MATH 461: Fourier Series and Boundary Value Problems

Chapter I: The Heat Equation

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Outline

Physical problem $\longrightarrow$ mathematical model $\longrightarrow$ approximate solution of problem (analytic or numeric)

Example

Growth of bacteria is often modeled using $\frac{dP}{dt} = kP$. The analytic solution is $P(t) = P_0 e^{kt}$. We could also solve the DE numerically (see MATH 350).

Why "approximate"?

- model usually idealized/simplified (e.g., infinite resources above; relativity theory applies to large scale problems, quantum mechanics to small scales $\rightarrow$ want unified theory (string theory?))
- modeling errors possible (e.g., different assumptions on how traffic or heat flows)
- data obtained from physical problem could be inaccurate (measurement errors)
- may need to truncate infinite series solutions to get practical answer
- possible roundoff or truncation errors in numerical solutions

Physical Problem

Cars traveling on the Chicago highway system.
How long does it take to get from *A* to *B*? How fast are cars able to travel at any specific position and time?

Math for traffic info services (e.g., GCM Travel)

Mathematical Model

Cars travel on an idealized one-lane road (no on- or off-ramps, no passing) – lots of simplification.

Consider a bunch of cars on our road. For each instance in time, t, each car will be at a specific position $x_i(t)$ moving with velocity $v_i(t)$, and we have

$$v_i(t) = \frac{\mathrm{d}x_i}{\mathrm{d}t}(t), \quad i = 1, \ldots, N.$$

If we view the traffic flow as a whole then it's more appropriate to introduce a velocity field v such that $v(x,t)$ denotes the velocity of the traffic at position x and time t.

Then the velocity of a car at position $x(t)$ (starting out at $x(t_0) = x_0$) is given by the solution of the first-order *ODE*

$$\frac{\mathrm{d}x}{\mathrm{d}t}(t) = v\left(x(t), t\right), \qquad x(t_0) = x_0.$$

See the example in the Mathematica notebook `Traffic.nb`.

Refined Mathematical Model

In addition to the velocity field, we now also consider

- the traffic density $\rho(x,t)$, i.e., the number of cars per unit length at any position x and time t [cars/km],
- the traffic flow rate or flux $\phi(x,t)$, i.e., the number of cars per unit time passing at position x and time t [cars/h].

The two are actually related via the velocity field:

$$\phi(x,t) = \rho(x,t)v(x,t) \qquad \left[\frac{\text{cars}}{\text{h}} = \frac{\text{cars}}{\text{km}}\frac{\text{km}}{\text{h}}\right]$$

How might we be able to compute one of these, say the density?

The fundamental assumption that allows us to build a (differential equation) model is a conservation law. We assume that no cars are added or removed between the starting point A and the ending point B.

Therefore,

$$\{\text{change in \# cars on } \overline{AB}\} = \{\text{\# cars entering at } A - \text{\# cars leaving at } B\}$$

or

$$\frac{\mathrm{d}}{\mathrm{d}t}N(t) = \phi(A,t) - \phi(B,t), \qquad (1)$$

where

$$N(t) = \int_A^B \rho(x,t)\mathrm{d}x. \qquad (2)$$

Combining (1) and (2) we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_A^B \rho(x,t)\mathrm{d}x = \phi(A,t) - \phi(B,t).$$

Using the FT of Calc we can express the difference in fluxes as

$$\phi(B,t) - \phi(A,t) = \int_A^B \frac{\partial}{\partial x}\phi(x,t)\mathrm{d}x.$$

Therefore, assuming the density ρ is continuous and A, B are const.,

$$\int_A^B \frac{\partial}{\partial t}\rho(x,t)\mathrm{d}x = -\int_A^B \frac{\partial}{\partial x}\phi(x,t)\mathrm{d}x$$

$$\iff \quad \int_A^B \left[\frac{\partial}{\partial t}\rho(x,t) + \frac{\partial}{\partial x}\phi(x,t)\right]\mathrm{d}x = 0$$

This gives rise to the partial differential equation (see Section 12.6 of [Haberman])

$$\frac{\partial}{\partial t}\rho(x,t) = -\frac{\partial}{\partial x}\phi(x,t)$$

$$\text{or} \quad \frac{\partial}{\partial t}\rho(x,t) = -\frac{\partial}{\partial x}\left[\rho(x,t)v(x,t)\right]$$

Even though the traffic flow equation

$$\frac{\partial}{\partial t}\rho(x,t) = -\frac{\partial}{\partial x}\left[\rho(x,t)v(x,t)\right]$$

is a first-order PDE it is more complicated to study than the second-order equations we will be looking at in this course since the traffic flow equation may develop a discontinuous solution or shock – even for a smooth initial condition (see the image in `Traffic.nb`).

The technique required to solve the traffic flow equation is discussed in MATH 489.

A nice Java applet simulating traffic flow (including shocks) can be found here and an html5 version here.

Modeling Summary

There are many other kinds of mathematical modeling situations such as

- *data fitting* (e.g., find the best approximation – from a certain linear/nonlinear function class – to given measurement data)
- *parameter estimation* (e.g., find the best parameters for one of the models used earlier – drag coefficient, birth/death rate, etc.)
- *statistical/probabilistic modeling* (e.g., non-deterministic models in finance or weather prediction)
- *discrete modeling* (e.g., determining the best location of a fire department or hospital on a network of roads)
- *geometric modeling* (e.g., used for CAD systems)
- *asymptotic modeling* (focus on extreme or limiting cases, can usually be done analytically)

An entertaining overview of the field of mathematical modeling is provided by Charlie's activities on the TV show *NUMB3RS*.

