KTH Computer Science
and Communication

Lecture Notes 1

Introduction to PDEs

- In *partial differential equations* (PDEs) the unknown function depends on several variables and the equation includes partial derivatives with respect to those, e.g.

$$au_{xx} + bu_{xy} + cu_{yy} = 0, \qquad u = u(x, y). \tag{1}$$

  Often one of the variables represents time and the rest space.

- PDEs an extremely useful tool for modeling of physical (and many other) processes. Some well-known examples are the Maxwell equations (electromagnetics), the Navier–Stokes equations (fluid dynamics), the Schrdinger equation (quantum mechanics), the wave equation etc.

- Seldom a closed form analytical solution for these equation. Numerical methods are the therefore very important.

1 Physical origins – conservation laws

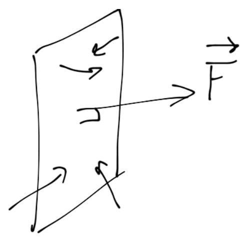
Many of the classical PDEs are based on conservation principles and derived as follows.

- Let $u(t, x)$ be the unknown, e.g. the number of particles per volume moving around in a fluid.

- Define the *flux* $\vec{F}(t, x)$ such that

$$|\vec{F}| := \text{number of particles flowing in direction } \vec{F} \text{ per area and time}$$

  (i.e. number of particles flowing through a m^2 surface orthogonal to $\vec{F}$ per second)



- Then the total number of particles passing through a given surface S is

$$Q_S(t) = \int_S \vec{F} \cdot \vec{n} dS,$$

  where $\vec{n}$ is the surface normal.

- Then because of *conservation* of particles (no new are created or destroyed) we must have that the change in the number of particles inside a given volume is completely determined by the flux of particles through the volume surface. Hence, for a given volume V with surface S,

$$\underbrace{\frac{d}{dt}\underbrace{\int_V udV}_{\#\text{ particles in } V}}_{\text{change in }\#\text{ particles}} = \underbrace{-Q_S(t)}_{\#\text{ particles flowing out through } S} = -\int_S \vec{F}\cdot\vec{n}dS. \tag{2}$$

This gives the *conservation law* for u in integral form,

$$\frac{d}{dt}\int_V udV + \int_S \vec{F}\cdot\vec{n}dS = 0. \tag{3}$$

- By applying the divergence theorem to the second term we obtain

$$\frac{d}{dt}\int_V udV + \int_V \nabla\cdot\vec{F}dV = 0.$$

This is true for any volume V and it will therefore also hold pointwise[1]. We get

$$u_t + \nabla\cdot\vec{F} = 0, \tag{4}$$

which is the conservation law in differential (or strong) form.

The conservation laws (3) and (4) is the mathematical encoding of the conservation property. Precisely the same arguments can be made for anything that is conserved, such as mass, momentum, heat, etc. The dynamics of these quantities will therefore all satisfy conservation laws of the type (3) and (4).

The conservation law as written above is not a closed system. There are $n+1$ unknowns (u and the n-dimensional flux vector $\vec{F}$) but only one equation. To close the system we need to express $\vec{F}$ in terms of u. This is done via *constitutive relations* based on more precise physics.

Example 1: Particles moving passively with constant (known) velocity $\vec{v}$. Then

$$\vec{F} = u\vec{v},$$

particles per unit area and time, and the PDE becomes

$$u_t + \nabla\cdot(u\vec{v}) = u_t + \vec{v}\cdot\nabla u = 0,$$

which is the *advection equation*.

Example 2: For large number of particles moving randomly the flux follows Fick's law,

$$\vec{F} = -d\nabla u,$$

which says that the net flow of particles go from regions with many particles to regions with fewer particles, i.e. in the direction of the negative gradient of the concentration. The proportionality constant d is called the diffusion coefficient of the system and the resulting PDE is the diffusion equation

$$u_t - \nabla\cdot(d\nabla u) = 0.$$

[1]This can be shown by shrinking the volume V to zero around a point.

The same equation also holds for heat conduction. Then u is the temperature and the heat flux satisfies Fourier's law

$$\vec{F} = -k\nabla u,$$

leading to the heat equation

$$u_t - \nabla \cdot (k\nabla u) = 0,$$

where k is the thermal conductivity of the medium.

