Scientific Computing for Partial Differential Equations

Understanding the models and utilizing efficient numerical methods

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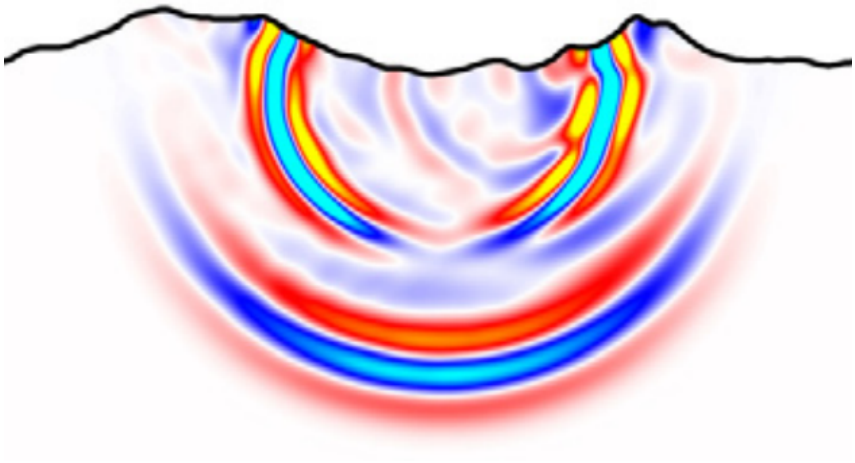

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Contents

1 Well-posedness of scalar PDE in 1D

1.1 The advection equation

One of the simplest examples of a partial differential equation (PDE) is the advection equation:

$$u_t + cu_x = 0, \quad x \in (0, W), \quad t > 0, \tag{1.1}$$

where subscripts denote partial derivatives, $W > 0$ is the domain width, and c is the wave speed (for now assumed to be constant and positive). We will refer to x as a spatial coordinate and t as time, although they could represent other physical quantities. We seek a solution $u = u(x, t)$ such that (1.1) is satisfied.

There are actually *infinitely* many solutions to (1.1). Given any differentiable function f we can construct a solution $u(x, t)$ as

$$u(x, t) = f(x - ct). \tag{1.2}$$

To verify that u satisfies (1.1), we compute its derivatives

$$u_t = -cf'(x - ct), \quad u_x = f'(x - ct) \tag{1.3}$$

and conclude that

$$u_t + cu_x = -cf'(x - ct) + cf'(x - ct) = 0. \tag{1.4}$$

The interpretation of the solution formula (1.2) is that, as time advances, the solution is simply translated (or *advected*) to the right, with speed c.

1.1.1 An introduction to well-posedness

We begin with the following somewhat loose definition of well-posedness, which we will later make more precise:

Definition 1. A PDE-problem is well posed if and only if:

1. A solution *exists*.
2. The solution is *unique*.
3. The solution depends smoothly on provided data (small changes in data lead to small changes in the solution).

Attempting to solve *ill-posed* (not well-posed) problems numerically is almost never worthwile. If no solution exists, then why are we trying to find one? If multiple solutions exist, which one are we hoping to find? Usually, if a PDE-problem is ill-posed, someone made a mistake and should go back to the drawing board.

We do not yet have enough background to discuss requirement 3, so we will revisit it later. Requirement 1 (existence) is often difficult to prove for complex PDE, so in general such proofs are outside the scope of this course. Note, however, that the formula (1.2)

proves existence for the advection equation. At the same time, it proves that requirement 2 is violated, because the solution is not unique! As we mentioned, there are infinitely many functions that satisfy (1.1). To ensure uniqueness, we will need to add more constraints so that we single out exactly one solution. Note that we need to be careful—if we add too many constraints there might not be a function that satisfies all of them! That is, we might violate requirement 1.

The usual way to construct a well-posed advection problem is to augment the PDE (1.1) with an *initial condition* and a *boundary condition*.

1.1.2 Initial condition

An initial condition specifies $u(x,t)$ at the initial time, usually taken to be $t = 0$ for simplicity. We can write the initial condition as

$$u(x,0) = u_0(x), \quad x \in [0,W], \tag{1.5}$$

where u_0 is a *known* function. We refer to u_0 as initial data.

1.1.3 Boundary conditions

In addition to the initial condition we need to specify a boundary condition at the *left* boundary, $x = 0$. The typical boundary condition for the advection equation (with $c > 0$) is

$$u(0,t) = g(t), \quad t > 0, \tag{1.6}$$

where g is a known function. We refer to g as *boundary data*. If $g = 0$, the boundary condition is said to be *homogeneous*, otherwise *inhomogeneous*.

Note that no boundary condition is prescribed at the right boundary. One way to understand this is to recall that waves travel *to the right*. That is, the flow of information is from left to right. The left boundary is an inflow boundary, so we need to specify what is "coming in" from the left. The right boundary is an outflow where information simply leaves the domain, so no boundary condition is needed.

If the wave speed c is negative, the situation is reversed. Waves now travel *to the left*, which means that the left boundary is an outflow and the right boundary is an inflow. In this case we need a condition on the right boundary.

Another possible boundary condition is the periodic condition

$$u(0,t) = u(W,t). \tag{1.7}$$

This condition has the effect that information that leaves the domain at the outflow re-enters at the inflow. It can be thought of as using the solution at the outflow as boundary data for the inflow.

1.1.4 The initial-boundary value problem

We summarize the discussion above by stating the advection equation augmented with appropriate initial and boundary conditions:

$$\begin{aligned} u_t + cu_x = 0, &\quad x \in (0, W), \quad t > 0, \\ u = u_0, &\quad x \in [0, W], \quad t = 0, \\ u = g, &\quad x = 0, \qquad\quad t > 0. \end{aligned} \tag{1.8}$$

The problem (1.8) is an example of an *initial-boundary value problem* (IBVP); it is a PDE augmented with initial and boundary conditions. IBVP are the center of attention in this course. So far we have hinted that this IBVP is well-posed, and we will soon have the tools to prove it.

1.2 Energy analysis

The so-called energy method is a powerful and versatile tool for analyzing IBVP. The point is to derive a bound on the solution in some norm. Such a bound shows that the solution cannot become arbitrarily "large". Before we introduce the energy method, we need to introduce some properties of the space L^2.

1.2.1 L^2 space

Let $L^2(\Omega)$ denote the space of complex-valued functions that are square-integrable over a domain $\Omega \subset \mathbb{R}^n$. That is,

$$L^2(\Omega) = \{f : \Omega \to \mathbb{C} \text{ such that } \int_\Omega |f(\vec{x})|^2 \, \mathrm{d}\vec{x} < \infty\}. \tag{1.9}$$

Let $u, v \in L^2(\Omega)$. The L^2 inner product is defined as

$$(u, v) = \int_\Omega u^*(\vec{x}) v(\vec{x}) \, \mathrm{d}\Omega, \tag{1.10}$$

where $*$ denotes conjugate transpose. The corresponding norm is

$$\|u\|^2 = (u, u)\,. \tag{1.11}$$

The inner product is conjugate symmetric:

$$(u, v) = (v, u)^*\,. \tag{1.12}$$

For real-valued functions $a > 0$, we introduce the weighted inner product and norm

$$(u, v)_a = (u, av)\,, \quad \|u\|_a^2 = (u, u)_a\,. \tag{1.13}$$

The norms $\|\cdot\|$ and $\|\cdot\|_a$ are equivalent in the sense that

$$\|u\|_a^2 \leq a_{max}\|u\|^2, \quad \|u\|^2 \leq \frac{1}{a_{min}}\|u\|_a^2. \tag{1.14}$$

where the constants a_{max} and a_{min} denote the maximum and minimum values of a over Ω.