Heat Flow

We will formulate a model which describes how the temperature u changes over time t in a region (1D $\to x$, 2D $\to (x, y)$, or 3D $\to (x, y, z)$).

Since u is always at least a function of two variables, e.g., $u = u(x, t)$, this will lead to a partial differential equation or PDE involving the unknown function u along with its (partial) derivatives with respect to space and time, i.e., u_t, u_x, u_y, u_{xx}, etc.

Our models will also require certain initial and boundary conditions such as the entire temperature distribution at the beginning and the temperature on the boundary at any time t.

We can model heat transfer in basically two different forms:

conduction – molecules stay put and heat energy is transferred to neighboring molecules (in a solid body)

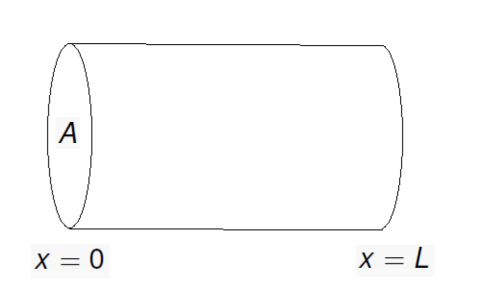
convection – molecules themselves move and generate heat energy (mostly in fluids or gases)

We will focus on heat conduction.

Our derivation will consist of two steps:

1. We use an energy conservation principle to derive a PDE for the heat energy in a one-dimensional rod.
2. Then we use Fourier's law of heat conduction to relate heat energy to temperature to obtain the so-called heat equation, a PDE that models the temperature in the rod at any position x and time t.

We consider a rod of length L and cross section A



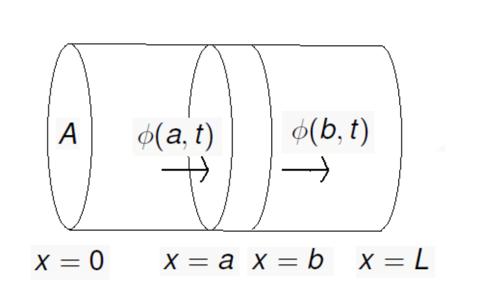
To understand the distribution of heat energy in the rod we consider the heat energy density $e = e(x, t)$, i.e., the heat energy per unit length at position x and time t.

Remark

We assume that e depends only on x and t. This means that the rod is insulated (except possibly at the ends) so that heat can only flow in the x-direction.

Similar to the traffic flow problem we also consider:

- The heat flux or heat flow rate $\phi(x,t)$, i.e., the amount of heat energy per unit time flowing (from left to right) through a unit cross-sectional area at x. Thus, $\phi(x,t) > 0$ denotes flow to right and $\phi(x,t) < 0$ flow to left.



- Possible heat sources $Q(x,t)$, i.e., the amount of heat energy per unit volume generated per unit time.

Conservation of Energy

This is the major physical assumption used:

{Rate of change of heat energy between $x = a$ and $x = b$}

$=$

{rate of heat energy flowing through ends}

$+$

{rate of heat energy generated inside segment of rod}

Remark

Note that all of these are rates of change per unit of time.

We express the ingredients for the conservation of energy principle:

Total heat energy between $x = a$ and $x = b$: $\quad A\int_a^b e(x,t)\mathrm{d}x,$

so that change of heat energy: $\quad \dfrac{\mathrm{d}}{\mathrm{d}t}\left[A\int_a^b e(x,t)\mathrm{d}x\right].$

Rate of heat energy flowing through ends: $\quad A\phi(a,t) - A\phi(b,t).$

Rate of heat energy generated inside: $\quad A\int_a^b Q(x,t)\mathrm{d}x.$

Together (conservation of energy – integral form):

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b e(x,t)\mathrm{d}x = \phi(a,t) - \phi(b,t) + \int_a^b Q(x,t)\mathrm{d}x \tag{3}$$

We can further manipulate (3):
First, provided that e is continuous and a, b are const. wrt t,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b e(x,t)\mathrm{d}x = \int_a^b \frac{\partial}{\partial t}e(x,t)\mathrm{d}x.$$

Second, by the FT of Calculus (provided $\phi \in C^1$),

$$\phi(a,t) - \phi(b,t) = \int_b^a \frac{\partial}{\partial x}\phi(x,t)\mathrm{d}x = -\int_a^b \frac{\partial}{\partial x}\phi(x,t)\mathrm{d}x.$$

So conservation of energy (3) becomes

$$\int_a^b \frac{\partial}{\partial t}e(x,t)\mathrm{d}x = -\int_a^b \frac{\partial}{\partial x}\phi(x,t)\mathrm{d}x + \int_a^b Q(x,t)\mathrm{d}x$$

or

$$\int_a^b \left[\frac{\partial}{\partial t}e(x,t) + \frac{\partial}{\partial x}\phi(x,t) - Q(x,t)\right]\mathrm{d}x = 0.$$

Since

$$\int_a^b \left[\frac{\partial}{\partial t}e(x,t) + \frac{\partial}{\partial x}\phi(x,t) - Q(x,t)\right] \mathrm{d}x = 0$$

holds for arbitrary a, b we have

$$\frac{\partial}{\partial t}e(x,t) + \frac{\partial}{\partial x}\phi(x,t) - Q(x,t) = 0$$

or

Conservation of energy (differential form):

$$\frac{\partial}{\partial t}e(x,t) = -\frac{\partial}{\partial x}\phi(x,t) + Q(x,t) \tag{4}$$

Remark

Equation (3) *is more general than* (4) *since it also applies if e and ϕ are not continuous.*

From Heat Energy to Temperature

We now introduce the following physical quantities:

- the temperature $u(x,t)$ at position x and time t,
- the specific heat $c(x)$ at position x (assumed not to vary over time t), i.e., the amount of heat energy required to raise the temperature of one unit of mass by one unit of temperature,
- the mass density $\rho(x)$ at position x (assumed not to vary over time t), i.e., the mass per unit volume.

