Example: Heat flow

Let us first solve the heat equation analytically before discussing the numerical method to solve it.

Example: Heat equation in one spatial dimension.

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2},$$

where κ is the thermal diffusivity.

Open boundaries: $T(x,t)$ defined on $-\infty < x < +\infty$ and $t \geq 0$.
Also, require that $T(x,t) \to 0$ as $x \pm \infty$

Initial value problem: $T(x, t = 0) = \Phi(x)$

We will use the Fourier transform in order to solve this problem.

Notes

Solving Heat flow with an integral transform

We have two independent variables x, t. Apply Fourier transform to spatial variables x *at constant* t:

$$\mathfrak{F}[T(x,t)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} T(x,t) e^{-ikx} dx$$

What is the Fourier transform of $\partial T / \partial x$?

$$\mathfrak{F}[T_x] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{\partial T}{\partial x} e^{-ikx} dx$$

Integrating by parts, we obtain

$$\mathfrak{F}[T_x] = \left[\frac{e^{-ikx}}{\sqrt{2\pi}} T(x,t) \right]_{-\infty}^{\infty} + \frac{ik}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} T(x,t) e^{-ikx} dx$$

Since $T(x,t)$ vanishes as $x \to \pm\infty$, the first term vanishes and we have

$$\mathfrak{F}[T_x] = ik\mathfrak{F}[T]$$

Notes

Solving Heat flow with an integral transform

The Fourier transform of $\partial T / \partial t$ is simply

$$\begin{aligned} \mathfrak{F}[T_t] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{\partial T}{\partial t} e^{-ikx} dx \\ &= \frac{\partial}{\partial t} \mathfrak{F}[T(x,t)] \end{aligned}$$

using Leibniz rule.

Similarly,

$$\begin{aligned} \mathfrak{F}[T_{tt}] &= \frac{\partial^2}{\partial t^2} \mathfrak{F}[T(x,t)] \\ \mathfrak{F}[T_{xx}] &= (ik)^2 \mathfrak{F}[T(x,t)] = -k^2 \mathfrak{F}[T(x,t)] \end{aligned}$$

Notes

Solving Heat flow with an integral transform

Now apply Fourier transform to the heat equation (at constant t):

$$\mathfrak{F}[T_t] = \mathfrak{F}[\kappa T_{xx}] \quad (1)$$

$$\frac{\partial}{\partial t} \mathfrak{F}[T] = -k^2 \kappa \mathfrak{F}[T] \quad (2)$$

Note: Fourier transform method for solving this problem is appropriate since $T(x,t)$ vanishes at $x \to \pm\infty$ according to the BC.

Let us denote $\tau(k,t) = \mathfrak{F}[T(x,t)]$

Notes

Solving Heat flow with an integral transform

$$\frac{\partial \tau(k,t)}{\partial t} = -k^2\kappa\tau(k,t) \qquad (3)$$

Equation (3) is now a simple ordinary differential equation. Heat equation is much easier to solve in the Fourier domain!

The solution is

$$\tau(k,t) = e^{-k^2\kappa t}\tau(k,0) \qquad (4)$$

Still need to transform the initial condition $T(x,0) = \Phi(x)$:

$$\mathfrak{F}[\Phi(x)] = \mathfrak{F}[T(x,t=0)] = \tau(k,0) \qquad (5)$$

Notes

Solving Heat flow with an integral transform

Combining eqs. (4) and (5)

$$\tau(k,t) = e^{-k^2\kappa t}\mathfrak{F}[\Phi(x)] \qquad (6)$$

In order to obtain solution in real space, apply the inverse Fourier transform:

$$T(x,t) = \mathfrak{F}^{-1}[\tau(k,t)] = \mathfrak{F}^{-1}[e^{-k^2\kappa t}\mathfrak{F}[\Phi(x)]] \qquad (7)$$

However, can use the *convolution theorem* on the right hand side. Recall

$$\mathfrak{F}[f \otimes g] = \mathfrak{F}[f]\mathfrak{F}[g]$$

Notes

Therefore,

$$f \otimes g = \mathfrak{F}^{-1}\left[\mathfrak{F}[f]\mathfrak{F}[g]\right] \qquad (8)$$

Now apply this to our solution (eq. (7)):
Let $\mathfrak{F}[f] = e^{-k^2\kappa t}$ and $\mathfrak{F}[g] = \mathfrak{F}[\Phi(x)]$.
It follows that $g = \mathfrak{F}^{-1}[\mathfrak{F}[\Phi(x)]] = \Phi(x)$ by definition.
Also,

$$\begin{aligned} f &= \mathfrak{F}^{-1}[e^{-k^2\kappa t}] && (9)\\ &= \frac{1}{\sqrt{2\kappa t}}e^{-x^2/(4\kappa t)} && (10)\end{aligned}$$

