12.1: Introduction to Partial Differential Equations

Many important equations in physical chemistry, engineering, and physics, describe how some physical quantity, such as a temperature or a concentration, varies with position and time. This means that one or more spatial variables and time serve as independent variables. For example, let's consider the concentration of a chemical around the point (x, y, z) at time t: $C = C(x, y, z, t)$. The differential equation that describes how C changes with time is

$$\nabla^2 C(x, y, z, t) = \frac{1}{D} \frac{\partial C(x, y, z, t)}{\partial t} \tag{12.1.1}$$

where ∇^2 is an operator known as the Laplacian. In cartesian three-dimensional coordinates:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

The constant D is the diffusion coefficient, and determines how far molecules move on average in a given period of time. The diffusion coefficient depends on the size and shape of the molecule, and the temperature and viscosity of the solvent.

The diffusion equation (Equation 12.1.1) is a partial differential equation because the dependent variable, C, depends on more than one independent variable, and therefore its partial derivatives appear in the equation.

Other important equations that are common in the physical sciences are:

The heat equation:

$$\nabla^2 T(x, y, z, t) = \frac{1}{\alpha} \frac{\partial T(x, y, z, t)}{\partial t} \tag{12.1.2}$$

which is in a way a diffusion equation, except that the quantity that diffuses is heat, and not matter. This translates into a change in temperature instead of a change in concentration.

The wave equation:

$$\nabla^2 u(x, y, z, t) = \frac{1}{v^2} \frac{\partial^2 u(x, y, z, t)}{\partial t^2} \tag{12.1.3}$$

which describes the displacement of all points of a vibrating thin string. Here, v has units of speed, and it's related to the elasticity of the string.

The time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(x, y, z) + V\psi(x, y, z) = E\psi(x, y, z) \tag{12.1.4}$$

which we have already introduced in previous chapters. Note that the Schrödinger equation becomes an Ordinary Differential Equation for one-dimensional problems (e.g. the one-dimensional particle in a box, page), but it is a PDE for systems where particles are allowed to move in two or more dimensions.

In this course, we will introduce the simplest examples of PDEs relevant to physical chemistry. As you will see, solving these equations analytically is rather complex, and the solutions depend greatly on initial and boundary conditions. Because solving these equations is time consuming, in your upper-level physical chemistry courses your teacher will often show you the solutions without going through the whole derivation. Yet, it is important that you go through all the work at least once for the simplest cases, so you know what it is involved in solving the PDEs you will see in the future.