These quantities are all related via the energy density. Namely,

$$e(x,t) = c(x)\rho(x)u(x,t).$$

Units:

$$\left[\frac{J}{m}\right] = \left[\frac{J}{kg\,^\circ C}\right]\left[\frac{kg}{m}\right]\left[^\circ C\right]$$

We can now modify the conservation of energy equation (4)

$$\frac{\partial}{\partial t} e(x,t) = -\frac{\partial}{\partial x}\phi(x,t) + Q(x,t)$$

to become

$$\frac{\partial}{\partial t}\left[c(x)\rho(x)u(x,t)\right] = -\frac{\partial}{\partial x}\phi(x,t) + Q(x,t)$$

or

$$c(x)\rho(x)\frac{\partial}{\partial t}u(x,t) = -\frac{\partial}{\partial x}\phi(x,t) + Q(x,t) \qquad (5)$$

Remark

This is still not ideal since it involves both temperature and energy flux. We need to unify further.

Fourier's Law of Heat Conduction

The final physical principle that makes everything come together.
Physical assumptions:

- If the temperature is constant, then no heat energy flows, i.e., $\phi = 0$.
- If there are temperature differences at different positions, then heat energy flows from hot to cold.
- The greater these differences, the greater the flux, i.e., $\phi \propto \frac{\partial}{\partial x} u$.
- Heat flow depends on the specific material of the rod.

The resulting formula is

$$\phi(x, t) = -K_0(x) \frac{\partial}{\partial x} u(x, t),$$

where the thermal conductivity K_0 depends on the material.

Remark

The "$-$" is needed since $\phi > 0$ indicates flow from left to right, but energy also flows from hot to cold and $\frac{\partial}{\partial x} u(x, t) < 0$ if it is warmer on the left.

Using Fourier's law of heat conduction

$$\phi(x,t) = -K_0(x)\frac{\partial}{\partial x}u(x,t),$$

we can rewrite (5) as

$$c(x)\rho(x)\frac{\partial}{\partial t}u(x,t) = \frac{\partial}{\partial x}\left[K_0(x)\frac{\partial}{\partial x}u(x,t)\right] + Q(x,t).$$

This is the heat equation in rather general form.
In most cases we will assume c, ρ, K_0 to be constant, i.e., we will use a uniform material. Then we get

$$c\rho\frac{\partial}{\partial t}u(x,t) = K_0\frac{\partial^2}{\partial x^2}u(x,t) + Q(x,t)$$

or

$$\frac{\partial}{\partial t}u(x,t) = k\frac{\partial^2}{\partial x^2}u(x,t) + q(x,t),$$

where $k = \frac{K_0}{c\rho}$, the thermal diffusivity and $q(x,t) = \frac{Q(x,t)}{c\rho}$.

Finally, if no sources are present, i.e., $Q(x, t) = 0$, then

$$\frac{\partial}{\partial t} u(x, t) = k \frac{\partial^2}{\partial x^2} u(x, t) \tag{6}$$

is the standard heat equation or diffusion equation.

Remark

The same form of equation also applies to many other situations, such as diffusion of pollutants, etc.

Initial Condition

In order to obtain a unique solution for a differential equation one needs to specify additional conditions – usually one for every derivative.

Since the heat equation contains $\frac{\partial u}{\partial t}$ we usually add an initial condition such as

$$u(x,0) = f(x), \quad 0 \le x \le L \qquad \text{(initial temperature distribution).}$$

The two conditions demanded by $\frac{\partial^2 u}{\partial x^2}$ are discussed next.

Remark

As we will see later, one cannot just add any set of conditions. They should be chosen such that the problem is well-posed, i.e., it should allow for the existence of a unique solution that depends continuously on the given conditions.

Boundary Conditions

We will consider three types of boundary conditions.

Controlled end temperature: e.g., using baths at the ends

$$\begin{aligned} u(0,t) &= u_{B_1}(t), \quad t > 0, \\ u(L,t) &= u_{B_2}(t), \quad t > 0. \end{aligned}$$

Insulated ends: Since the heat flow is $\phi(x,t) = -K_0 \frac{\partial u}{\partial x}(x,t)$ insulation (i.e, no heat flow) implies $\frac{\partial u}{\partial x} = 0$. Therefore,

$$\frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(L,t) = 0, \quad t > 0.$$

Newton's law of cooling: e.g., cooler air is passed by ends of rod

For Newton's law of cooling we assume there is only partial insulation governed by a positive heat transfer (or convection) coefficient H, e.g.,

$$\phi(0,t) = -H\left[u(0,t) - u_{B_1}(t)\right] \qquad \text{(Newton's law)}$$

Note "$-$" which indicates that – for a rod that is hotter than its environment – heat flow is negative, i.e., flows to the cooler environment (on the "left").
In terms of u we get (Fourier's law)

$$\frac{\partial u}{\partial x}(0,t) = \frac{H}{K_0}\left[u(0,t) - u_{B_1}(t)\right]$$

