18.303 Problem Set 3

Due Wednesday, 25 September 2013.

Problem 1: Damping 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 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.

(a) 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 length Δx, 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 show that you obtain a diffusion equation for $u(x)$, where $u(m\Delta x) = u_m$. Don't worry about the boundary conditions; just look at the interior $1 < m < M$.

(b) 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?

(c) Suppose that we seal the ends of the straw, so that no salt 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 ($d\mathbf{u}/dt = A\mathbf{u}$), and write the corresponding boundary condition on $u(x)$ in the continuum limit.

(d) 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 $\frac{\partial u}{\partial t} = \hat{A}u$? What changes if you let $R = 0$?

Problem 2: Early curly

Consider the space of three-component vector fields $\mathbf{u}(\mathbf{x})$ on some finite-volume 3d domain $\Omega \subset \mathbb{R}^3$. One linear operator on these fields is the curl $\nabla\times$, which is important in electromagnetism (which we will study in more detail later in 18.303). Define the inner product of two vector fields $\mathbf{u}$ and $\mathbf{v}$ by the volume integral $\langle \mathbf{u}, \mathbf{v} \rangle = \int_\Omega \bar{\mathbf{u}} \cdot \mathbf{v}$.

(a) An 18.02 exercise: derive the identity $\nabla \cdot (\mathbf{u} \times \mathbf{v}) = (\nabla \times \mathbf{u}) \cdot \mathbf{v} - \mathbf{u} \cdot (\nabla \times \mathbf{v})$.

(b) Figure out how to do integration by parts with the curl: show that $\langle \mathbf{u}, \nabla \times \mathbf{v} \rangle = \langle \nabla \times \mathbf{u}, \mathbf{v} \rangle + \oiint_{\partial\Omega} \mathbf{w} \cdot d\mathbf{S}$, where $d\mathbf{S}$ is the usual outward surface-normal area element, and the $\mathbf{w}$ appearing in the surface integral over the boundary ($\partial\Omega$) is some vector field to be determined. (*Hint:* use the identity you derived in the previous part, combined with the divergence theorem.)

(c) Give a possible boundary condition on our space of vector fields such that $\nabla\times$ is self-adjoint with this inner product. (Boundary conditions can only involve one vector field at a time! No fair giving an equation that relates $\mathbf{u}$ to $\mathbf{v}$!) You should *not* have to specify *all* the components of $\mathbf{u}$ on the boundary. It may be convenient to define a vector field $\mathbf{n}(\mathbf{x})$ on $\partial\Omega$ to denote the outward normal vector at each point on the boundary.[1]

(d) Show that $\nabla \times \nabla \times$ is self-adjoint for this inner product under *either* some boundary condition on $\mathbf{u}$ (similar to above) or some boundary condition on *derivatives* of $\mathbf{u}$. Is it positive or negative definite or semidefinite?

(e) Two of Maxwell's equations in vacuum are $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$ and $\nabla \times \mathbf{B} = \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}$ where c is the speed of light. Take the curl of both sides of the second equation to obtain a PDE in $\mathbf{E}$ alone. Suppose that Ω is the interior of a hollow metal container, where the boundary conditions are that $\mathbf{E}$ is perpendicular to the metal at the surface (i.e. $\mathbf{E} \times \mathbf{n}|_{\partial\Omega} = 0$).[2] Combining these facts with the previous parts, explain why you would expect to obtain *oscillating* solutions to Maxwell's equations (*standing electromagnetic waves*, essentially light bouncing around inside the container).

(This kind of system exists, for example, in the microwave regime where metals have high conductivity, and such containers are called *microwave resonant cavities*.)

---

[1]Technically, we are assuming here that the boundary is a differentiable surface so that the normal vector is well defined. Actually, it is sufficient to assume that it is differentiable except for isolated corners and edges (a "set of measure zero") since those isolated kinks won't contribute anything to the $\oiint_{\partial\Omega}$ surface integral.

[2]In a perfect conductor, any nonzero component of $\mathbf{E}$ parallel to the surface would generate an infinite current parallel to the surface, in which charges instantaneously rearrang to cancel the field. For a real conductor with finite conductivity, matters are more complicated because we must consider what the fields do inside the conductor, but a perfect conductor is a good approximation at microwave and lower frequencies where the penetration of the field into the conductor (the *skin depth*) is much smaller than the wavelength of light.