

Conservation and dissipation principles for PDEs

1 Modeling through conservation principles

The notion of conservation - of number, energy, mass, momentum - is a fundamental property of many systems that can be used to derive and analyze familiar partial differential equations.

Let $u(\mathbf{x}, t)$ be the density of any quantity - heat, momentum, probability, population, etc. For any subregion $R \subset \Omega$ of the entire domain, the amount of u in R is

$$\int_R u \, d\mathbf{x}.$$

To say that a quantity is *locally conserved* means that it is only gained or lost either (1) through domain boundaries or (2) because of sources and sinks in the domain. The flow or *flux*, of $u(\mathbf{x}, t)$ can be thought of as a vector field $\mathbf{J}(\mathbf{x}, t)$, defined so that $\mathbf{J} \cdot \hat{\mathbf{n}} dA$ is the amount of u flowing in direction $\hat{\mathbf{n}}$ per unit time across a small area dA . Suppose there is also a source which produces u at a rate $Q(x, t)$ (if $Q < 0$, then this is a sink instead). Conservation of u on any subdomain $R \subset \Omega$ implies the balance

$$\frac{d}{dt} \int_R u \, d\mathbf{x} = \int_R \frac{\partial u}{\partial t} \, d\mathbf{x} = - \int_{\partial R} \mathbf{J} \cdot \hat{\mathbf{n}} \, d\mathbf{x} + \int_R Q(x, t) \, d\mathbf{x}. \quad (1)$$

Equation (1) says that the change in u is due to flow out of R and source terms in R .

The boundary integral in (1) can be converted to a integral over the domain R by using the divergence theorem.

$$\int_{\partial R} \mathbf{J} \cdot \hat{\mathbf{n}} \, d\mathbf{x} = \int_R \nabla \cdot \mathbf{J} \, d\mathbf{x},$$

which gives

$$\int_R \left(\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{J} - Q \right) \, d\mathbf{x} = 0.$$

The important point is that this is true for *every* region R , which means that the integrand must be exactly zero. This gives the differential equation

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{J} = Q. \quad (2)$$

In some contexts, this is called the transport or continuity equation. This equation is valid for any spatial dimension. Note that in one dimension, divergence is just the regular derivative $\partial/\partial x$. Because the flux and source terms are problem specific, a wide variety of PDEs take the form (2). Some examples are given below.

1.1 Boundary Conditions

If a quantity is locally conserved, it still may be gained or lost by flowing through the boundaries of the physical domain. A common situation is when flow through the boundary is prohibited, leading to the *no-flux* boundary condition

$$\mathbf{J} \cdot \hat{\mathbf{n}} = 0, \quad \mathbf{x} \in \partial\Omega. \quad (3)$$

Notice that \mathbf{J} itself is not zero on the boundary; this reflects the possibility that material flows along the boundary but not through it.

The actual boundary condition that (3) represents depends on how the flux \mathbf{J} is modeled. For example, in the diffusion equation, the flux is $\mathbf{J} = -D\nabla u$, so (3) becomes

$$\nabla u \cdot \hat{\mathbf{n}} = 0, \quad \mathbf{x} \in \partial\Omega,$$

which is simply the homogeneous Neumann boundary condition.

For flow of a viscous fluid film, the conserved quantity $h(\mathbf{x}, t)$ (actually the film thickness) has a corresponding flux $\mathbf{J} = -h^3\nabla\Delta h$. In this case, the no-flux boundary condition would read

$$h^3(\nabla\Delta h) \cdot \hat{\mathbf{n}} = 0, \quad \mathbf{x} \in \partial\Omega.$$

This means either $h = 0$ or $(\nabla\Delta h) \cdot \hat{\mathbf{n}} = 0$ on the boundary.

Note that other types of boundary conditions can be used in conservation laws. For example, if the temperature is fixed on the boundary in a heat diffusion model, this corresponds to a Dirichlet-type boundary condition

$$u = U(\mathbf{x}), \quad \mathbf{x} \in \partial\Omega$$

instead. In this case, the flux across the boundary is generally not zero, but is simply whatever flux is needed to maintain the Dirichlet boundary condition.