At the other end

$$\frac{\partial u}{\partial x}(L,t) = -\frac{H}{K_0}\left[u(L,t) - u_{B_2}(t)\right]$$

We also note that

- $H \to 0$ corresponds to perfect insulation
- $H \to \infty$ corresponds to controlled temperature

We are now ready to solve our first heat equation PDEs. We

- consider different types of boundary conditions
  - fixed end temperature
  - insulated ends
- under the fundamental simplifying assumption that we have observed the temperature distribution process for a long time and it has settled down to an equilibrium temperature distribution, i.e., the temperature no longer changes with time.

Controlled End Temperature

Problem:

$$\begin{aligned}
\frac{\partial u}{\partial t}(x,t) &= k\frac{\partial^2 u}{\partial x^2}(x,t) \\
u(x,0) &= f(x) \qquad \text{(initial condition)} \\
u(0,t) &= T_1(t) \qquad \text{(left-end BC)} \\
u(L,t) &= T_2(t) \qquad \text{(right-end BC)}
\end{aligned}$$

This is easy to solve if there is no time dependence, i.e., if

$$\frac{\partial u}{\partial t} \equiv 0 \quad \Longrightarrow \quad \text{equilibrium}$$

Then

$$\frac{\partial^2 u}{\partial x^2}(x,t) = 0 \quad \text{or really just} \quad u''(x) = 0$$

The IC becomes meaningless[1], and the BCs become

$$u(0) = T_1, \qquad u(L) = T_2.$$

[1] but should be consistent with the BCs

We solve $u''(x) = 0$ by integrating twice, i.e.,

$$u(x) = C_1 x + C_2$$

and use the BCs to determine C_1, C_2:

$$\begin{aligned} u(0) &= T_1 = C_2 \\ u(L) &= T_2 = C_1 L + T_1 \quad \Rightarrow \quad C_1 = \frac{T_2 - T_1}{L} \end{aligned}$$

Therefore

$$u(x) = T_1 + \frac{T_2 - T_1}{L} x,$$

i.e., the temperature distribution interpolates linearly between the fixed end temperatures.

Remark

We will later see that the time dependent PDE problem

$$\begin{aligned} \frac{\partial u}{\partial t}(x,t) &= k\frac{\partial^2 u}{\partial x^2}(x,t) \\ u(x,0) &= f(x) \end{aligned}$$

with time independent BCs

$$u(0,t) = T_1, \qquad u(L,t) = T_2$$

has (in the limit – for very large time) the steady-state solution we just computed, so in this case one can just solve the simple equilibrium problem from the previous slide.

Insulated Boundaries

Now we have

Problem:

$$\begin{aligned}
\frac{\partial u}{\partial t}(x,t) &= k\frac{\partial^2 u}{\partial x^2}(x,t) \\
u(x,0) &= f(x) \qquad \text{(initial condition)} \\
\frac{\partial u}{\partial x}(0,t) &= \frac{\partial u}{\partial x}(L,t) = 0 \qquad \text{(BCs)}
\end{aligned}$$

The steady-state ($\frac{\partial u}{\partial t} \equiv 0$) ODE problem then is

$$\begin{aligned}
u''(x) &= 0 \\
u'(0) &= u'(L) = 0
\end{aligned} \tag{7}$$

Its general solution (again via integration) is

$$u(x) = C_1 x + C_2.$$

If we try to use our BCs to determine C_1, C_2 we note that either one of the BCs implies

$$C_1 = 0 \qquad (\text{since } u'(x) = C_1)$$

This leaves us with a constant temperature distribution

$$u(x) = C_2.$$

But which constant C_2 specifies the “correct” temperature?

Remark

- *Note that the ODE problem* (7) *is not well posed. It does not have a unique solution.*
- *One might expect that the initial temperature distribution $f(x)$ should affect C_2.*
- *In general one should not expect $u(x) = f(x)$, but rather that the initial distribution somehow “levels out”.*

Since thermal energy is conserved inside the rod, we can go back to the integral form of the conservation of energy law (3):

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L e(x,t)\mathrm{d}x = \phi(0,t) - \phi(L,t) + \int_0^L Q(x,t)\mathrm{d}x$$

In terms of u this becomes (using $e = c\rho u$, Fourier's law and assuming $Q = 0$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L c\rho u(x,t)\mathrm{d}x = -K_0 \underbrace{\frac{\partial u}{\partial x}(0,t)}_{\overset{\mathrm{BC}}{=}0} + K_0 \underbrace{\frac{\partial u}{\partial x}(L,t)}_{\overset{\mathrm{BC}}{=}0}$$

so that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L c\rho u(x,t)\mathrm{d}x = 0$$

or

$$\int_0^L c\rho u(x,t)\mathrm{d}x = \text{const} \qquad (\text{total heat energy})$$

Since the total heat energy is constant for all time we must have

$$\underbrace{\{\text{initial energy}\}}_{u(x)=f(x)} = \underbrace{\{\text{equilibrium energy}\}}_{u(x)=C_2}$$

$$\int_0^L c\rho f(x)\mathrm{d}x = \int_0^L c\rho C_2 \mathrm{d}x$$

or

$$\int_0^L f(x)\mathrm{d}x = \int_0^L C_2\mathrm{d}x = LC_2$$

so that

$$C_2 = \frac{1}{L}\int_0^L f(x)\mathrm{d}x.$$

In summary, we get

$$u(x) = \frac{1}{L}\int_0^L f(x)\mathrm{d}x,$$

i.e., the steady-state temperature distribution is the average of the initial temperature distribution.

