MATH 546: Partial Differential Equations II

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Lectures: Engineering E 206, Mondays/Wednesdays/Fridays, 11-11:50am
Office hours: Wednesdays, 1-2pm; or by appointment.

Homework assignment 1 – due Friday 3/1/2019

Problem 1 (Modeling temperature-dependent chemical reactions).   In class we have derived the equations the concentrations ρ_A, ρ_B, ρ_B of three chemical species A, B, C have to satisfy as these species diffuse and advect in an ambient medium (air, water) that moves with velocity β, and that undergo reactions of the form $A + B \to C$ with a reaction constant k. Namely, they had to satisfy the equations

$$\frac{\partial}{\partial t}\rho_A - D_A \Delta \rho_A + \nabla \cdot (\beta \rho_A) + k\rho_A \rho_B = 0,$$

$$\frac{\partial}{\partial t}\rho_B - D_B \Delta \rho_B + \nabla \cdot (\beta \rho_B) + k\rho_A \rho_B = 0,$$

$$\frac{\partial}{\partial t}\rho_C - D_C \Delta \rho_C + \nabla \cdot (\beta \rho_C) - k\rho_A \rho_B = 0.$$

We have also discussed how these equations have to be modified if the reaction doesn't just involve a single molecule of A and B reacting into one C, but instead something of the form $2A + 3B \to 4C$.

In reality, however, this kind of description is often incomplete. This is because of two factors: (i) reactions are either endothermic or exothermic, i.e., to combine A and B into C either takes energy (reducing the temperature at those locations where the reactions are happening) or produces energy (raising the temperature); and (ii) the reaction rate k is typically a function of the temperature T and grows exponentially with the temperature.

Derive an extended model that takes this into account in the following way:

- The model should describe the evolution of densities $\rho_A(\mathbf{x}, t), \rho_B(\mathbf{x}, t), \rho_C(\mathbf{x}, t)$ as well as the temperature $T(\mathbf{x}, t)$.

- k is a function of temperature T so that it grows exponentially with T. Explain all of the units that appear in this relationship.

- The reaction is of the form $2A + B \to 2C$ (for example $2H_2 + O_2 \to 2H_2O$) and each such reaction happening releases a (fixed) amount of thermal energy Q (measured in Joule, i.e., $\mathrm{kg\,m^2/s^2}$). If the reaction is endothermic, you will have $Q < 0$ and if it is exothermic $Q > 0$, though this distinction will not be important to you when writing down the equations (i.e., the equations will have the same form involving Q, whether this constant is positive or negative).

- The temperature (which somehow describes the amount of energy per volume – you should clarify this) will have to evolve in response to this release of energy Q.

- Everything happens in a medium that moves with velocity $\beta = \beta(\mathbf{x}, t)$ and both concentrations and temperature also diffuse with their respective diffusion constants.

(40 points)

Problem 2 (The Helmholtz equation "with the bad sign"). Let's start with the wave equation that describes, for example, the vertical displacement of a vibrating membrane, or the vertical height of a water surface. In both cases, the solution $u(\mathbf{x}, t)$ has to satisfy the equation

$$\partial_t^2 u(\mathbf{x}, t) - c^2 \Delta u(\mathbf{x}, t) = f(\mathbf{x}, t) \qquad\qquad \forall \mathbf{x} \in \Omega, t \in \mathbb{R},$$
$$u(\mathbf{x}, t) = g(\mathbf{x}, t) \qquad\qquad \forall \mathbf{x} \in \partial\Omega, t \in \mathbb{R}.$$

Assume now the interior forces $f(\mathbf{x}, t)$ as well as the boundary values $g(\mathbf{x}, t)$ all oscillate at a given frequency ω, though these oscillations may have different phases at different locations. In other words, we assume that $f(\mathbf{x}, t) = \hat{f}(\mathbf{x}, t)\cos(\omega t - \phi(\mathbf{x}))$ and $g(\mathbf{x}, t) = \hat{g}(\mathbf{x}, t)\cos(\omega t - \psi(\mathbf{x}))$ where ϕ and ψ describe the spatially dependent phases. We assume that these oscillations have gone on forever so that initial conditions are not relevant.

Our goal is to derive the following statement: *The solution $u(\mathbf{x}, t)$ at every point also oscillates at frequency ω and that its amplitude satisfies the Helmholtz equation with the bad sign.* As we will see, this statement is not entirely correct (it isn't the amplitude, but something related that satisfies the Helmholtz equation) but close enough to be intuitively correct.

To prove this statement – and derive its correct form – assume that you can write

$$u(\mathbf{x}, t) = \hat{u}(\mathbf{x})\cos(\omega t - \mu(\mathbf{x})).$$

If you put this into the wave equation, you will not achieve very much. But you can improve the situation if you note that

$$
\begin{aligned}
u(\mathbf{x}, t) &= \hat{u}(\mathbf{x})\cos(\omega t - \mu(\mathbf{x})) \\
&= \mathrm{Re}\left[\hat{u}(\mathbf{x})e^{i(\omega t - \mu(\mathbf{x}))}\right] \\
&= \mathrm{Re}\left[\hat{u}(\mathbf{x})e^{-i\mu(\mathbf{x})}e^{i\omega t}\right] \\
&= \mathrm{Re}\left[U(\mathbf{x})e^{i\omega t}\right],
\end{aligned}
$$

where $U(\mathbf{x}) = \hat{u}(\mathbf{x})e^{-i\mu(\mathbf{x})} : \Omega \to \mathbb{C}$ combines both the *amplitude* of the oscillations at each point $\mathbf{x}$ and the *phase shift*, whereas the term $e^{i\omega t}$ encodes the actual oscillation in time. (In other words, we are attempting a separation of variables approach. As discussed last semester, such an attempt is not guaranteed to succeed, but it sometimes does and it should sure here or I wouldn't give you this assignment.)

Similarly, you can write

$$f(\mathbf{x}, t) = \mathrm{Re}\left[F(\mathbf{x})e^{i\omega t}\right],$$
$$g(\mathbf{x}, t) = \mathrm{Re}\left[G(\mathbf{x})e^{i\omega t}\right].$$

Now show that $U(\mathbf{x})$ satisfies the Helmholtz equation with the bad sign. Specifically discuss whether this is only true for the real part of U, for both the real and imaginary parts separately, or whether real and imaginary parts actually satisfy two equations that are coupled.

(30 points)