2 General properties

There are three main classes of PDEs: hyperbolic, parabolic and elliptic. In this section we list the simplest examples and general properties for each category.

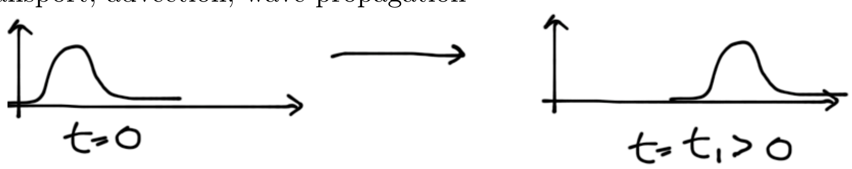
1. **Hyperbolic equations**

   Model equations

   $$u_t + u_x = 0, \qquad \text{advection equation,}$$
   $$u_{tt} - u_{xx} = 0, \qquad \text{wave equation.}$$

   Phenomena

   Transport, advection, wave propagation



   u time-dependent, no steady state, $\vec{F}$ depends on u, $b^2 - 4ac > 0$ in (1)

   Physics

   Fluid flow, electromagnetic, acoustic and elastic waves

2. **Parabolic equations**

   Model equation

   $$u_t - u_{xx} = 0, \qquad \text{diffusion/heat equation.}$$

   Phenomena

   Diffusion, "smearing"

   u time-dependent, has steady state, $\vec{F}$ depends on ∇u, $b^2 - 4ac = 0$ in (1)

   Physics

   Heat conduction, diffusion. Also e.g. option pricing via the Black–Scholes equation

   $$u_t + \frac{1}{2}\sigma^2 x^2 u_{xx} + rxu_x - ru = 0,$$

   where $u(t, x)$ is the option price at time t if the stock price is x; σ is the volatility and r the risk free interest rate.

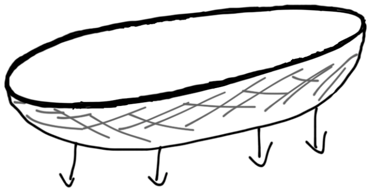
3. **Elliptic equations**

Model equation

$$-\Delta u = f(x), \qquad\qquad \text{Poisson equation.}$$

Phenomena

Equilibrium (e.g. deflection of membrane under a load)



Not a conservation law, u not time-dependent, but represents steady state as $t \to \infty$ in parabolic equation, $b^2 - 4ac < 0$ in (1)

Physics

Electric potential, structural mechanics, potential flow

3 Adding realism

The simple versions of the heat, advection and Poisson equations above are the model equations for the parabolic, hyperbolic and elliptic classes of PDEs. They represent idealized situations but capture the main characteristics and numerical difficulties for all equations in these classes. Of course, reality is more complicated. To add realism we must consider a number of additional issues, for instance:

Higher dimensions

For instance,

$$\begin{aligned} u_t + u_x &= 0 \quad \Rightarrow \quad & u_t + \vec{v}\cdot\nabla u &= 0 \qquad \text{(advection equation)}\\ u_{tt} - u_{xx} &= 0 \quad \Rightarrow \quad & u_{tt} - \Delta u &= 0 \qquad \text{(wave equation)}\\ u_t - u_{xx} &= 0 \quad \Rightarrow \quad & u_t - \Delta u &= 0 \qquad \text{(heat equation)} \end{aligned}$$

Systems of equations

Many PDEs actually have vectors as unknowns,

$$u_t + u_x = 0 \quad \Rightarrow \quad \vec{u}_t + A\vec{u}_x = 0.$$

For instance, the hyperbolic Maxwell equations for electromagnetics are of this form, where $\vec{u}$ contains the components of the $\vec{B}$ and $\vec{H}$ fields.