Remark. We will often consider real-valued functions only, in which case the complex conjugate can be omitted. The conjugate symmetry of the inner product then reduces to symmetry.

1.2.2 The energy method

The energy method consists of the following steps:

1. Identify the highest-order time derivative appearing in the PDE. Suppose that the highest order is qth order. That is, the PDE contains a term $\frac{\partial^q u}{\partial t^q}$. Then take the inner product of the PDE and $\frac{\partial^{q-1} u}{\partial t^{q-1}}$ (one derivative order lower).

2. Take the conjugate transpose of the relation that you derived in step 1. (The transpose operation is only necessary for systems of equations, not scalar equations. Similiarly, the complex conjugate can be omitted if all quantities are real.)

3. Add the relations from step 1 and 2 and integrate by parts in space "as many times as necessary". This is best explained by examples.

1.2.3 Example: the energy method for the advection equation

Consider the 1D advection equation with variable wave speed $c = c(x) > 0$:

$$\begin{aligned} u_t + cu_x = 0, &\quad x \in (0, W), \quad t > 0, \\ u = u_0, &\quad x \in [0, W], \quad t = 0, \\ u = g, &\quad x = 0, \qquad\quad t > 0. \end{aligned} \tag{1.15}$$

Assume for simplicity that the solution is real. Here, our domain is $\Omega = [0, W]$, so the inner product is simply

$$(u, v) = \int_0^W u(x)v(x)\,\mathrm{d}x. \tag{1.16}$$

The PDE contains a first derivative in time (u_t), so we shall multiply it by u. After some trial and error one realizes that it is clever to first divide the PDE through by c to obtain

$$c^{-1}u_t = -u_x. \tag{1.17}$$

Taking the inner product with u yields

$$\left(u, c^{-1}u_t\right) = -\left(u, u_x\right). \tag{1.18}$$

Since the inner product is symmetric and c is assumed to be constant in *time*, we have

$$\left(u, c^{-1}u_t\right) = \left(u_t, c^{-1}u\right) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(u, c^{-1}u\right) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{c^{-1}}. \tag{1.19}$$

We can now write (1.18) as

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{c^{-1}} = -\left(u, u_x\right). \tag{1.20}$$

Next, we integrate the right-hand side by parts to obtain

$$-\left(u, u_x\right) = -u^2|_{x=0}^{x=W} + \left(u_x, u\right), \tag{1.21}$$

which simplifies to

$$-\left(u, u_x\right) = -\frac{1}{2}u^2|_{x=0}^{x=W}. \tag{1.22}$$

Using (1.22) in (1.20) leads to

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{c^{-1}} = -\frac{1}{2}u^2|_{x=0}^{x=W}. \tag{1.23}$$

We may define the mathematical energy (the connection to a physical energy is not obvious in this case)

$$E = \|u\|^2_{c^{-1}}, \tag{1.24}$$

which highlights that (1.23) describes the rate of change of energy:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -u^2|_{x=0}^{x=W}. \tag{1.25}$$

We note that energy can only enter and leave the system via the boundaries. There is no dissipation or growth of energy in the domain interior in this model.

Remark. As we will later see, the energy method usually derives the rate of change of the physical energy of he system, but sometimes the "energy" is a purely mathematical construction. Just like physical energies, mathematical energies are always non-negative quantities.

It is possible to use the energy rate (1.25) to determine how many boundary conditions are required for well-posedness. We have

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -u^2|_{x=0}^{x=W} = -u(W,t)^2 + u(0,t)^2 \leq u(0,t)^2. \tag{1.26}$$

The right boundary (the outflow, at $x = W$) does not contribute to energy growth. Therefore, no boundary condition is required there. To control the growth of energy stemming from the left boundary, we need to specify $u(0,t)$. The boundary condition $u(0,t) = g(t)$ yields the energy rate

$$\frac{\mathrm{d}E}{\mathrm{d}t} \leq g(t)^2. \tag{1.27}$$

Integrating in time yields

$$E(t) \le E(0) + \int_0^t g(s)^2 \, \mathrm{d}s, \tag{1.28}$$

which we can write as

$$\|u(\cdot,t)\|_{c^{-1}}^2 \le \|u_0\|_{c^{-1}}^2 + \int_0^t g(s)^2 \, \mathrm{d}s. \tag{1.29}$$

The bound (1.29) is an *energy estimate*, because it bounds (estimates) the energy at time t in terms of initial and boundary data.

1.2.4 Proof of uniqueness

We may use the energy estimate to prove that any solution to the IBVP (1.15) is unique. Assume that u and v are two solutions and define $w = u - v$. Since both u and v satisfy (1.15), w must satisfy the same IBVP but with homogeneous boundary and initial data ($g = 0, u_0 = 0$). The energy estimate (1.29) yields

$$\|w(\cdot,t)\|_{c^{-1}}^2 \le 0 + 0 = 0. \tag{1.30}$$

This implies that $0 = w = u - v$, which means that u must equal v and hence the solution is unique.

Note that specifying appropriate boundary conditions was essential in proving uniqueness. Without the boundary condition at the left boundary we could not have derived the energy estimate (1.29), and hence not completed this proof.

In this case one boundary condition is enough to guarantee uniqueness. We will see examples of other PDEs that require multiple conditions.

1.3 Well-posedness for general IBVP

Consider the general linear IBVP

$$\begin{aligned} u_t &= \mathcal{D}u + F, & x &\in (0,W), & t &> 0, \\ u &= u_0, & x &\in [0,W], & t &= 0, \\ \mathcal{L}_\ell u &= g_\ell, & x &= 0, & t &> 0, \\ \mathcal{L}_r u &= g_r, & x &= W, & t &> 0, \end{aligned} \tag{1.31}$$

where $\mathcal{D}$ is a differential operator in space, and $\mathcal{L}_{\ell,r}$ are boundary operators at the left and right boundary, respectively. The boundary operators determine the boundary conditions and can, for example, be identity or differential operators. One of them could be zero, if a boundary condition is not needed at that boundary. Note that the PDE is first order in time, but may be of higher order in space (we will discuss PDE that are second order in time later). The restriction that the PDE is linear implies that the operator $\mathcal{D}$ does not depend on u. As usual, $g_{\ell,r} = g_{\ell,r}(t)$ are boundary data functions and $u_0 = u_0(x)$ is

the initial data. The function $F = F(x,t)$ is called a *forcing* function. The functions F, $g_{\ell,r}$, and u_0 are assumed to be known.

Gustafsson [1] (p. 32) uses the following definition of well-posedness, which we will henceforth adopt:

Definition 2. The IBVP (1.31) is well-posed if, for $F = 0$, $g_\ell = 0$, $g_r = 0$, there is a unique solution satisfying

$$\|u\| \leq Ke^{\alpha t}\|u_0\|, \tag{1.32}$$

where K and α are constants independent of u_0.

The definition states that the IBVP is well-posed if the solution does not grow "too quickly" in time. Note that the definition is quite relaxed in the sense that it allows for exponential growth. This bound on the growth rate ensures that the solution depends smoothly on initial and boundary data, so it replaces Requirement 3 in Definition 1.