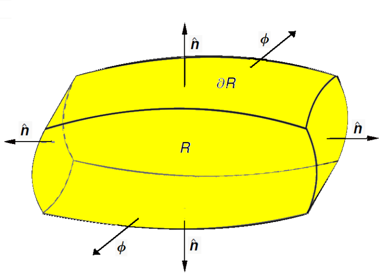
Derivation of the Heat Equation in 2D and 3D

We will discuss the 3D case since it is more realistic than 2D (whose derivation is quite similar).

In order to understand the following you should review volume and surface integrals from Calculus III (mostly Ch. 16 in [Stewart]).

Notation and quick refresher:

- R will denote the 3D region under consideration.
- The heat flux ϕ is now a vector field, i.e., $\phi = \phi(x, y, z, t)$. It specifies the amount of heat energy per unit time flowing through a unit of area of the boundary surface ∂R in the outward direction.
- The unit outer normal vector to R is denoted by $\hat{\boldsymbol{n}}$.

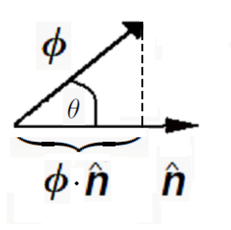


We will need only the normal component of the flux, i.e., the component of ϕ along $\hat{\boldsymbol{n}}$.

From Calc III:

- Projection (component of ϕ along $\hat{\boldsymbol{n}}$):

$$\text{proj}_{\hat{\boldsymbol{n}}}\phi = \|\phi\| \cos\theta$$



- Relation between angle and dot product:

$$\cos\theta = \frac{\phi \cdot \hat{\boldsymbol{n}}}{\|\phi\| \underbrace{\|\hat{\boldsymbol{n}}\|}_{=1}}$$

- Therefore

$$\text{proj}_{\hat{\boldsymbol{n}}}\phi = \phi \cdot \hat{\boldsymbol{n}} \qquad (8)$$

Of fundamental importance is also

Theorem (Divergence/Gauss/Ostrogradsky)

Suppose R is a bounded region in $\mathbb{R}^3$ with piecewise smooth boundary ∂R. If $\boldsymbol{f} = (f_1, f_2, f_3) \in C^1$ in an open region that contains R then

$$\iiint_R \nabla \cdot \boldsymbol{f}(x,y,z)\,\mathrm{d}V = \iint_{\partial R} \boldsymbol{f}(x,y,z) \cdot \hat{\boldsymbol{n}}(x,y,z)\,\mathrm{d}S,$$

where $\nabla \cdot \boldsymbol{f} = \frac{\partial}{\partial x} f_1 + \frac{\partial}{\partial y} f_2 + \frac{\partial}{\partial z} f_3 = \operatorname{div} \boldsymbol{f}$ and $\hat{\boldsymbol{n}}(x,y,z)$ is the unit outward normal vector to R at the point (x,y,z) of ∂R.

Remark

- *This is the 3D-analogue of the FT of Calculus.*
- *In 2D we would be using Green's theorem.*

Conservation of Energy (again)

$$\{\text{Rate of change of heat energy}\}$$
$$=$$
$$\{\text{rate of heat energy generated inside of } R\}$$
$$+$$
$$\{\text{rate of heat energy flowing through boundary surface}\}$$

We need to derive formulas for each one of these three parts.

Total heat energy:

$$\iiint\limits_R e(x,y,z,t)\,\mathrm{d}V = \iiint\limits_R c(x,y,z)\rho(x,y,z)u(x,y,z,t)\,\mathrm{d}V$$

Therefore, the rate of change of heat energy is

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint\limits_R c(x,y,z)\rho(x,y,z)u(x,y,z,t)\,\mathrm{d}V \tag{9}$$

Similarly, the rate of heat energy generated inside of R is

$$\iiint\limits_R Q(x,y,z,t)\,\mathrm{d}V \tag{10}$$

Using only the normal component of the heat flux (see (8)) we get the rate of heat energy flowing through boundary surface:

$$-\iint_{\partial R} \phi(x,y,z,t)\cdot\hat{\boldsymbol{n}}(x,y,z)\,\mathrm{d}S \tag{11}$$

Remark

The "$-$" sign appears since outward flow ϕ is positive, but such a flow reduces the heat energy.

Combining (9–11) the conservation of energy principle gives:

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint\limits_R c\rho u\,\mathrm{d}V = -\iint\limits_{\partial R} \boldsymbol{\phi}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S + \iiint\limits_R Q\,\mathrm{d}V \tag{12}$$

In order to get the heat equation in PDE form we need to convert the surface integral

$$\iint\limits_{\partial R} \boldsymbol{\phi}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S$$

into a volume integral.
This is where we will use the divergence theorem, i.e.,

$$\iint\limits_{\partial R} \boldsymbol{\phi}\cdot\hat{\boldsymbol{n}}\,\mathrm{d}S = \iiint\limits_R \nabla\cdot\boldsymbol{\phi}\,\mathrm{d}V \tag{13}$$

Using the divergence theorem for ϕ, (13), equation (12)