Variable coefficients

When the physical properties of the system vary in space or time we get PDEs with variable coefficients. For instance, if the velocity in Example 1 above varies in space, $\vec{v} = \vec{v}(x)$ we get the variable coefficient advection equation,

$$u_t + \vec{v}\cdot\nabla u = 0 \quad \Rightarrow \quad u_t + \nabla\cdot(\vec{v}(x)u) = 0.$$

Similarly, if the heat conduction coefficient varies in space in Example 2,

$$u_t - \nabla \cdot (k\nabla u) = 0 \quad \Rightarrow \quad u_t - \nabla \cdot (k(x)\nabla u) = 0.$$

Source terms

Source terms are added to a conservation law if the conserved quantity, e.g. the particles in the derivation above, are created/destroyed by some external process. E.g. if $f(t,x)$ particles per unit time and volume are created/destroyed, the balance equation (2) becomes

$$\frac{d}{dt}\int_V u dV = -\int_S \vec{F}\cdot\vec{n} dS + \underbrace{\int_V f dV}_{\#\text{ particles created/time in } V},$$

for any volume V with surface S. In the same way as before, this gives a PDE with the source f in the right hand side,

$$u_t + \nabla \cdot \vec{F} = f(t,x).$$

Nonlinearities

When the flux is not a linear function of u (or ∇u) the resulting PDE will be nonlinear, such as the nonlinear advection equation,

$$u_t + u_x = 0 \quad \Rightarrow \quad u_t + f(u)_x = 0.$$

For instance, in Burger's equation, which is the simplest model of fluid dynamics, $f(u) = u^2/2$. This can be interpreted as $v = v(u) = u/2$ in the derivation of the advection equation. Hence, the velocity depends on the solution itself, which would happen e.g. if u represents the momentum or the kinetic energy.

4 Well-posedness

We say that a mathematical problem is well-posed if

1. There is a solution (existence),
2. The is only one solution (uniqueness),
3. The solution depends continuously on the data for the problem (stability).

Otherwise the problem is ill-posed. Well-posedness is the basic condition for a problem to be solvable by numerical methods. It is therefore a fundamental concept in applied mathematics. Note that, even if there exists a unique solution, i.e. if 1) and 2) holds, the problem cannot be solved if 3) does not hold.

Example 3: Suppose we want to solve the equation $f(x) = \delta$ for $\delta = 0$, when

$$f(x) = \begin{cases} x, & x \neq 0,\ x \neq 1, \\ 0, & x = 1, \\ 1, & x = 0. \end{cases}$$

Clearly, $x = 1$ is the unique solution to the problem. It is, however, impossible to find this solution by a numerical root-finding algorithm. The problem is ill-posed, since the solution does not depend continuously on δ.

In the preceding example the difficulty for a numerical method was quite clear. For PDEs the well-posedness issue is more subtle.

Example 4: The backward heat equation (note the plus sign),

$$u_t + u_{xx} = 0, \qquad u(0,x) = f(x),$$

is ill-posed, eventhough it has a unique solution. (This equation comes from changing $t \to -t$ in the heat equation, i.e. solving it backwards in time. However, physically we know that the heat transfer process is irreversible by the second law of thermodynamics.)

Example 5: Boundary conditions are important. For instance,

$$u_t + u_x = 0, \qquad u(0,x) = f(x), \qquad u(t,0) = u(t,1) = 0,$$

is ill-posed if $f \neq 0$, because it does not have a solution.

Note the relation between point 3) and the concept of *conditioning*. In a well-conditioned problem, a small change in the data results in a small change in the solution. In an ill-conditioned problem, a small change in the data can result in a large change in the solution. For both cases there is an upper bound of how much a change in input can be amplified as a change in output, namely the condition number – small for well-posed problems and large for ill-conditioned problems. In an ill-posed problem, however, there is no such bound and the condition number is formally infinite.

For linear PDE initial value problems

$$\begin{aligned} u_t &= Lu + F(t,x), \quad x \in \mathbb{R}^n, \quad t > 0 \\ u(0,x) &= f(x), \end{aligned} \tag{5}$$

where L is some linear differential operator, the last point in the requirements for well-posedness (stability) is made precise as follows. Suppose $\delta(t,x)$ and $\varepsilon(x)$ are small perturbations of $F(t,x)$ and $f(x)$ respectively. If $\tilde{u}$ solves the perturbed version of (5),

$$\begin{aligned} \tilde{u}_t &= L\tilde{u} + F(t,x) + \delta(t,x), \quad x \in \mathbb{R}^n, \quad t > 0 \\ \tilde{u}(0,x) &= f(x) + \varepsilon(x), \end{aligned} \tag{6}$$

then the difference $u - \tilde{u}$, in a fixed time interval, should become small when δ and ε becomes small, all in suitable norms.