Definition 2 is very useful in practice, because it tells us that for well-posedness, it is enough to study the IBVP with $F = 0$ and homogeneous boundary conditions ($g_{\ell,r} = 0$):

$$\begin{aligned} u_t &= \mathcal{D}u, && x \in (0,W), && t > 0, \\ u &= u_0, && x \in [0,W], && t = 0, \\ \mathcal{L}_\ell u &= 0, && x = 0, && t > 0, \\ \mathcal{L}_r u &= 0, && x = W, && t > 0 \end{aligned} \tag{1.33}$$

We will refer to (1.33) as *the homogeneous version* (THV) of (1.31). If THV (1.33) is well-posed, then so is the original IBVP (1.31). We will use this result frequently. A hand-waving explanation of the result is that growth that violates well-posedness (faster than exponential) must be caused by a feedback mechanism where a growing solution causes increased growth. Known data F and $g_{\ell,r}$ cannot cause this kind of growth—it must stem from the structure of the homogeneous IBVP.

We will sometimes encounter energy growth of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u\|_a^2 \leq \beta\|u\|_a^2. \tag{1.34}$$

Solving the ODE and using the initial condition leads to the estimate

$$\|u\|_a^2 \leq \|u_0\|_a^2 e^{\beta t}. \tag{1.35}$$

Because the norms $\|\cdot\|_a$ and $\|\cdot\|$ are equivalent (recall (1.14)), we have

$$\|u\|^2 \leq \frac{1}{a_{min}}\|u\|_a^2 \leq \frac{1}{a_{min}}\|u_0\|_a^2 e^{\beta t} \leq \frac{a_{max}}{a_{min}}\|u_0\|^2 e^{\beta t} \tag{1.36}$$

Taking the square root yields the desired estimate

$$\|u\| \leq Ke^{\alpha t}\|u_0\| \tag{1.37}$$

with

$$K = \sqrt{\frac{a_{max}}{a_{min}}}, \quad \alpha = \frac{\beta}{2}. \tag{1.38}$$

This shows that an estimate of the form (1.34) is sufficient for well-posedness.

1.3.1 Well-posed boundary conditions

For a general, linear, *scalar* PDE of the form

$$u_t = Du + F \tag{1.39}$$

where the spatial differential operator D is of order r, we should always impose exactly r boundary conditions in total. In general, for systems of linear PDE, where u is a vector with m components, we should always impose *at most* rm conditions. There are systems with singular matrices for which fewer conditions should be imposed.

With too few conditions, the solution will not be unique. With too many conditions, no solution will exist. So, to ensure well-posedness, we need to select the *minimial number* of boundary conditions that allows a bound of the form (1.32).

1.4 The heat equation

The heat equation in 1D reads

$$\rho c_p u_t = (\kappa u_x)_x + F, \quad x \in (0, W), \quad t > 0, \tag{1.40}$$

where u is temperature, $\kappa = \kappa(x)$ is the thermal conductivity, c_p is specific heat capacity and ρ is density. Let us for simplicity assume that ρ and c_p are constant, in which case the equation can be written as

$$u_t = (au_x)_x + G, \quad x \in (0, W), \quad t > 0, \tag{1.41}$$

where the coefficient $a > 0$ is called the thermal diffusivity. The heat equation is identical to the *diffusion* equation, where a would instead be the diffusion coefficient.

Exercise: Which of the following sets of boundary conditions are well-posed for the heat equation? The coefficient b in condition e) is a real constant.

a) $u(0,t) = 0, \quad u(W,t) = 0$ (Dirichlet conditions on both sides)

b) $u_x(0,t) = 0, \quad u_x(W,t) = 0$ (Neumann conditions on both sides)

c) $u(0,t) = 0, \quad u_x(W,t) = 0$ (Dirichlet on one side, Neumann on the other)

d) $u(0,t) = 0, \quad u_x(0,t) = 0$ (two conditions on one side)

e) $u(0,t) = 0, \quad a(W)u_x(W,t) + bu(W,t) = 0,$ (Dirichlet + Robin)

f) $u(0,t) = 0$

g) $u(0,t) = 0, \quad u(W,t) = 0, \quad u_x(W,t) = 0$

Solution: We can immediately say that f) and g) are ill-posed. The PDE is linear, scalar, and of second order in space. We need exactly 2 boundary conditions.

We know that when it comes to well-posedness, it is sufficient to study THV, so we set the forcing function G to zero. We will apply the energy method. The PDE contains u_t, so we multiply by u. Here it is reasonable to assume that all quantities are real. We obtain, using integration by parts:

$$(u, u_t) = (u, (au_x)_x) = uau_x|_0^W - (u_x, au_x)\,. \tag{1.42}$$

In this case it is not necessary to add the complex conjugate. Note that

$$(u, u_t) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2, \quad (u_x, au_x) = \|u_x\|_a^2. \tag{1.43}$$

We obtain the energy rate

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2 = uau_x|_0^W - \|u_x\|_a^2 \leq uau_x|_0^W. \tag{1.44}$$

Note that $\|u\|^2$ does not correspond to the physical energy, so this energy rate is purely mathematical. The term $-\|u_x\|_a^2$ corresponds to dissipation. It is characteristic of the heat/diffusion equations that sharp features of u are dissipated quickly. The solution tends to flatten out.

Writing out the boundary terms explicitly yields

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2 \leq a(W)u(W,t)u_x(W,t) - a(0)u(0,t)u_x(0,t) \tag{1.45}$$

Any set of exactly two boundary conditions that allows us to bound the growth of u according to Definition 2 yields a well-posed IBVP.

For a)-c), we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2 \leq a(W)u(W,t)u_x(W,t) - a(0)u(0,t)u_x(0,t) = 0. \tag{1.46}$$

The boundary conditions do not produce growth or dissipation. They preserve (mathematical) energy. We see that $\|u\|$ does not grow with time, so the IBVP is clearly well posed.

For d), we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2 \leq a(W)u(W,t)u_x(W,t). \tag{1.47}$$

Here it is not possible to bound the growth rate, so we cannot prove well-posedness. It is nontrivial to prove that the IBVP is actually ill-posed, but it is, and it would be a good guess to say that it is.

For e), we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2 \leq a(W)u(W,t)u_x(W,t) = -bu(W,t)^2. \tag{1.48}$$

The Dirichlet condition at the left boundary conserves energy. The boundary condition $au_x + bu = 0$ at the right boundary yields dissipation (and is therefore well posed) for $b > 0$. This is called a *Robin* boundary condition. For $b = 0$, it reduces to a Neumann condition. For $b < 0$, the condition yields growth and is ill-posed.

1.5 The Schrödinger equation

The Schrödinger equation for a single particle in one dimension reads

$$i\hbar u_t = -\frac{\hbar^2}{2m}u_{xx} + Vu, \quad x \in (0, W), \quad t > 0. \tag{1.49}$$

where u is the wave function, m is the particle's mass, $V = V(x,t) \in \mathbb{R}$ is the potential, and $\hbar$ is the reduced Planck constant. The equation is often posed on the real line ($x \in (-\infty, \infty)$), but here we assume that it is posed on a finite domain.

Before applying the energy method, it is convenient to divide through by $i\hbar$ to obtain

$$u_t = i\frac{\hbar}{2m}u_{xx} + \frac{i}{\hbar}Vu. \tag{1.50}$$

We now multiply by u^* (since there are complex quantities the complex conjugate is important) and integrate to obtain

$$(u, u_t) = i\frac{\hbar}{2m}(u, u_{xx}) + \frac{i}{\hbar}(u, Vu). \tag{1.51}$$

Integrating by parts leads to

$$(u, u_t) = i\frac{\hbar}{2m}u^*u_x|_0^W - i\frac{\hbar}{2m}(u_x, u_x) + \frac{i}{\hbar}(u, Vu). \tag{1.52}$$

Taking the complex conjugate of (1.52) yields

$$(u_t, u) = -i\frac{\hbar}{2m}u_x^*u|_0^W + i\frac{\hbar}{2m}(u_x, u_x) - \frac{i}{\hbar}(u, Vu). \tag{1.53}$$

Adding (1.52) and (1.53) yields the energy rate

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2 = i\frac{\hbar}{2m}(u^*u_x - u_x^*u)|_0^W. \tag{1.54}$$

Notice that all the volume integrals cancelled and we are left with only boundary terms. The "energy" $\|u\|^2$ is not actually the physical energy, but rather the probability of finding the particle in the domain $(0, W)$, so at least it is an important physical quantity.