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint_R c\rho u \,\mathrm{d}V = -\iint_{\partial R} \phi \cdot \hat{\boldsymbol{n}} \,\mathrm{d}S + \iiint_R Q \,\mathrm{d}V$$

now becomes

$$\iiint_R c\rho \frac{\partial}{\partial t} u \,\mathrm{d}V = -\iiint_R \nabla \cdot \phi \,\mathrm{d}V + \iiint_R Q \,\mathrm{d}V$$

or

$$\iiint_R \left[c\rho \frac{\partial}{\partial t} u + \nabla \cdot \phi - Q \right] \mathrm{d}V = 0.$$

Since this holds for arbitrary R we get (compare with (5))

$$c(x,y,z)\rho(x,y,z)\frac{\partial}{\partial t}u(x,y,z,t) = -\nabla \cdot \phi(x,y,z,t) + Q(x,y,z,t).$$

As in 1D we now use Fourier's law of heat conduction:

In its 3D form the flux ϕ is proportional to the temperature gradient $\nabla u = \left(\frac{\partial}{\partial x}u, \frac{\partial}{\partial y}u, \frac{\partial}{\partial z}u\right)$, i.e.,

$$\phi(x,y,z,t) = -K_0(x,y,z)\nabla u(x,y,z,t)$$

and so we get the

Heat equation in 3D:

$$c\rho\frac{\partial}{\partial t}u = \nabla\cdot(K_0\nabla u) + Q \tag{14}$$

Special case:

$Q = 0$ with $c, \rho, K_0 = \text{const}$ results in

$$\frac{\partial}{\partial t} u = k \nabla^2 u, \qquad k = \frac{K_0}{c\rho},$$

or

$$\frac{\partial}{\partial t} u = k \Delta u,$$

where the Laplacian is defined as

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

or

$$\Delta u = \nabla \cdot \nabla u = \frac{\partial}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial}{\partial y}\frac{\partial u}{\partial y} + \frac{\partial}{\partial z}\frac{\partial u}{\partial z}$$

i.e.,

$$\Delta u = \text{div}(\text{grad}\, u).$$

Initial and Boundary Conditions

- Initial temperature distribution:

$$u(x,y,z,0) = f(x,y,z) \quad \text{for } (x,y,z) \in R$$

- Boundary conditions
  - Prescribed boundary temperature:

$$u(x,y,z,t) = T(x,y,z,t) \quad \text{for } (x,y,z) \in \partial R$$

  - Perfectly insulated boundary: this means no heat flux through the boundary (normal component of ϕ is zero), i.e., $\phi \cdot \hat{\boldsymbol{n}} = 0$. Using Fourier's law ($\phi = -K_0 \nabla u$) we have for all $(x,y,z) \in \partial R$

$$\phi \cdot \hat{\boldsymbol{n}} = 0 \quad \iff \quad \nabla u \cdot \hat{\boldsymbol{n}} = 0,$$

i.e., the normal derivative of u is zero.

- Boundary conditions (cont.)
  - Newton's law of cooling:

$$\nabla u \cdot \hat{\boldsymbol{n}} = -\frac{H}{K_0}[u - u_B] \quad \text{on the boundary } \partial R$$

Remark

- *If $u > u_B$ then heat flows outward, i.e., the temperature gradient is negative. Thus we need to have $H > 0$ for everything to make sense.*
- *Note that $\hat{\mathbf{n}} = \boldsymbol{i}$ and $\hat{\mathbf{n}} = -\boldsymbol{i}$ correspond to 1D end conditions. For example,*

$$\nabla u \cdot \boldsymbol{i} = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z}\right) \cdot (1, 0, 0) = \frac{\partial u}{\partial x}$$

Steady State Problems

As in 1D, steady state is characterized by $\frac{\partial}{\partial t}u \equiv 0$.
Therefore the heat equation (14)

$$c\rho \frac{\partial}{\partial t}u = \nabla \cdot (K_0 \nabla u) + Q$$

becomes

$$\nabla \cdot (K_0 \nabla u) = -Q.$$

If $K_0 = \text{const}$, then we get

Poisson's equation

$$\nabla^2 u(x, y, z, t) = -\frac{Q(x, y, z, t)}{K_0}.$$

If in addition $Q = 0$, then we get

Laplace's equation

$$\nabla^2 u(x, y, z, t) = 0.$$

Remark

- *Now the steady state equations are PDEs, and we need to postpone their solution until later.*
- *In 2D these equations look the same, except that we use the 2D Laplacian*

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

Other Coordinate Systems

- The Laplacian of u

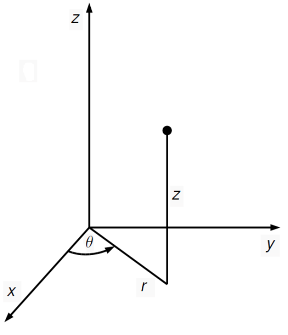
$$\nabla^2 u$$

  plays a central role in the formulation of the heat equation.
- We often have to deal with regions R that are better expressed in cylindrical or spherical coordinates.

$\Longrightarrow$ need to convert the Laplacian to cylindrical and spherical coordinates

Cylindrical Coordinates

$$
\begin{aligned}
x &= r\cos\theta \\
y &= r\sin\theta \\
z &= z
\end{aligned}
$$



These coordinates imply $r = \sqrt{x^2 + y^2}$ and $\theta = \tan^{-1}\frac{y}{x}$ and so

$$u(x, y, z) = u(r(x, y), \theta(x, y), z).$$

Therefore the derivatives $\frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 u}{\partial y^2}, \frac{\partial^2 u}{\partial z^2}$ can be expressed using the chain rule.