We will now show that for (5) both the points 2) (uniqueness) and 3) (stability) follow if we have an estimate of how big the solution can be in terms of the initial data. This is called an *energy estimate* (or growth estimate). The estimate should state that for every $T > 0$ there is a number C such that whenever $F \equiv 0$, the solution of (5) satisfies

$$||u(t,\cdot)|| \leq C||f||, \qquad \text{for } \ 0 \leq t \leq T, \tag{7}$$

where $||\ \cdot\ ||$ is some appropriate norm, for instance the L^2-norm,

$$||v||_2^2 := \int_{\mathbb{R}^n} v^2(x)dx.$$

The number C may depend on T and the choice of norm, but it should be independent of f. Showing this kind of estimates is thus of great interest as it leads to both stability and uniqueness. Indeed, we can show the following theorem, where for simplicity we assume that L is independent of t.

Theorem 1 *Suppose a solution to (5) exists for every sufficiently smooth f and F. Let u, $\tilde{u}$ solve (5), (6) respectively when $L = L(x)$. If (7) holds, then*

$$||u(t,\cdot) - \tilde{u}(t,\cdot)|| \leq C\left(||\varepsilon|| + \int_0^T ||\delta(\tau,\cdot)||d\tau\right), \qquad \text{for} \quad 0 \leq t \leq T.$$

where C and $||\cdot||$ are the same as in (7). Moreover, the solution to (5) is unique.

We start by proving the uniqueness. Suppose u_1 and u_2 are two solutions to (5) and let $w = u_1 - u_2$. Then w solves

$$\begin{aligned} w_t &= Lw, \quad x \in \mathbb{R}^n, \quad t > 0, \\ w(0,x) &= 0. \end{aligned} \tag{8}$$

The energy estimate (7) can now be applied, giving $||w|| \leq 0$, i.e. $u_1 = u_2$, which shows uniqueness. To prove the first part of the theorem we use *Duhamel's principle* which says that a the solution to an inhomogeneous linear PDE with zero initial data, can be written as an integral over solutions to the corresponding homogeneous PDE. More precisely, if $L = L(x)$, F are sufficiently smooth and $\bar{z}(t,x,s)$ solves

$$\begin{aligned} \bar{z}_t &= L\bar{z}, \quad x \in \mathbb{R}^n, \quad t > 0, \\ \bar{z}(0,x,s) &= F(s,x), \end{aligned}$$

then

$$z(t,x) = \int_0^t \bar{z}(t-s,x,s)ds, \tag{9}$$

solves

$$\begin{aligned} z_t &= Lz + F(t,x), \quad x \in \mathbb{R}^n, \quad t > 0, \\ z(0,x) &= 0. \end{aligned} \tag{10}$$

This is easily verified by just plugging (9) into (10). We now let $\bar{q}(t,x,s)$ solve

$$\begin{aligned} \bar{q}_t &= L\bar{z}, \quad x \in \mathbb{R}^n, \quad t > 0, \\ \bar{q}(0,x,s) &= \delta(s,x), \end{aligned}$$

and let $v(t,x)$ solve

$$\begin{aligned} v_t &= Lv, \quad x \in \mathbb{R}^n, \quad t > 0, \\ v(0,x) &= \varepsilon(x). \end{aligned}$$

We then claim that

$$\tilde{u}(t,x) - u(t,x) = v(t,x) + \int_0^t \bar{q}(t-s,x,s)ds. \tag{11}$$

By the uniqueness established above it suffices to show that the functions in the left and right hand sides satisfy the same PDE. Since for $\tilde{u} - u$ we have

$$\begin{aligned} (\tilde{u} - u)_t &= L(\tilde{u} - u) + \delta(t,x), \quad x \in \mathbb{R}^n, \quad t > 0, \\ \tilde{u}(0,x) - u(t,x) &= \varepsilon(x), \end{aligned}$$

the claim (11) then follows from Duhamel's principle above and the linearity of the PDE. Finally, as the constant C in the energy estimate (7) is independent of f we get for $\tilde{u} - u$,

$$||\tilde{u}(t,\cdot) - u(t,\cdot)|| = \left\| v(t,\cdot) + \int_0^t \bar{q}(t-s,\cdot,s)ds \right\| \leq ||v(t,\cdot)|| + \int_0^t ||\bar{q}(t-s,\cdot,s)||ds$$
$$\leq C\left(||\varepsilon|| + \int_0^t ||\delta(s,\cdot)||ds \right).$$

Hence, with fixed T we see that $||\tilde{u}(t,\cdot) - u(t,\cdot)|| \to 0$ when $\varepsilon, \delta \to 0$ and $0 \leq t \leq T$, which means that u is continuous with respect to ε and δ.