Exercise: Determine a set of well-posed (non-periodic) boundary conditions that corresponds to

a) conservation of probability.

b) dissipation of probability at both boundaries.

Solution: The PDE is second order in space, so we need two boundary conditions in total.

For a), imposing $u = 0$ at both boundaries leads to conservation of probability:

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2 = 0. \tag{1.55}$$

The same holds for $u_x = 0$ at both boundaries, as well as $u = 0$ at one and $u_x = 0$ at the other.

For b), we note that the boundary terms are products of u and u_x. To control the sign of these terms, we would like to be able to write them as $C|u|^2$ or $C|u_x|^2$. We therefore try the boundary conditions

$$u - au_x = 0,\ x = 0, \quad u - bu_x = 0,\ x = W, \tag{1.56}$$

where the coefficients a, b are to be determined. We obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2 &= i\frac{\hbar}{2m}(u^*u_x - u_x^*u)|_0^W \\
&= i\frac{\hbar}{2m}\left(u_x^*b^*u_x - u_x^*bu_x\right)\Big|_{x=W} - i\frac{\hbar}{2m}\left(u_x^*a^*u_x - u_x^*au_x\right)\Big|_{x=0} \\
&= i\frac{\hbar}{2m}(b^* - b)|u_x^2|\Big|_{x=W} - i\frac{\hbar}{2m}(a^* - a)|u_x^2|\Big|_{x=0}
\end{aligned} \tag{1.57}$$

Note that $i(a^* - a) = 2\mathcal{I}(a)$, where $\mathcal{I}$ denotes the imaginary part. For dissipation of probability, we need $\mathcal{I}(a) > 0$ and $\mathcal{I}(b) < 0$. The real part does not cause dissipation or growth, and therefore does not affect well-posedness.

2 Well-posedness of first-order systems and the second-order wave equation in 1D

2.1 First order hyperbolic systems

Consider the following system of linear PDE:

$$\mathbf{u}_t = A\mathbf{u}_x + \mathbf{F}, \quad x \in (0, W), \quad t > 0, \tag{2.1}$$

where the solution vector $\mathbf{u} = [u_1, \ldots, u_m]^T$ is a vector-valued function with m components and $A = A(x)$ is an $m \times m$ matrix.

Example: A system of $m = 2$ equations is given by

$$\mathbf{u}(x,t) = \begin{bmatrix} u_1(x,t) \\ u_2(x,t) \end{bmatrix}, \quad A(x) = \begin{bmatrix} a_{11}(x) & a_{12}(x) \\ a_{21}(x) & a_{22}(x) \end{bmatrix}, \quad \mathbf{F}(x,t) = \begin{bmatrix} F_1(x,t) \\ F_2(x,t) \end{bmatrix}. \tag{2.2}$$

This system can equivalently be written

$$\begin{cases} u_{1,t} = a_{11}u_{1,x} + a_{12}u_{2,x} + F_1 \\ u_{2,t} = a_{21}u_{1,x} + a_{22}u_{2,x} + F_2 \end{cases}. \tag{2.3}$$

Definition 3. The PDE (2.1) is *hyperbolic* if $A(x)$ is diagonalizable and has only real eigenvalues for all $x \in [0, W]$.

Recall that hyperbolic PDEs describe wave propagation. The fact that A can be diagonalized with real eigenvalues means that we have

$$A(x) = T(x)\Lambda(x)T(x)^{-1}, \tag{2.4}$$

where Λ is a diagonal matrix that holds the eigenvalues of A. That is, if λ_i denotes the ith eigenvalue of A, then

$$\Lambda_{ii} = \lambda_i. \tag{2.5}$$

If A is Hermitian, then all its eigenvalues are real and (2.4) holds with a unitary matrix T (implying $T^{-1} = T^*$), yielding

$$A(x) = T(x)\Lambda(x)T(x)^*. \tag{2.6}$$

2.1.1 Constant coefficients

If A is constant we can decouple the equations in (2.1) by a change of variables. Let $\mathbf{w} = T^{-1}\mathbf{u}$. Multiplying (2.1) by T^{-1} from the left yields

$$T^{-1}\mathbf{u}_t = T^{-1}ATT^{-1}\mathbf{u}_x + T^{-1}\mathbf{F}, \tag{2.7}$$

where we used that $TT^{-1} = I$. Since A is assumed to be constant, so is T. This implies that $T^{-1}\mathbf{u}_x = (T^{-1}\mathbf{u})_x = \mathbf{w}_x$. Using also that $T^{-1}AT = \Lambda$ and introducing $\tilde{\mathbf{F}} = T^{-1}\mathbf{F}$, we obtain

$$\mathbf{w}_t = \Lambda \mathbf{w}_x + \tilde{\mathbf{F}}. \tag{2.8}$$

Notice that we have decoupled the equations, since the matrix Λ is diagonal! Every equation in the system (2.8) is a scalar advection equation. The new variables (the components of $\mathbf{w}$), which satisfy advection equations, are called the *characteristic variables*. The wave speeds are given by the eigenvalues of A. The i:th equation in (2.8) is (assuming zero forcing, for simplicity)

$$w_{i,t} = \lambda_i w_{i,x}. \tag{2.9}$$

Notice that this corresponds to an advection equation with wave speed $-\lambda_i$.

Exercise: Consider the problem

$$\begin{aligned} \mathbf{u}_t = A\mathbf{u}_x + \mathbf{F}, \quad x \in (0, W), \quad t > 0, \\ \mathbf{u} = \mathbf{u}_0, \quad x \in [0, W], \quad t = 0, \end{aligned} \tag{2.10}$$

Suppose that A is constant and diagonalizable with only real eigenvalues, with m_+ positive eigenvalues, m_- negative eigenvalues, and m_0 zero eigenvalues, where $m_+ + m_- + m_0 = m$. How many (scalar) boundary conditions must be imposed at each boundary for (2.10) to be well posed? Any linear boundary condition can be written in the form

$$\sum_{i=1}^{m} \alpha_i u_i = g, \tag{2.11}$$

for some coefficients α_i and boundary data g.

Solution: This question can be answered with very few calculations. We know that the forcing function F does not affect well-posedness, so we will study the homogeneous version. The PDE can be transformed into diagonal form:

$$\mathbf{w}_t = \Lambda \mathbf{w}_x. \tag{2.12}$$

Since the problems are equivalent, if one of them is well posed, then so is the other. It is therefore enough to study the diagonal form. Equation number i reads

$$w_{i,t} = \lambda_i w_{i,x}. \tag{2.13}$$

If $\lambda_i > 0$, this corresponds to an advection equation with left-going waves. We know that a BC is required on the inflow, the right boundary. Conversely, if $\lambda_i < 0$, a BC is required on the left boundary. If $\lambda_i = 0$, the PDE collapses to

$$w_{i,t} = 0 \tag{2.14}$$

which simply states that w_i is constant in time. No BC is required for this equation.

Conclusion: We need to impose m_+ BC on the right boundary and m_- BC on the left boundary, for a total of $m - m_0$ BC.

Remark. Note that there are typically many different sets of well-posed BC. They do not have to be of the simple form $w_i = 0$. The discussion above just answers *how many* BC are required at each boundary.