1.2 Examples

Simple transport in one space dimension. Suppose that a quantity with density $u = u(x, t)$ is transported at velocity c . Note that flux in one dimension is a scalar, and from dimensional considerations

$$\begin{aligned} & J(\text{some quantity per unit time}) \\ &= \text{velocity (length per unit time)} \times \text{density (some quantity per unit length)} = cu. \end{aligned}$$

Without source terms, (2) becomes

$$u_t + cu_x = 0. \tag{4}$$

Traffic flow. Unlike simple transport, automobiles do not generally travel at a uniform speed. The simplest way of modeling this situation is taking the speed $c = c(u)$ as a decreasing function of the density of cars u . This makes sense most of the time: greater densities lead to slower speeds. Then the scalar flux is $J = c(u)u$ and (2) becomes

$$u_t + (c(u)u)_x = 0. \tag{5}$$

This has the form of a hyperbolic conservation law $u_t + f(u)_x = 0$. The choice $f = u^2/2$ gives rise to what is known as *Burger's equation*.

Diffusion. The idea of a quantity diffusing means that its flux has a direction toward regions of less density. Mathematically, this can be modeled as $\mathbf{J} = -D\nabla u$ since the gradient points in the direction of greatest increase. (The constant D is known as the diffusivity, and is measured in units of length squared per unit time). This is known as Fick's law, or Fourier's law for the case of heat diffusion. The basic form (2) becomes

$$u_t = D\nabla \cdot \nabla u = D\Delta u, \tag{6}$$

which is known as the diffusion equation. This is one of the most fundamental PDEs.

Diffusion with a nonlinear source. Suppose that the source term $Q(x, t)$ is a function $f(u)$ of u itself. This might be the case for a chemical reaction (where Q is reaction rate) or biological reproduction (for example, $Q = u(1 - u)$ as in the logistic equation). Then one obtains

$$u_t = \Delta u + f(u), \quad (7)$$

which is a simple example of a *reaction-diffusion equation*.

Chemotaxis. Various cells and microorganisms move in response to chemical gradients. For example, certain bacteria are drawn toward oxygen, and white blood cells may move in response to chemicals produced at the site of an infection.

Let $u(\mathbf{x}, t)$ be the time-dependent density of cells, and let $c(\mathbf{x}, t)$ be the density of chemoattractant concentration. The main idea is that the flux of cells is in the same direction as the (spatial) gradient of c - in other words, the cells seek a direction where there is the greatest concentration. The magnitude of the flux is, on the other hand, typically a fixed number M , which has to do with the mobility of cells. It follows that the flux of cells due to chemotaxis is

$$\mathbf{J}_c = M \frac{\nabla c}{|\nabla c|}.$$

In real situations, one also has standard diffusion of cells modeled as the diffusive flux $\mathbf{J}_d = -D\nabla u$. The equations of motion are a combination of these fluxes:

$$u_t = -\nabla \cdot (\mathbf{J}_c + \mathbf{J}_d) = -M\nabla \cdot \left(\frac{\nabla c}{|\nabla c|} \right) + D\Delta u. \quad (8)$$

Of course, one can also consider the evolution of chemoattractant by diffusion. If the organism produces the chemoattractant itself (as in the famous slime mold example), one arrives at a coupled system for u and c known as the *Keller-Segel* equations.

Wave equation. Suppose that $u(\mathbf{x}, t)$ represents the vertical displacement of an elastic membrane at (\mathbf{x}, t) . For wave propagation, the conserved quantity is the *momentum*, which is the time derivative u_t instead of u . Momentum flux is proportional to $-\nabla u$, which comes from the way in which elastic forces depend on the displacement. Setting the proportionality constant to one, the fact that momentum is conserved means

$$(u_t)_t - \nabla \cdot \nabla u = 0$$

which is known as the wave equation.