Remark 1 *For linear PDEs with standard boundary conditions, the well-posedness issue is essentially resolved, in particular for the parabolic, hyperbolic and elliptic equations mentioned before. For nonlinear PDEs, however, well-posedness can be very difficult to verify and there are many open mathematical questions. For instance, the widely used Navier-Stokes equations,*[2]

$$\vec{u}_t + (\vec{u}\cdot\nabla)\vec{u} = \nu\Delta\vec{u} - \nabla p + f,$$
$$\nabla\cdot\vec{u} = 0.$$

describing incompressible fluids, still lack a proof of well-posedness (in 3D).[3] *Even for systems of* one-dimensional *hyperbolic conservation laws*

$$\vec{u}_t + \vec{f}(\vec{u})_x = 0,$$

with some reasonable conditions on $\vec{f}(\vec{u})$ and initial data, full well-posedness was not proved until the late nineties.[4]

4.1 Proving energy estimates

We saw above that proving energy estimates for a problem is important to be able to verify well-posedness. For linear problems an energy estimate implies stability and uniqueness. There are a couple of standard approaches for making such proofs. We discuss two here: Fourier analysis and the energy method.

4.1.1 Fourier analysis

When the problem has constant coefficients one can often solve it explicitly by using the Fourier transform. This is true when there are no boundaries (e.g. the Cauchy problem, when the problem is set on the whole real line) or if the boundary conditions are periodic. From Parseval's theorem one can then get an expression for the L^2 norm of the solution at any time, which can be bounded to obtain (7). We show two examples.

Example 6: Consider the constant coefficient heat equation on $\mathbb{R}$,

$$u_t = u_{xx}, \qquad x \in \mathbb{R},\ t > 0,$$
$$u(0,x) = f(x).$$

[2] The gradient ∇ and Laplace operator Δ are applied elementwise here.

[3] This is one of the Millennium Problems. There is a one million dollar prize for solving it. See `www.claymath.org/millennium/Navier-Stokes_Equations`

[4] A. Bressan, G. Crasta, B. Piccoli. Well-posedness of the Cauchy problem for $n \times n$ systems of conservation laws. *Mem. Amer. Math. Soc.*, 146, 2000.

Let $\hat{u}(t,\xi)$ be the Fourier transform of $u(t,x)$ in space,

$$\hat{u}(t,\xi) = \frac{1}{2\pi}\int u(t,x)e^{-i\xi x}dx.$$

Since the Fourier transform of $u_x(t,x)$ is $i\xi\hat{u}(t,\xi)$ the PDE transforms into

$$\begin{aligned} \hat{u}_t &= -\xi^2\hat{u}, \qquad \xi\in\mathbb{R},\ t>0,\\ \hat{u}(0,\xi) &= \hat{f}(\xi). \end{aligned}$$

We can solve this explicitly,

$$\hat{u}(t,\xi) = \hat{u}(0,\xi)e^{-t\xi^2} = \hat{f}(\xi)e^{-t\xi^2}.$$

Parseval's theorem says that for a function $v\in L^2(\mathbb{R})$,

$$||v||_2 = ||\hat{v}||_2.$$

Applying this to our solution we obtain

$$||u(t,\cdot)||_2 = \left\|\hat{f}(\xi)e^{-t\xi^2}\right\|_2 \le ||\hat{f}||_2 = ||f||_2,$$

which is the desired energy estimate with $C=1$. (Here C is actually independent of T and (7) holds for all t.)

