School of Natural Sciences
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MATH 132: Numerical Analysis II
Final Project—Spring 2020
Due Friday, May 13, 2022 on Catcourses

Modeling biological patterns

Figure 1: Skin patterns of the giant pufferfish (Tetraodon mbu)

We are interested in modeling the biological patterns such as the spots found on leopard and giraffe, the stripes on tiger and zebra or the intricated ones on the giant pufferfish (see figure 1). To do so we consider the class of coupled PDE systems

$$\frac{\partial u}{\partial t} = D\triangle u + f(u, v, x, y) \qquad \forall x \in \Omega \tag{1}$$

$$\frac{\partial v}{\partial t} = D\triangle v + g(u, v, x, y) \qquad \forall x \in \Omega \tag{2}$$

where u and v are the concentration of two chemical species responsible for the animal skin pigmentation. The domain Ω is $(0, 1) \times (0, 1)$. D is the diffusivity of the chemicals. The non linear functions f and g represent the chemical reaction between u and v. The initial concentration profiles $u(x, y, 0)$ and $v(x, y, 0)$ are known. Both solutions are assumed to be periodic in both direction:

$$u(x+1, y, t) = u(x, y, t), \qquad u(x, y+1, t) = u(x, y, t), \tag{3}$$

$$v(x+1, y, t) = v(x, y, t), \qquad v(x, y+1, t) = v(x, y, t). \tag{4}$$

The Laplacian operator Δ is defined as $\Delta u = \nabla \cdot \nabla u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$. We would like to approximate the solution using the semi-implicit scheme:

$$\frac{U^{n+1} - U^n}{\Delta t} = DAU^{n+1} + F(U^n, V^n) \tag{5}$$

$$\frac{V^{n+1} - V^n}{\Delta t} = DAV^{n+1} + G(U^n, V^n) \tag{6}$$

where A is the discrete Laplacian operator constructed using the standard five points scheme, and uniform spatial resolution $\Delta x = \frac{1}{N-1}$ in both direction

1. Justify why the diffusive term is treated implicitly.
2. What are the advantages and disadvantages of treating the non-linear reactive term explicitly?
3. Define the local truncation error and prove that it is $\mathcal{O}(\Delta t + \Delta x^2)$.
4. In this question we would like to construct and verify the implementation of the discrete Laplacian operator. To do so we consider the test problem

   $$u - \triangle u = \sin^2(\pi x)\sin^2(\pi y) - 2\pi^2[\cos(2\pi x)\sin^2(\pi y) + \sin^2(\pi x)\cos(2\pi y)] \qquad \forall x \in \Omega \tag{7}$$

   with periodic boundary conditions.

   (a) What is the corresponding linear system the numerical solution U is the solution of ? Write it in terms of the matrix A.

   (b) Verify that
   $$u_{\text{true}}(x, y) = \sin^2(\pi x)\sin^2(\pi y). \tag{8}$$
   is the exact solution of the above test problem (hint: two things should be verified .....)

   (c) Write a Matlab function that take the grid resolution N as an input and return the corresponding discrete laplacian operator A for peridodic conditions.

   (d) Print your matrix for N=5. Does it look right ?

   (e) Compute the numerical solution of the test problem for N=5,10,20, and compute the corresponding errors. Is your implementation correct?

5. Reformulate the above semi-implicit method in the form

   $$MU^{n+1} = R_u(U^n, V^n) \tag{9}$$
   $$MV^{n+1} = R_v(U^n, V^n), \tag{10}$$

   and explicit what the matrix M and vectors R_u and R_u are.

6. In this question we would like to study the stability and convergence of the numerical method. We start by considering the linear problem with $f(u, v) = g(u, v) = 0$.

   (a) Why are we interested in the linear problem?

   (b) What are the vectors R_u and R_v in this case? Is the system decoupled in this case?

   (c) Prove that the eigenvalues of M are greater than 1 (in absolute value) and that the method is unconditionally stable for the linear problem.

   (d) Write a Matlab function that takes N, D and Δt as input and return the matrix M using the function from question 4).

   (e) Compute (and show) the eigenvalues of the matrix M for a a few values of N and D and verify that they are greater than 1 (in absolute value).

7. Estimate the stability condition for the full non-linear problem in terms of the derivative of $\frac{\partial f}{\partial U}, \frac{\partial f}{\partial V}$ and $\frac{\partial g}{\partial U}, \frac{\partial g}{\partial V}$.

8. Implement a Matlab function that solve the system 5, 6, for any given $t_0, t_f, \Delta t, N, f, g, D$.

9. For this final question, we define the function f and g as

$$
\begin{aligned}
f(u,v) &= -uv^2 + F(1-u), \qquad (11)\\
g(u,v) &= uv^2 - (F+k)v, \qquad (12)
\end{aligned}
$$

where F and k are two constant parameters. For this choice of functions, the coupled system of PDE is known as the Gray-Scott model. We set $D = 10^{-5}$.

(a) Take $F = 0.09$ and $k = 0.059$, run your code for uniform, random and localized initial conditions and plot your results (your figures must be included in the report).

(b) Using any available ressources (such as https://mrob.com/pub/comp/xmorphia/ or https://itp.uni-frankfurt.de/ gros/StudentProjects/Projects_2020/projekt_schulz_kaefer/) estimate what parameters F and k produce a pattern similar to the one on the giant pufferfish (see figure 1). Run your code for that set of parameter and plot your results.

(c) (**extra credit**) Pick your own F and f, simulate the system and make a video of the evolution of either concentration.