1.3 Steady state problems

Often dynamical processes “settle down” over time. Mathematically this means that $u_t \rightarrow 0$ as $t \rightarrow \infty$. In the context of conservation laws, a *steady state solution* is a solution of (2) for which the time derivative is suppressed:

$$\nabla \cdot \mathbf{J}(u) = Q. \quad (9)$$

Note that this does not mean that the flux is zero; it simply says that the amount flowing away from a point balances the sources at that point. Often (9) is supplemented with inhomogeneous boundary conditions.

As an example, consider diffusion described by the flux $\mathbf{J} = -D\nabla u$, with a given time-independent source $Q(\mathbf{x})$. A steady state solution is a solution $u = u(\mathbf{x})$ solving (9) which in this case reads

$$D\nabla \cdot \nabla u = \Delta u = Q(\mathbf{x}). \quad (10)$$

This is known as *Poisson’s equation*; If $Q \equiv 0$, it is called *Laplace’s equation*, which is one of the fundamental equations along with the diffusion and wave equations.

2 Conserved and dissipated quantities

Any function, especially one with several independent variables, carries a huge amount of information. The questions we want to answer about PDEs are often simple, and don't require a complete knowledge of the solution. It is useful to study coarse grained quantities that arise in PDEs in order to circumvent a complete analysis of these problems. Note that this philosophy has a long history in science: physicists and chemists like to talk about a system's energy or entropy, which can be understood without any intimate knowledge of the microscopic details.

For some solution of a PDE $u(x, t)$, we can define a coarse-grained quantity as a *functional*, which is a mapping from u to the real numbers. For example,

$$\int_{\Omega} u dx, \quad \int_{\Omega} u_x^2 dx, \quad \int_{\Omega} u_{xx}^4 dx$$

are all examples of functionals. It often happens that functionals represent quantities of physical interest – mass, energy, momentum, etc. – but such an interpretation is not essential for these objects to be useful.

Suppose F is some functional of $u(x, t)$ of the form

$$F[u] = \int_{\Omega} f(u, u_x, \dots) dx.$$

so that F depends on t , but not on the variable x which has been integrated out. There are two common properties which depend on the time evolution of F . If $dF/dt = 0$, then F is called *conserved*. If $dF/dt \leq 0$, then F is called *dissipated*.

Suppose u solves the wave equation and boundary conditions

$$u_{tt} = u_{xx}, \quad u(0, t) = 0 = u(L, t).$$

Then the energy functional (essentially the sum of kinetic and potential energy)

$$E = \int_0^L \frac{1}{2} u_t^2 + \frac{1}{2} u_x^2 dx$$

is conserved. Indeed,

$$\frac{dE}{dt} = \int_0^L u_t u_{tt} + u_x u_{xt} dx = u_x u_t \Big|_{x=0}^{x=L} + \int_0^L u_t u_{tt} - u_{xx} u_t dx = 0,$$

where integration by parts and the boundary condition was used for the second equality (we leave out a technical issue: is it always appropriate to move the derivative d/dt inside the integral and replace it with a partial derivative?)

The fact that E remains the same for all t has profound qualitative implications. Any solution which has wave oscillations initially (so that the energy is positive) must continue to have oscillations for all time - they never die out, for example. Conversely, if the initial conditions are quiescent, so that $E = 0$, then this must happen forever. Notice we learn these things without ever finding a solution of the equation!

As another example, suppose u solves the diffusion equation

$$u_t = u_{xx}, \quad u(0, t) = 0 = u(L, t).$$

Then the quantity

$$F = \int_0^L \frac{1}{2} u_x^2 dx$$

is dissipated, since

$$\frac{dF}{dt} = \int_0^L u_x u_{xt} dx = - \int_0^L u_{xx} u_t dx = - \int_0^L u_{xx}^2 dx < 0,$$

where again integration by parts and the boundary condition was used.

We can interpret F as follows. The arclength of x -cross sections of u can be approximated for small u_x as

$$\int_0^L \sqrt{1 + u_x^2} dx \approx \int_0^L 1 + \frac{1}{2} u_x^2 dx.$$

Since, $dF/dt \leq 0$, the approximate arclength must also diminish over time. This means the graph of $u(x, \cdot)$ gradually becomes smoother, and oscillations die away. This statement will be made perfectly quantitative by solving the equation outright later on.