Example 7: Consider the constant coefficient advection equation with periodic boundary conditions,

$$\begin{aligned} u_t + u_x &= 0, \qquad x\in[0,2\pi],\ t>0,\\ u(t,0) &= u(t,2\pi),\\ u(0,x) &= f(x). \end{aligned}$$

In this case we write u as a Fourier series,

$$u(t,x) = \sum_{n=-\infty}^{\infty}\hat{u}_n(t)e^{inx}, \qquad \hat{u}_n(t) = \frac{1}{2\pi}\int_0^{2\pi}u(t,x)e^{-inx}dx.$$

As before, we use the simple expression of the Fourier coefficient $in\hat{u}_n$ for u_x to simplify the PDE,

$$\begin{aligned} \partial_t\hat{u}_n + in\hat{u}_n &= 0, \qquad n\in\mathbb{Z},\ t>0,\\ \hat{u}_n(0) &= \hat{f}_n. \end{aligned}$$

The solution is

$$\hat{u}_n(t) = \hat{u}_n(0)e^{-int} = \hat{f}_n e^{-int}.$$

In this case we have the following version of Parseval's theorem for an L^2 function v on $[0,2\pi]$,

$$||v||_2^2 = \int_0^{2\pi}|v(x)|^2dx = 2\pi\sum_{n=-\infty}^{\infty}|\hat{v}_n|^2 := ||\hat{v}||_2^2.$$

(We take the last equality as the definition of the norm for the infinite sequence $\{\hat{v}_n\}$.) Then we can do precisely as in the previous example to obtain the energy estimate,

$$||u(t,\cdot)||_2 = \left\|\left\{\hat{f}_n e^{-int}\right\}\right\|_2 = \left\|\left\{\hat{f}_n\right\}\right\|_2 = ||\hat{f}||_2 = ||f||_2.$$

Again we get the estimate with $C=1$.

4.1.2 Energy method

When the PDE has variable coefficients Fourier analysis does not work and one must resort to other methods such as the energy method. We show an example here for the advection equation. In Lecture notes 2 there is another, simpler, example showing how the energy method is used for the heat equation.

Example 8: Consider the variable coefficient advection equation with periodic boundary conditions and periodic coefficient $a(0) = a(2\pi)$,

$$\begin{aligned} u_t + (a(x)u)_x &= 0, \qquad x \in [0, 2\pi],\ t > 0, \\ u(t,0) &= u(t,2\pi), \\ u(0,x) &= f(x). \end{aligned}$$

We analyze the time derivative of the L^2 norm and assume the functions are all real,

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}||u(t,\cdot)||^2 &= \int_0^{2\pi} u(t,x)u_t(t,x)dx = \{\text{use the PDE}\} = \\ &= -\int_0^{2\pi} u(a(x)u)_x dx = \left\{2u(au)_x = u^2 a_x + (u^2 a)_x\right\} = \\ &= -\frac{1}{2}\int_0^{2\pi} (u^2 a(x))_x dx - \frac{1}{2}\int_0^{2\pi} u^2 a_x(x)dx \\ &= -\frac{1}{2}\int_0^{2\pi} u^2 a_x(x)dx. \end{aligned}$$

We can bound

$$\int_0^{2\pi} u^2 a_x(x)dx \le |a_x|_\infty \int_0^{2\pi} u^2 dx = |a_x|_\infty ||u(t,\cdot)||^2,$$

giving us

$$\frac{d}{dt}||u(t,\cdot)||^2 \le |a_x|_\infty ||u(t,\cdot)||^2.$$

Now let

$$z(t) = e^{-|a_x|_\infty t}||u(t,\cdot)||^2. \tag{12}$$

Then

$$\frac{dz}{dt} = -|a_x|_\infty z + e^{-|a_x|_\infty t}\frac{d}{dt}||u(t,\cdot)||^2 \le -|a_x|_\infty z + |a_x|_\infty e^{-|a_x|_\infty t}||u(t,\cdot)||^2 = 0.$$

Hence,

$$z(t) \le z(0),$$

or upon multiplying both sides by $\exp(|a_x|_\infty t)$,

$$||u(t,\cdot)||^2 \le e^{|a_x|_\infty t}||u(0,\cdot)||^2 = e^{|a_x|_\infty t}||f||^2.$$

We thus get (7) with $C = e^{|a_x|_\infty T/2}$.

5 Acknowledgement

Part of these notes are based on earlier notes by Prof. Jesper Oppelstrup.