P.

6 References

[1] T.E. Woolley, R.E. Baker, E.A. Gaffney, P.K. Maini, How long can we survive? In Mathematical Modelling of Zombies, ed R. Smith?, University of Ottawa Press, 93-115 (2014).
URL: https://people.maths.ox.ac.uk/maini/PKM%20publications/384.pdf