First calculate

$$\begin{aligned}
\frac{\partial u}{\partial x} &= \frac{\partial u}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial u}{\partial \theta}\frac{\partial \theta}{\partial x} \\
&= \frac{\partial u}{\partial r}\frac{2x}{2\underbrace{\sqrt{x^2+y^2}}_{=r}} + \frac{\partial u}{\partial \theta}\underbrace{\frac{-\frac{y}{x^2}}{1+\left(\frac{y}{x}\right)^2}}_{=\frac{-y}{x^2+y^2}=\frac{-y}{r^2}} \\
&= \frac{\partial u}{\partial r}\frac{x}{r} - \frac{\partial u}{\partial \theta}\frac{y}{r^2}
\end{aligned}$$

Using $x = r\cos\theta$ and $y = r\sin\theta$ we get

$$\frac{\partial u}{\partial x} = \cos\theta\frac{\partial u}{\partial r} - \frac{\sin\theta}{r}\frac{\partial u}{\partial \theta}$$

and so the differential operator

$$\frac{\partial}{\partial x} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}$$

Next, using $\frac{\partial}{\partial x} = \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}$ three times we get

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) = \cos\theta \frac{\partial}{\partial r}\left(\frac{\partial u}{\partial x}\right) - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\left(\frac{\partial u}{\partial x}\right) \\ &= \cos\theta \frac{\partial}{\partial r}\left[\cos\theta \frac{\partial u}{\partial r} - \frac{\sin\theta}{r}\frac{\partial u}{\partial \theta}\right] - \frac{\sin\theta}{r}\frac{\partial}{\partial \theta}\left[\cos\theta \frac{\partial u}{\partial r} - \frac{\sin\theta}{r}\frac{\partial u}{\partial \theta}\right]\end{aligned}$$

Differentiation using the product rule along with $\frac{\partial^2}{\partial r \partial \theta} = \frac{\partial^2}{\partial \theta \partial r}$ gives us

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} &= \cos\theta \left[\cos\theta \frac{\partial^2 u}{\partial r^2} + \frac{\sin\theta}{r^2}\frac{\partial u}{\partial \theta} - \frac{\sin\theta}{r}\frac{\partial^2 u}{\partial r \partial \theta}\right] \\ &\quad - \frac{\sin\theta}{r}\left[-\sin\theta \frac{\partial u}{\partial r} + \cos\theta \frac{\partial^2 u}{\partial r \partial \theta} - \frac{\cos\theta}{r}\frac{\partial u}{\partial \theta} - \frac{\sin\theta}{r}\frac{\partial^2 u}{\partial \theta^2}\right]\end{aligned}$$

Therefore

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} &= \cos^2\theta \frac{\partial^2 u}{\partial r^2} + 2\frac{\sin\theta\cos\theta}{r^2}\frac{\partial u}{\partial \theta} - 2\frac{\sin\theta\cos\theta}{r}\frac{\partial^2 u}{\partial r \partial \theta} \\ &\quad + \frac{\sin^2\theta}{r}\frac{\partial u}{\partial r} + \frac{\sin^2\theta}{r^2}\frac{\partial^2 u}{\partial \theta^2}\end{aligned}$$

We just calculated

$$\frac{\partial^2 u}{\partial x^2} = \cos^2\theta \frac{\partial^2 u}{\partial r^2} + 2\frac{\sin\theta\cos\theta}{r^2}\frac{\partial u}{\partial\theta} - 2\frac{\sin\theta\cos\theta}{r}\frac{\partial^2 u}{\partial r\partial\theta} + \frac{\sin^2\theta}{r}\frac{\partial u}{\partial r} + \frac{\sin^2\theta}{r^2}\frac{\partial^2 u}{\partial\theta^2}$$

Analogously

$$\frac{\partial^2 u}{\partial y^2} = \sin^2\theta \frac{\partial^2 u}{\partial r^2} - 2\frac{\sin\theta\cos\theta}{r^2}\frac{\partial u}{\partial\theta} + 2\frac{\sin\theta\cos\theta}{r}\frac{\partial^2 u}{\partial r\partial\theta} + \frac{\cos^2\theta}{r}\frac{\partial u}{\partial r} + \frac{\cos^2\theta}{r^2}\frac{\partial^2 u}{\partial\theta^2}$$

Therefore

$$\begin{aligned}\nabla^2 u &= \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \\ &= \left(\cos^2\theta + \sin^2\theta\right)\frac{\partial^2 u}{\partial r^2} + \left(\frac{\sin^2\theta}{r} + \frac{\cos^2\theta}{r}\right)\frac{\partial u}{\partial r} + \left(\frac{\sin^2\theta}{r^2} + \frac{\cos^2\theta}{r^2}\right)\frac{\partial^2 u}{\partial\theta^2} + \frac{\partial^2 u}{\partial z^2}\end{aligned}$$

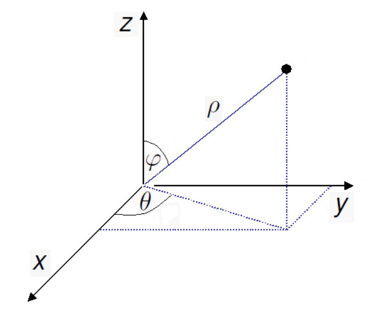
or

Laplacian in cylindrical coordinates:

$$\nabla^2 u = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2} + \frac{\partial^2 u}{\partial z^2}$$

