446-2 Numerical Solution of Partial Differential Equations

Spring 2007

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Problem Set 6, May 19, 2007 due Monday June 4, 2007

Directional Sensing in Chemotaxis

Use Chebyshev polynomials to simulate the one-dimensional version of a model by Levine, Kessler, and Rappel for the directional sensing in amoeba (see also lecture notes). The model consists of a diffusing inhibitor

$$\frac{\partial B}{\partial t} = D\frac{\partial^2 B}{\partial x^2} \qquad \text{inside the cell } -1 < x < +1,$$

which is generated at the cell wall in proportion to the chemical S that is to be sensed,

$$D\frac{\partial B}{\partial n} = k_a S - k_b B.$$

Here $\partial/\partial n$ is the outward normal derivative. In a one-dimensional system its sign is opposite on the two sides of the system, $\partial/\partial n = -\partial/\partial x$ at $x = -1$ whereas $\partial/\partial n = +\partial/\partial x$ at $x = +1$. The reactions of the activator A, which is confined to the cell membrane, and of the membrane-bound fraction B_m of the inhibitor are given by

$$\begin{aligned} \frac{dA}{dt} &= k_a S - k_{-a} A - k_i A B_m \\ \frac{dB_m}{dt} &= k_b B - k_{-b} B_m - k_i A B_m. \end{aligned}$$

Use the semi-implicit Crank-Nicholson scheme (see notes) to solve these equations. Implement it with a variable factor α that allows you to switch easily between Crank-Nicholson and backward and forward Euler.

1. Validate your implementation of the diffusion equation with its boundary condition:
   (a) Choosing k_a and k_b equal and large you can fix the value of B at the boundary to be equal to S. Use an initial condition that allows you to solve the diffusion equation with this boundary condition exactly. Check the code by comparing the decay time of the numerical solution with that of the analytical solution.
   (b) Choose $k_b = 0$ to validate the normal derivative part of your implementation by comparing with a suitable exact stationary solution.
   (c) For $k_i = 0$ the stationary solutions for A and B_m are easy to read off. Check your numerical result against that analytical result.
   (d) For $k_i \neq 0$ but with $S(x = -1) = S(x = +1)$ - implying $B = B(t)$ independent of space - the stationary solution for A and B_m can easily determined. Check your code against that result.
2. Determine the stability limits of the forward Euler version of the code as a function of the number of Chebyshev modes. Does it agree with your expectations?
3. Perform a convergence test of the Crank-Nicholson version of the code to check the order of the implementation of the time-stepping.
4. Measure the dependence of the model's ability to sense small differences in the concentration of S at the front and the back of the cell ($x = \mp 1$) on the strength of the coupling coefficient k_i. Use the same parameter values as in Fig.1 of the original paper, except for fixing $p = 0.1$ and increasing k_i from $k_i = 0$ to $k_i = 1,000$ in suitable steps and use a sufficiently large t_{max} to ensure that the system has converged to a fixed point. Plot the final value of the ratio $A(x = -1)/A(x = +1)$ as a function of k_i.