2.1.2 Energy analysis with constant coefficients

Consider the IBVP

$$\begin{aligned} \mathbf{u}_t = A\mathbf{u}_x, &\quad x \in (0,W), &\quad t > 0, \\ \mathbf{u} = \mathbf{u}_0, &\quad x \in [0,W], &\quad t = 0, \\ \mathcal{L}_\ell \mathbf{u} = g_\ell, &\quad x = 0, &\quad t > 0, \\ \mathcal{L}_r \mathbf{u} = g_r, &\quad x = W, &\quad t > 0, \end{aligned} \tag{2.15}$$

where the boundary conditions (described by $\mathcal{L}_{\ell,r}$) are yet to be prescribed. The diagonal form of the PDE and IC is

$$\begin{aligned} \mathbf{w}_t = \Lambda \mathbf{w}_x, &\quad x \in (0,W), &\quad t > 0, \\ \mathbf{w} = T^{-1}\mathbf{u}_0, &\quad x \in [0,W], &\quad t = 0. \end{aligned} \tag{2.16}$$

where $\mathbf{w} = T^{-1}\mathbf{u}$. Let us apply the energy method to the diagonal form. That is, we multiply by $\mathbf{w}^*$ from the left and integrate in space:

$$(\mathbf{w}, \mathbf{w}_t) = (\mathbf{w}, \Lambda \mathbf{w}_x) = [IBP] = \mathbf{w}^* \Lambda \mathbf{w}|_0^W - (\mathbf{w}_x, \Lambda \mathbf{w}) \,. \tag{2.17}$$

The conjugate transpose is

$$(\mathbf{w}_t, \mathbf{w}) = (\mathbf{w}_x, \Lambda^* \mathbf{w}) \,. \tag{2.18}$$

Adding the two equations above yields the energy rate

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{w}\|^2 = \mathbf{w}^* \Lambda \mathbf{w}|_0^W + (\mathbf{w}_x, (\Lambda^* - \Lambda)\mathbf{w}) \,. \tag{2.19}$$

Recall that the PDE is hyperbolic only if all eigenvalues of A are real, which implies $\Lambda^* = \Lambda$. We now obtain only boundary terms in the energy rate, which we can write as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{w}\|^2 = \mathbf{w}^* \Lambda \mathbf{w}|_0^W = \sum_{i=1}^m \lambda_i |w_i|^2 \Big|_0^W = \left[\sum_{i \in I_+} \lambda_i |w_i|^2 + \sum_{i \in I_-} \lambda_i |w_i|^2 \right]_0^W , \tag{2.20}$$

where I_+ and I_- denote the set of indices corresponding to positive and negative eigenvalues, i.e.

$$I_+ = \{i : \lambda_i > 0\}, \quad I_- = \{i : \lambda_i < 0\}. \tag{2.21}$$

For well-posedness we need to impose the minimal number of BC ($m - m_0$ conditions, as discussed above) that allows us to bound the right-hand side in the homogeneous version (zero boundary data). One option that yields dissipation in THV is so-called *characteristic boundary conditions*, which amounts to specifiying the ingoing characteristic variables:

$$w_i = g_i \; \forall i \in I_- \text{ at } x = 0, \quad w_i = g_i \; \forall i \in I_+ \text{ at } x = W. \tag{2.22}$$

This corresponds to the usual inflow boundary condition that we saw for the scalar advection equation, applied to each of the characteristic variables separately. After imposing characteristic BC, the energy rate (2.20) becomes (with zero boundary data)

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{w}\|^2 = -\sum_{i\in I_+}\lambda_i|w_i|^2\Big|_0 + \sum_{i\in I_-}\lambda_i|w_i|^2\Big|_W \leq 0. \tag{2.23}$$

Integrating in time leads to the energy estimate

$$\|\mathbf{w}(\cdot,t)\|^2 \leq \|\mathbf{w}(\cdot,0)\|^2 = \|T^{-1}\mathbf{u}_0\|^2. \tag{2.24}$$

We can transform this bound back to the original variables, $\mathbf{u}$. We have

$$\|\mathbf{u}\| = \|T\mathbf{w}\| \leq \|T\|\|\mathbf{w}\| \leq \|T\|\|T^{-1}\mathbf{u}_0\| \leq \|T\|\|T^{-1}\|\|\mathbf{u}_0\| = cond(T)\|\mathbf{u}_0\|, \tag{2.25}$$

which shows well-posedness in the original variables too. The norm of $\mathbf{u}$ may grow, but only by a factor of the condition number of T.

Remark. Characteristic boundary conditions are not the only well-posed option. There are usually many options. In fact, one can show that any set of conditions that uses the outgoing characteristic variables as data for one of the ingoing characterstic variables is well-posed. Thas is, conditions of the form

$$w_i = \sum_{j\in I_+}\alpha_{ij}w_j + g_i \;\forall i \in I_- \text{ at } x = 0, \quad w_i = \sum_{j\in I_-}\beta_{ij}w_j + g_i \;\forall i \in I_+ \text{ at } x = W, \tag{2.26}$$

are well posed.

2.1.3 The acoustic wave equation with variable material parameters

As a first example of a hyperbolic system with variable coefficients, let us study the acoustic wave equation:

$$\begin{aligned} \rho v_t + p_x &= 0, \quad x \in (0,W), \quad t > 0, \\ \tfrac{1}{K}p_t + v_x &= 0, \quad x \in (0,W), \quad t > 0, \\ v &= v_0, \quad x \in [0,W], \quad t = 0, \\ p &= p_0, \quad x \in [0,W], \quad t = 0, \end{aligned} \tag{2.27}$$

where the material parameters are density ($\rho = \rho(x) > 0$) and bulk modulus ($K = K(x) > 0$). The unknowns v and p are particle velocity and pressure, respectively. We will discuss appropriate boundary conditions later.

Let $\mathbf{u} = [v,p]^T$. The acoustic wave equation can be written in matrix-vector form:

$$\begin{aligned} C\mathbf{u}_t &= B\mathbf{u}_x, \quad x \in (0,W), \quad t > 0, \\ \mathbf{u} &= \mathbf{u}_0, \quad x \in [0,W], \quad t = 0, \end{aligned} \tag{2.28}$$

where $C = C(x)$ is Hermitian positive definite and B is constant and Hermitian. These properties are important. In fact, Maxwell's equations and the elastic wave equation can also be written in the form of (2.28). Most of the following analysis is therefore generally applicable.

In the specific case of the acoustic wave equation, we have

$$C = \begin{bmatrix} \rho & \\ & K^{-1} \end{bmatrix}, \quad B = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}. \tag{2.29}$$

Applying the energy method to (2.28) yields:

$$(\mathbf{u}, \mathbf{u}_t)_C = (\mathbf{u}, B\mathbf{u}_x) = [IBP] = \mathbf{u}^* B \mathbf{u}|_0^W - (\mathbf{u}_x, B\mathbf{u}). \tag{2.30}$$

The conjugate transpose is:

$$(\mathbf{u}_t, \mathbf{u})_C = (\mathbf{u}_x, B^*\mathbf{u}). \tag{2.31}$$

Adding the two equations, using $B = B^*$ (and dividing by 2), yields

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}\|_C^2 = \frac{1}{2}\mathbf{u}^* B \mathbf{u}|_0^W. \tag{2.32}$$

Finally, this a *physical* energy rate! For the acoustic wave equation, we have the energy

$$\frac{1}{2}\|\mathbf{u}\|_C^2 = \frac{1}{2}(v, \rho v) + \frac{1}{2}\left(p, K^{-1}p\right) =: E, \tag{2.33}$$

where $\frac{1}{2}(v, \rho v)$ is the kinetic energy and $\frac{1}{2}(p, K^{-1}p)$ is the potential energy. We further have

$$\frac{1}{2}\mathbf{u}^* B \mathbf{u}|_0^L = -pv|_0^L \tag{2.34}$$

which can be interpreted as a *work rate* (units of power), i.e., work being done on the system per unit time. The energy rate reads

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -pv|_0^W. \tag{2.35}$$

Boundary conditions that lead to energy conservation, and thus well-posedness, are:

$$v = 0 \text{ or } p = 0, \ x = 0, \quad v = 0 \text{ or } p = 0, \ x = W. \tag{2.36}$$

There are many other well-posed BC.