Spherical Coordinates

$$\begin{aligned} x &= \rho \sin\varphi \cos\theta \\ y &= \rho \sin\varphi \sin\theta \\ z &= \rho \cos\varphi \end{aligned}$$



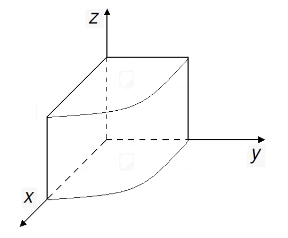
Proceeding similarly as for cylindrical coordinates one can obtain

Laplacian in spherical coordinates:

$$\nabla^2 u = \frac{1}{\rho^2}\frac{\partial}{\partial \rho}\left[\rho^2 \frac{\partial u}{\partial \rho}\right] + \frac{1}{\rho^2 \sin\varphi}\frac{\partial}{\partial \varphi}\left[\sin\varphi \frac{\partial u}{\partial \varphi}\right] + \frac{1}{\rho^2 \sin^2\varphi}\frac{\partial^2 u}{\partial \theta^2}$$

Example

Let $u(r,\theta)$ denote the temperature, independent of z, in a long rod parallel to the z-axis whose cross-section in the xy-plane is given by the circular sector $0 \le r \le 1$, $0 \le \theta \le \frac{\pi}{2}$.

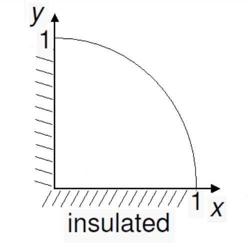


(a) Show

$$\frac{\partial u}{\partial \theta} = -y\frac{\partial u}{\partial x} + x\frac{\partial u}{\partial y}$$

(b) Use the result of (a) to show that if the rod is insulated on its planar surfaces, where $\theta = 0$ and $\theta = \frac{\pi}{2}$, then u must satisfy the boundary conditions

$$\frac{\partial u}{\partial \theta}(r,0) = 0, \quad \frac{\partial u}{\partial \theta}(r,\frac{\pi}{2}) = 0, \quad 0 < r < 1.$$



Solution

(a) We use polar coordinates

$$x = r\cos\theta, \quad y = r\sin\theta$$

Then $u(x,y) = u(x(r,\theta), y(r,\theta))$ and the chain rule gives

$$\begin{aligned}
\frac{\partial u}{\partial \theta} &= \frac{\partial u}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial \theta} \\
&= \frac{\partial u}{\partial x}(-r\sin\theta) + \frac{\partial u}{\partial y}(r\cos\theta) \\
&= -y\frac{\partial u}{\partial x} + x\frac{\partial u}{\partial y}
\end{aligned}$$

(b) Let $\hat{\boldsymbol{n}}$ be the unit outer normal vector and remember that insulated means that

$$\phi \cdot \hat{\boldsymbol{n}} = 0 \quad \overset{\text{Fourier's law}}{\Longleftrightarrow} \quad -K_0 \nabla u \cdot \hat{\boldsymbol{n}} = 0$$

so that $\nabla u \cdot \hat{\boldsymbol{n}} = 0$, where $\nabla u = (u_x, u_y)$.

Face $\theta = 0$: Here $\hat{\boldsymbol{n}} = (0, -1)$ (in cartesian coordinates). Therefore

$$\nabla u \cdot \hat{\boldsymbol{n}} = (u_x, u_y) \cdot (0, -1) = -\frac{\partial u}{\partial y}$$

Now

$$\begin{aligned}
\frac{\partial u}{\partial \theta}(r, 0) &\overset{\text{(a)}}{=} -y(r,0)\frac{\partial u}{\partial x}(r,0) + x(r,0)\frac{\partial u}{\partial y}(r,0) \\
&= -\underbrace{r \sin\theta|_{\theta=0}}_{=0} \frac{\partial u}{\partial x}(r,0) + r\cos\theta|_{\theta=0} \underbrace{\frac{\partial u}{\partial y}(r,0)}_{=0\ (\nabla u \cdot \hat{\boldsymbol{n}}=0)}
\end{aligned}$$

Therefore

$$\frac{\partial u}{\partial \theta}(r, 0) = 0.$$

(b) (cont.)

Face $\theta = \frac{\pi}{2}$: Here $\hat{\boldsymbol{n}} = (-1, 0)$ so that $\nabla u \cdot \hat{\boldsymbol{n}} = -\frac{\partial u}{\partial x}$.

Now

$$\begin{aligned}\frac{\partial u}{\partial \theta}(r, \frac{\pi}{2}) &\overset{(a)}{=} -y(r, \frac{\pi}{2})\frac{\partial u}{\partial x}(r, \frac{\pi}{2}) + x(r, \frac{\pi}{2})\frac{\partial u}{\partial y}(r, \frac{\pi}{2}) \\ &= -r\sin\frac{\pi}{2}\underbrace{\frac{\partial u}{\partial x}(r, \frac{\pi}{2})}_{=0\ (\nabla u \cdot \hat{\boldsymbol{n}}=0)} + r\underbrace{\cos\frac{\pi}{2}}_{=0}\frac{\partial u}{\partial y}(r, \frac{\pi}{2})\end{aligned}$$

Therefore

$$\frac{\partial u}{\partial \theta}(r, \frac{\pi}{2}) = 0.$$

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