

Conservation and dissipation principles for PDE models

1 Modeling through conservation laws

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

Let $u(\mathbf{x}, t)$ be the density of any quantity - heat, momentum, probability, bacteria, etc. The amount of u in a (say 3-dimensional) region Ω is

$$\int_{\Omega} u dV.$$

To say that a quantity is *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 $u(x, t)$ can be thought of as a vector field $\mathbf{J}(x, t)$. This is 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 . If $Q(x, t)$ is the rate of inflow of u (outflow if negative) then the conservation of u on any domain Ω implies

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

Here $\partial\Omega$ denotes the boundary of Ω and $\hat{\mathbf{n}}$ is the outward normal. Equation (1) says that the change in u is due to flow out of Ω and source terms in Ω .

The surface flux integral in (1) can be converted to a volume integral by using the divergence theorem, giving

$$\int_{\Omega} \left(\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{J} - Q \right) dV = 0.$$

The important point is that this is true for *every* region Ω , 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 (divergence in one dimension is just the regular derivative $\partial/\partial x$). The flux and source terms are problem specific. Some examples are given below.

1.1 Boundary Conditions

If a quantity is conserved, it still may be gained or lost by flowing through the boundaries of the physical domain. This implies that the flux $\mathbf{J}$ must be specified on the domain boundary. For example, in the diffusion equation, the flux is $-D\nabla u$, so a valid boundary condition could be written

$$-D\nabla u \cdot \hat{\mathbf{n}} = \mathbf{J}_0(\mathbf{x}), \quad \mathbf{x} \in \partial\Omega,$$

where $\hat{\mathbf{n}}$ is the outward normal to the domain boundary $\partial\Omega$. Often the boundaries are called “no-flux” or “insulating” (in the case of heat diffusion), which leads to the very common “Neumann” boundary condition

$$\nabla u \cdot \hat{\mathbf{n}} = 0.$$

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

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

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

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

Without source terms, (2) becomes

$$u_t + cu_x = 0. \tag{3}$$

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

$$u_t + (c(u)u)_x = 0. \quad (4)$$

This has the form of a *one-dimensional* 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 if u is heat. In this case, (2) becomes

$$u_t = D\nabla \cdot \nabla u = D\Delta u, \quad (5)$$

which is known as the diffusion equation.

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

$$u_t = \Delta u + f(u), \quad (6)$$

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:

$$u_t = -\nabla \cdot (\mathbf{J}_c + \mathbf{J}_d) = -M \nabla \cdot \left(\frac{\nabla c}{|\nabla c|} \right) + D \Delta u. \quad (7)$$

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. This example is different from the rest. In this case, the conserved quantity is *momentum*, which is the time derivative of the displacement u (properly speaking, one needs to multiply by mass density). Momentum flux occurs because forces (if the wave arises from, say, an elastic body) are transmitted spatially, and are proportional to $-\nabla u$. With a constant of proportionality equal to one, the fact that momentum is conserved means

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

which is the wave equation with unit speed.

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:

$$\nabla \cdot \mathbf{J}(u) = Q. \quad (8)$$

Note that this does not mean that the flux is zero; it simply says that the amount flowing into a region in space equals the amount flowing out. Often (8) 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 $Q(x, y)$. A steady state solution is a solution $u = u(x, y)$ solving (8) which in this case reads

$$D \nabla \cdot \nabla u = \Delta u = Q(x, y). \quad (9)$$

This is known as *Poisson's equation*; if $Q \equiv 0$, it is called *Laplace's equation*.

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, however. Complete knowledge of the details of an equation's solution are frequently unavailable, and would be overkill in any event. It is therefore useful to study coarse grained quantities that arise in PDEs in order to circumvent a complete analysis of these problems. Notice 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 using separation of variables.