2.1.4 Characteristic variables of the acoustic wave equation

The aoustic wave equation can be written in the form $\mathbf{u}_t = A\mathbf{u}_x$, where

$$A = C^{-1}B = \begin{bmatrix} 0 & -\rho^{-1} \\ -K & 0 \end{bmatrix}. \tag{2.37}$$

The eigenvalues of A are $\pm c$, where $c = \sqrt{K/\rho}$ is the sound speed. A can be diagonalized by the matrix T:

$$T^{-1} = \begin{bmatrix} \rho c & 1 \\ -\rho c & 1 \end{bmatrix}, \quad T = \frac{1}{2}\begin{bmatrix} \frac{1}{\rho c} & -\frac{1}{\rho c} \\ 1 & 1 \end{bmatrix} \tag{2.38}$$

Proof:

$$\begin{aligned} T\Lambda T^{-1} &= \frac{1}{2}\begin{bmatrix} \frac{1}{\rho c} & -\frac{1}{\rho c} \\ 1 & 1 \end{bmatrix}\begin{bmatrix} -c & \\ & c \end{bmatrix}\begin{bmatrix} \rho c & 1 \\ -\rho c & 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} \frac{1}{\rho c} & -\frac{1}{\rho c} \\ 1 & 1 \end{bmatrix}\begin{bmatrix} -\rho c^2 & -c \\ -\rho c^2 & c \end{bmatrix} \\ &= \begin{bmatrix} 0 & -\rho^{-1} \\ -K & 0 \end{bmatrix} = A. \end{aligned} \tag{2.39}$$

Since A has real eigenvalues and can be diagonalized, the acoustic wave equation is a *hyperbolic* PDE. The characteristic variables are given by $\mathbf{w} = T^{-1}\mathbf{u}$ and are $p \pm \rho c v$. Note however, that the PDE can only be written in diagonal form if ρ and K are constant.

2.1.5 General hyperbolic systems with variable coefficients

As mentioned above, the acoustic and elastic wave equations as well as Maxwell's equations with variable material properties can all be written in the form

$$C\mathbf{u}_t = B\mathbf{u}_x \tag{2.40}$$

where $C = C(x)$ is Hermitian positive definite and B is constant and Hermitian. The energy method yields the energy rate

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}\|_C^2 = \frac{1}{2}\mathbf{u}^* B\mathbf{u}\Big|_0^W. \tag{2.41}$$

To determine how many BC are needed at each boundary, it is sufficient to study the eigenvalues of B. Note that B is assumed to be Hermitian and therefore has only real eigenvalues and can be diagonalized by a unitary matrix T, i.e.,

$$B = T\Lambda T^*. \tag{2.42}$$

We can write the energy rate as

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{u}\|_C^2 = \frac{1}{2}\mathbf{u}^* B\mathbf{u}\Big|_0^W = \frac{1}{2}\mathbf{u}^* T\Lambda T^*\mathbf{u}\Big|_0^L = \frac{1}{2}\mathbf{w}^*\Lambda\mathbf{w}\Big|_0^W = \frac{1}{2}\sum_{i=1}^{m}\lambda_i|w_i|^2\Big|_0^W, \tag{2.43}$$

where $\mathbf{w} = T^*\mathbf{u}$ and λ_i are the eigenvalues of B. This shows that for every positive eigenvalue we need one BC at $x = W$ and for every negative eigenvalue we need one at $x = 0$. Zero eigenvalues do not require a BC.

2.2 The acoustic wave equation in second-order form

The acoustic wave equation can be written as a scalar, second-order PDE (often called simply "the wave equation") and is often solved in this form. One way to derive the second-order form is to start from the first-order system:

$$\begin{aligned} \rho v_t &= -p_x, \\ \tfrac{1}{K} p_t &= -v_x, \end{aligned} \tag{2.44}$$

and then apply ∂_x to the first equation and ∂_t to the second, yielding

$$\begin{aligned} v_{tx} &= -(\rho^{-1} p_x)_x, \\ \tfrac{1}{K} p_{tt} &= -v_{xt}. \end{aligned} \tag{2.45}$$

Eliminating v yields a scalar equation for p:

$$\frac{1}{K} p_{tt} = (\rho^{-1} p_x)_x. \tag{2.46}$$

It is common to solve this equation for p. However, this form of the equation suffers from the annoying property that the energy method does not yield the physical energy. It might therefore be preferrable to introduce the *momentum potential*, ϕ, which by definition satisfies

$$\phi_x = \rho v, \quad \phi_t = -p. \tag{2.47}$$

Using (2.47) and (2.44), we can derive

$$\frac{1}{K}\phi_{tt} = -\frac{1}{K} p_t = v_x = (\rho^{-1}\phi_x)_x, \tag{2.48}$$

i.e.,

$$\frac{1}{K}\phi_{tt} = (\rho^{-1}\phi_x)_x. \tag{2.49}$$

Notice that ϕ satisfies the same PDE as p.

Remark. If ρ is constant the acoustic wave equation can be written in the canonical form

$$\phi_{tt} = c^2 \phi_{xx}, \tag{2.50}$$

where $c = \sqrt{K/\rho}$ is the sound speed.

2.2.1 Energy analysis

Since the PDE contains ϕ_{tt}, the energy method starts by mutiplying with ϕ_t. Let us assume that all quantities are real. We have

$$\underbrace{\left(\phi_t, K^{-1}\phi_{tt}\right)}_{=\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(\phi_t, K^{-1}\phi_t)} = \left(\phi_t, (\rho^{-1}\phi_x)_x\right) = [IBP] = \phi_t \rho^{-1}\phi_x\Big|_0^W - \underbrace{\left(\phi_{tx}, \rho^{-1}\phi_x\right)}_{=\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(\phi_x, \rho^{-1}\phi_x)}. \tag{2.51}$$

We obtain the energy rate

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \phi_t \rho^{-1} \phi_x \big|_0^W , \tag{2.52}$$

where the energy is

$$E = \frac{1}{2} \left(\phi_t, K^{-1} \phi_t \right) + \frac{1}{2} \left(\phi_x, \rho^{-1} \phi_x \right) . \tag{2.53}$$

Using the definition of the momentum potential, we can show that this energy rate is identical to what we obtained for the first-order system, given by (2.35) and (2.33).

