Problem Set 3

Due Wednesday, March 20th

March 2, 2019

1 Solving a Semilinear Heat Equation

Use the Method of Lines (MOL) with a finite difference discretization to solve the 2D Brusselator equation:

$$\frac{\partial u}{\partial t} = 1 + u^2 v - 4.4u + \alpha \Delta u + f(x, y, t)$$
$$\frac{\partial v}{\partial t} = 3.4u - u^2 v + \alpha \Delta v$$

with $\Delta x = \Delta y = \frac{1}{32}$,

$$f(x, y, t) = \begin{cases} 5 & (x - 0.3)^2 + (y - 0.6)^2 \leq 0.1^2 \ \ \& \ \ t \geq 1.1 \\ 0 & o.w. \end{cases}$$

initial conditions

$$u(x, 0) = 22y(1 - y)^{\frac{3}{2}}$$
$$v(x, 0) = 27x(1 - x)^{\frac{3}{2}}$$

with periodic boundary conditions

$$u(x, t) = u(x + 1, t)$$
$$u(y, t) = u(y + 1, t)$$
$$v(x, t) = v(x + 1, t)$$
$$v(y, t) = v(y + 1, t)$$

and parameters

$$A = 3.4$$
$$B = 1.0$$
$$\alpha = 10.0$$

over a timespan of $[0, 22.0]$. Plot the time course of the solution of u and v at $x = y = \frac{1}{4}$, along with a 2D surface plot of u and v.

Hints: it's highly suggested that you use a stiff ODE solver with a Newton-Krylov method. CVODE_BDF(linear_solver=:GMRES) is a good choice. Additionally, it will not be viable to save the full PDE's time course. Instead, use save_everystep=false and use a tool like the SavingCallback from DiffEqCallbacks.jl to more selectively save the time series.

2 Derivation of dempened diffusion

When we put a strong acid, such as hydrochloric acid (HCl), into water, it does two things. First, it diffuses into the water, becoming more and more evenly distributed. Second, it *dissociates* by ionizing (releasing a proton, e.g. HCl becomes Cl– plus a proton that attaches to nearby water molecules) and releasing heat. If the concentration of the acid is$u(x,t)$, the rate of dissociation is (to a first approximation, for low concentrations) proportional to$u$.

In this problem, you will be deriving the PDE describing this process by starting with a discrete system, applying the fact that a diffusion equation results from any microscopic picture in which the flow of solute is proportional to the gradient or difference in solute concentration ("Fick's law"), and taking the continuum limit.

1. Consider the case of HCl diffusing in water within a narrow straw of length L, which we will approximate as a one-dimensional system. Imagine dividing the straw into$M$ small pieces of lengthΔx, and call the mass of HCl in the m-th piece $u_m \Delta x$ for $m = 1, \ldots, M$, where u_m is a concentration (mass per Δx). Suppose that the rate at which mass flows from one piece to the next is proportional to the difference in concentrations (u_m), and is inversely proportional to the distance to the mass must travel (Δx), so that the *mass per unit time* flowing from $m+1$ to m is given by:

$$D\frac{u_{m+1} - u_m}{\Delta x}$$

   for some constant *diffusion coefficient* D. In addition to the HCl flowing out of each piece, the acid is also dissociating (the mass $u_m \Delta x$ of acid is decreasing) at a rate $R u_m \Delta x$ for some "rate" constant$R > 0$. Derive an equation for the net rate of change du_m/dt of the concentration in piece m. Take the limit $\Delta x \to 0$ and find a PDE for $u(x)$, where $u(m\Delta x) = u_m$; you should get a diffusion equation in the limit $R \to 0$. Don't worry about the boundary conditions; just look at the interior $1 < m < M$.

2. Suppose that any HCl that reaches the ends of the straw is immediately removed (there is a little HCl-eating demon sitting at each end of the straw). What boundary condition on u_0 and u_{M+1} does that imply in the discrete model? What boundary condition on $u(x)$ in the continuum limit?

3. Suppose that we seal the ends of the straw, so that no HCl can enter or leave through the ends. Write down a boundary condition on u_0 and u_{M+1}

that reflects this situation in the discrete model, write the corresponding matrix A in the discrete system ($d\vec{u}/dt = A\vec{u}$), and write the corresponding boundary condition on $u(x)$ in the continuum limit.

4. For the two continuum-limit cases in your previous parts (b and c), show that the resulting PDE operator $\hat{A}$ is Hermitian and negative-definite; what do you conclude about the solutions of $\frac{\partial u}{\partial t} = \hat{A}u$ as $t \to \infty$? What changes if you let $R = 0$?

5. How does the PDE from part (a) change if $D(x)$ and $R(x)$ are (real, positive) functions of x? In the discrete approximation, use $D_{m+0.5}\frac{u_{m+1}-u_m}{\Delta x}$ and $R_m u_m \Delta x$ terms, where $D_{m+0.5} = D([m+0.5]\Delta x)$ and $R_m = R(m\Delta x)$.