We know that we need two BC in total because the PDE is scalar and second order in space. BC that yield energy conservation (with zero boundary data) are

$$\phi = 0 \text{ or } \phi_x = 0, \ x = 0, \quad \phi = 0 \text{ or } \phi_x = 0, \ x = W. \tag{2.54}$$

2.2.2 Well-posed IBVP

For PDE that are second order in time, we need two initial conditions. An IBVP for the wave equation is thus

$$\begin{aligned} \tfrac{1}{K}\phi_{tt} = (\rho^{-1}\phi_x)_x + F, &\quad x \in (0, W), &\quad t > 0, \\ \phi = \phi_0, &\quad x \in [0, W], &\quad t = 0, \\ \phi_t = \varphi_0, &\quad x \in [0, W], &\quad t = 0, \\ \mathcal{L}_\ell \phi = g_\ell, &\quad x = 0, &\quad t > 0, \\ \mathcal{L}_r \phi = g_r, &\quad x = W, &\quad t > 0. \end{aligned} \tag{2.55}$$

This IBVP is well-posed if the boundary operators $\mathcal{L}_{\ell,r}$ are such that the homogeneous version of the IBVP (where $F = 0$, $g_{\ell,r} = 0$) does not allow for energy growth, i.e., the energy rate satisfies

$$\frac{\mathrm{d}E}{\mathrm{d}t} \leq 0. \tag{2.56}$$

3 The energy method in 2D and 3D

3.1 Integration by parts in higher dimensions

Let Ω denote a bounded domain in $\mathbb{R}^n$, with boundary $\partial\Omega$ and outward unit normal $\hat{\mathbf{n}}$. For a (sufficiently smooth) scalar function $u \in L^2(\Omega)$ and a (sufficiently smooth) vector field $\mathbf{v} \in L^2(\Omega)$, we have

$$\int_\Omega u\nabla\cdot\mathbf{v}\,\mathrm{d}\Omega = \oint_{\partial\Omega} u(\mathbf{v}\cdot\hat{\mathbf{n}})\,\mathrm{d}S - \int_\Omega \nabla u\cdot\mathbf{v}\,\mathrm{d}\Omega. \tag{3.1}$$

This is a consequence of the divergence theorem and can be viewed as a higher-dimensional version of the integration-by-parts formula. Substituting $\mathbf{v} = \alpha\nabla w$ in (3.1), where α and w are scalar functions, yields the following useful relation:

$$\int_\Omega u\nabla\cdot\alpha\nabla w\,\mathrm{d}\Omega = \oint_{\partial\Omega} u(\alpha\nabla w\cdot\hat{\mathbf{n}})\,\mathrm{d}S - \int_\Omega \nabla u\cdot\alpha\nabla w\,\mathrm{d}\Omega. \tag{3.2}$$

The normal derivative $\frac{\partial}{\partial\hat{\mathbf{n}}}$ is defined by

$$\frac{\partial w}{\partial\hat{\mathbf{n}}} = \nabla w\cdot\hat{\mathbf{n}}. \tag{3.3}$$

We can therefore write (3.2) as

$$\int_\Omega u\nabla\cdot\alpha\nabla w\,\mathrm{d}\Omega = \oint_{\partial\Omega} u\alpha\frac{\partial w}{\partial\hat{\mathbf{n}}}\,\mathrm{d}S - \int_\Omega \nabla u\cdot\alpha\nabla w\,\mathrm{d}\Omega. \tag{3.4}$$

Introducing the inner product for (possibly) vector-valued functions $\boldsymbol{\phi}, \boldsymbol{\psi}$ in $L^2(\Omega)$,

$$(\boldsymbol{\phi},\boldsymbol{\psi}) = \int_\Omega \boldsymbol{\phi}^*\boldsymbol{\psi}\,\mathrm{d}\Omega, \tag{3.5}$$

we can write (3.1) and (3.4) as

$$(u,\nabla\cdot\mathbf{v}) = \oint_{\partial\Omega} u^*(\mathbf{v}\cdot\hat{\mathbf{n}})\,\mathrm{d}S - (\nabla u,\mathbf{v}) \tag{3.6}$$

and

$$(u,\nabla\cdot\alpha\nabla w) = \oint_{\partial\Omega} u^*\alpha\frac{\partial w}{\partial\hat{\mathbf{n}}}\,\mathrm{d}S - (\nabla u,\alpha\nabla w)\,. \tag{3.7}$$

The relation (3.7) is useful when applying the energy method to, for example, the wave equation, the heat equation, and the Schrödinger equation.

3.2 Example: the heat equation

The heat equation can be written

$$\rho c_p u_t = \nabla \cdot \kappa \nabla u + F, \quad \mathbf{x} \in \Omega, \quad t > 0 \tag{3.8}$$

where u is temperature, $\kappa = \kappa(\mathbf{x})$ is the thermal conductivity, $c_p = c_p(\mathbf{x})$ is specific heat capacity, $\rho = \rho(\mathbf{x})$ is density, and $F = F(\mathbf{x}, t)$ is the volumetric heat source. We assume that all quantities are real. The energy method yields (with $F = 0$)

$$\underbrace{(u, u_t)_{\rho c_p}}_{=\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{\rho c_p}} = (u, \nabla \cdot \kappa \nabla u) = [\text{IBP, using (3.7)}] = \oint_{\partial\Omega} u\kappa \frac{\partial u}{\partial \hat{\mathbf{n}}} \,\mathrm{d}S - \underbrace{(\nabla u, \kappa \nabla u)}_{=\|\nabla u\|^2_\kappa}. \tag{3.9}$$

We obtain the energy rate

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{\rho c_p} = \oint_{\partial\Omega} u\kappa \frac{\partial u}{\partial \hat{\mathbf{n}}} \,\mathrm{d}S - \|\nabla u\|^2_\kappa \leq \oint_{\partial\Omega} u\kappa \frac{\partial u}{\partial \hat{\mathbf{n}}} \,\mathrm{d}S. \tag{3.10}$$

For well-posedness, we need a boundary condition on the entire boundary $\partial\Omega$. For example, the boundary integral vanishes if we impose homogeneous Dirichlet conditions,

$$u = 0, \quad \mathbf{x} \in \partial\Omega, \tag{3.11}$$

or homogeneous Neumann conditions,

$$\kappa \frac{\partial u}{\partial \hat{\mathbf{n}}} = 0, \quad \mathbf{x} \in \partial\Omega. \tag{3.12}$$

We then obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{\rho c_p} \leq 0, \tag{3.13}$$

and thus well-posedness. Since boundary data do not affect well-posedness, corresponding inhomogeneous conditions are also well-posed. There are many other well-posed BC, including Robin conditions. It is also possible to divide $\partial\Omega$ into parts and impose, for example, Dirichlet conditions on one part and Neumann conditions on the other.

3.2.1 The heat equation on a rectangular domain

As an example of a domain, let $\Omega = [0, W_x] \times [0, W_y] \subset \mathbb{R}^2$. The boundary, $\partial\Omega$, can be divided into four vertical or horizontal lines (with subscripts corresponding to compass directions):

$$\begin{aligned} \Gamma_W &= \{(x, y) \in \partial\Omega : x = 0\} \\ \Gamma_E &= \{(x, y) \in \partial\Omega : x = W_x\} \\ \Gamma_S &= \{(x, y) \in \partial\Omega : y = 0\} \\ \Gamma_N &= \{(x, y) \in \partial\Omega : y = W_y\} \end{aligned} \tag{3.14}$$

For this specific domain, the general energy rate (3.10) can be written

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{\rho c_p} = \int_{\Gamma_E} u\kappa u_x \,\mathrm{d}S - \int_{\Gamma_W} u\kappa u_x \,\mathrm{d}S + \int_{\Gamma_N} u\kappa u_y \,\mathrm{d}S - \int_{\Gamma_S} u\kappa u_y \,\mathrm{d}S - \|\nabla u\|^2_\kappa. \tag{3.15}$$

4 Fourier analysis of well-posedness for periodic problems

So far, we have used the energy method to analyze well-posedness. The energy method is useful because it provides insight into which boundary conditions are well posed and whether they cause dissipation or growth of energy. The energy method also allows for variable coefficients in many cases. However, to determine if a PDE with constant coefficients is well posed in itself (that is, with periodic boundary conditions), it is often easier to use the so-called Fourier method.

4.1 Fourier series

The Fourier-series representation of a W-periodic function $u = u(x)$ is

$$u(x) = \sum_{k \in K_\infty} \widehat{u}_k e^{ikx}, \tag{4.1}$$

where $\widehat{u}_k$ is the Fourier coefficient corresponding to wavenumber k and K_∞ is the set of wavenumbers corresponding to W-periodic Fourier modes, i.e.,

$$K_\infty = \left\{ 0, \pm\frac{2\pi}{W}, \pm\frac{4\pi}{W}, \dots \right\}. \tag{4.2}$$

The Fourier coefficients are given by

$$\widehat{u}_k = \frac{1}{W} \int_0^W e^{-ikx} u(x) \, \mathrm{d}x. \tag{4.3}$$

Parselval's relation connects the norm of u and the magnitude of the Fourier coefficients:

$$\|u\|^2 = \sum_{k \in K_\infty} |\widehat{u}_k|^2. \tag{4.4}$$

4.2 Example: the advection equation

Consider the 1D advection equation,

$$u_t = -cu_x, \quad x \in (0, W), \quad t > 0, \tag{4.5}$$

with constant c and *periodic* boundary conditions. For any fixed time, we can decompose the solution into Fourier modes (e^{ikx}) and represent it as a Fourier series according to (4.1). This implies that the solution can be represented as a Fourier series with time-dependent coefficients:

$$u(x,t) = \sum_{k \in K_\infty} \widehat{u}_k(t) e^{ikx}. \tag{4.6}$$

Inserting this representation in the PDE yields

$$\sum_{k\in K_\infty} \frac{\mathrm{d}\widehat{u}_k}{\mathrm{d}t} e^{ikx} = -c \sum_{k\in K_\infty} ik\widehat{u}_k e^{ikx}. \tag{4.7}$$

Since the Fourier modes are *orthogonal*, the equality must hold mode by mode, i.e.,

$$\frac{\mathrm{d}\widehat{u}_k}{\mathrm{d}t} = -cik\widehat{u}_k, \quad \forall k \in K_\infty. \tag{4.8}$$

This is a set of scalar ODE for the Fourier coefficients. The solutions are

$$\widehat{u}_k(t) = \widehat{u}_k(0)e^{-ikct}, \tag{4.9}$$

where $\widehat{u}_k(0)$ are the Fourier coefficients of the initial data. In this case, we can see that the Fourier coefficients do not grow or decay in time, since $|e^{-ikct}| = 1$. The same holds for $\|u\|$ according to Parseval's relation:

$$\|u(\cdot,t)\|^2 = \sum_{k\in K_\infty} |\widehat{u}_k(t)|^2 = \sum_{k\in K_\infty} |\widehat{u}_k(0)|^2 = \|u(\cdot,0)\|^2, \tag{4.10}$$

which matches the energy estimates that we have derived for the advection equation.

This example illustrates that we can analyze well-posedness of periodic problems by studying the growth of the Fourier coefficients.

4.3 General 1D PDEs

Consider a general linear and periodic problem

$$u_t = \mathcal{D}u + F, \quad x \in (0, W), \quad t > 0, \tag{4.11}$$

where $\mathcal{D}$ is a differential operator. For well-posedness it is sufficient to study the homogeneous version, so we set $F = 0$. The Fourier coeffiecients satisfy the ODE

$$\frac{\mathrm{d}\widehat{u}_k}{\mathrm{d}t} = \widehat{\mathcal{D}}(k)\widehat{u}_k, \tag{4.12}$$

where $\widehat{\mathcal{D}}(k)$ is the Fourier transform of $\mathcal{D}$, which can be obtained by replacing every $\frac{\partial}{\partial x}$ by ik, just like in the example with the advection equation. $\widehat{\mathcal{D}}(k)$ is sometimes referred to as the *symbol* of $\mathcal{D}$.

Let c be a real constant and $a > 0$ a real, positive constant. Examples of $\widehat{\mathcal{D}}(k)$ are

$$\begin{aligned}
&\mathcal{D} = -c\frac{\partial}{\partial x} \longrightarrow \quad \widehat{\mathcal{D}}(k) = -cik && \text{(advection equation)} \\
&\mathcal{D} = a\frac{\partial^2}{\partial x^2} \longrightarrow \quad \widehat{\mathcal{D}}(k) = a(ik)^2 = -ak^2 && \text{(heat equation)} \\
&\mathcal{D} = ic\frac{\partial^2}{\partial x^2} \longrightarrow \quad \widehat{\mathcal{D}}(k) = ic(ik)^2 = -ick^2 && \text{(Schrödinger equation).}
\end{aligned} \tag{4.13}$$

The Fourier coefficients satisfy

$$\widehat{u}_k(t) = \widehat{u}_k(0) e^{\widehat{\mathcal{D}}(k)t}, \tag{4.14}$$

and hence the periodic problem is well posed if there are constants K and α such that

$$|e^{\widehat{\mathcal{D}}(k)t}| \leq K e^{\alpha t} \tag{4.15}$$

for all k. See [1], page 19.

For our three example PDEs, we have

advection equation:	$\mathcal{D} = -c\dfrac{\partial}{\partial x}$,	$\widehat{\mathcal{D}}(k) = -cik$, $\quad \lvert e^{\widehat{\mathcal{D}}(k)t}\rvert = 1$	(conservation)
heat equation:	$\mathcal{D} = a\dfrac{\partial^2}{\partial x^2}$,	$\widehat{\mathcal{D}}(k) = -ak^2$, $\quad \lvert e^{\widehat{\mathcal{D}}(k)t}\rvert = e^{-ak^2 t} \leq 1$	(dissipation)
Schrödinger equation:	$\mathcal{D} = ic\dfrac{\partial^2}{\partial x^2}$,	$\widehat{\mathcal{D}}(k) = -ick^2$, $\quad \lvert e^{\widehat{\mathcal{D}}(k)t}\rvert = 1$	(conservation)

All three examples are clearly well posed (they satisfy (4.15) with $K = 1$, $\alpha = 0$). We can see that a purely imaginary $\widehat{\mathcal{D}}$ conserves the magnitude of all Fourier coefficients and is therefore characteristic of wave propagation (advection and Schrödinger equations). A negative real part of $\widehat{\mathcal{D}}$ implies decay (the heat equation) while a positive real part indicates growth. In the heat equation, the rate of dissipation depends on the wavenumber, k. Large wavenumbers dissipate the fastest.

An example of an ill-posed problem is the *backwards* heat equation:

$$\begin{aligned} &u_t = a u_{xx}, \quad && x \in (0, W), \quad && 0 \leq t < T, \\ &u = u_T, && x \in [0, W], && t = T, \end{aligned} \tag{4.16}$$

where the temperature at some time T is known and we are trying to determine the temperature at previous times. After the change of variables $\tau = T - t$, the problem reads

$$\begin{aligned} &u_\tau = -a u_{xx}, \quad && x \in (0, W), \quad && 0 \leq \tau < T, \\ &u = u_T, && x \in [0, W], && \tau = 0. \end{aligned} \tag{4.17}$$

The symbol of the spatial operator is

$$\widehat{\mathcal{D}}(k) = ak^2 \tag{4.18}$$

and therefore

$$|e^{\widehat{\mathcal{D}}(k)\tau}| = e^{ak^2\tau}, \tag{4.19}$$

which cannot be bounded by $Ke^{\alpha\tau}$, since k may be arbitrarily large. This shows that the backwards heat equation is ill posed.

References

[1] B. Gustafsson. *High Order Difference Methods for Time Dependent PDE.* Springer, 2007. doi:10.1007/978-3-540-74993-6.