In the last step we used the known inverse Fourier transform of a Gaussian (see table of Fourier transforms - lecture 2):

$$\mathfrak{F}[e^{-\alpha x^2}] = \frac{1}{\sqrt{2\alpha}}e^{-k^2/(4\alpha)}$$

Notes

Solving Heat flow with an integral transform

Since

$$T(x,t) = f \otimes g \qquad (11)$$

according to eqs. (8) and (7) we have

$$\begin{aligned} T(x,t) &= \frac{1}{\sqrt{2\kappa t}}e^{-x^2/(4\kappa t)} \otimes \Phi(x) && (12)\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\frac{1}{\sqrt{2\kappa t}}e^{-(x-\xi)^2/(4\kappa t)}\Phi(\xi)d\xi && (13)\\ &= \frac{1}{\sqrt{4\pi\kappa t}}\int_{-\infty}^{+\infty}e^{-(x-\xi)^2/(4\kappa t)}\Phi(\xi)d\xi && (14)\end{aligned}$$

This is the *fundamental* solution of the heat equation with open boundaries for an initial condition $T(x,t=0) = \Phi(x)$.

Notes

Green's function

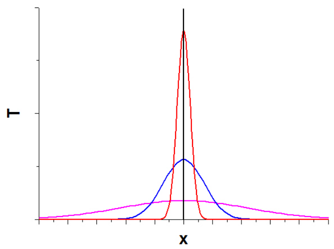
The fundamental solution is the the convolution of the initial conditions with the *Green's function*.
Once the Green's function of a linear PDE is known (for given B.C.'s), it can be solved for arbitrary initial conditions via a convolution integral (eq. (14)).
The Green's function is the solution of the PDE for a delta (impulse) function.
Let the initial condition be $\Phi(x) = \delta(x)$. Then

$$\begin{aligned} T(x,t) &= \frac{1}{\sqrt{4\pi\kappa t}} \int_{-\infty}^{+\infty} e^{-(x-\xi)^2/(4\kappa t)} \delta(\xi) d\xi \\ &= \frac{1}{\sqrt{4\pi\kappa t}} e^{-x^2/(4\kappa t)} \end{aligned}$$

Note: $T(x,t) \to \delta(x)$ as $t \to 0$.

Notes

Heat diffusion from delta function impulse



The delta function at $t = 0$ becomes spread out as time goes on.

Notes

Finite difference methods

In the following, let's see how to solve PDE's using finite difference methods.

For simplicity, assume u to be a function of two independent variables x and t, only.

The continuous function u is then discretized on a grid in the x, t plane where the points are separated by Δx and Δt, respectively.

Notation: $u(x,t) \to u(j\Delta x, n\Delta t)$, where j and n are integers.

Notes

Approximating the derivatives

In order to discretize the PDE we need to approximate the derivatives appearing in the PDE by finite differences.
There are three possible approximations for the first order (partial) derivative: $\partial u(j\Delta x, n\Delta t)/\partial x$

- The forward (Euler) difference:
$$\frac{u^n_{j+1} - u^n_j}{\Delta x}$$
- The backward difference:
$$\frac{u^n_j - u^n_{j-1}}{\Delta x}$$
- The centered difference:
$$\frac{u^n_{j+1} - u^n_{j-1}}{2\Delta x}$$

Notes

Approximating the derivatives

The same applies for the temporal partial derivative, except that j is kept constant. e.g. the forward difference is

$$\frac{\partial u(j\Delta x, n\Delta t)}{\partial t} \approx \frac{u_j^{n+1} - u_j^n}{\Delta t}$$

The finite differences follow from the Taylor expansion of $u(x)$ (at constant t):

$$\begin{aligned} u(x+\Delta x) = \quad & u(x) + u'(x)\Delta x + \frac{1}{2}u''(x)(\Delta x)^2 && (15) \\ & +\frac{1}{6}u'''(x)(\Delta x)^3 + O(\Delta x)^4 && (16) \\ u(x-\Delta x) = \quad & u(x) - u'(x)\Delta x + \frac{1}{2}u''(x)(\Delta x)^2 && (17) \\ & -\frac{1}{6}u'''(x)(\Delta x)^3 + O(\Delta x)^4 && (18) \end{aligned}$$

where in the last line $\Delta x \to -\Delta x$

Notes

Approximating the derivatives

From the Taylor series expansion we can find the *local* errors:

- The forward (Euler) difference (eq.(17)):

$$\frac{u(x+\Delta x) - u(x)}{\Delta x} + O(\Delta x)$$

- The backward difference (eq.(18)):

$$\frac{u(x) - u(x-\Delta x)}{\Delta x} + O(\Delta x)$$

- The centered difference(subtract eq.(18) from eq. (17)):

$$\frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} + O(\Delta x)^2$$

Note that the global (accumulated) error may be different from the local one.

Notes

Approximating the derivatives

What about the second derivative? By adding the two Taylor expansions (17) and (18) and solving for $u''(x)$ we obtain

$$u''(x) = \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{(\Delta x)^2} + O(\Delta x)^2 \qquad (19)$$

In index notation, this reads for a partial second derivative at constant t:

$$\frac{\partial u(j\Delta x, n\Delta t)}{\partial x^2} \approx \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} \qquad (20)$$

This is the **second centered difference**.
Similar expression for partial time derivative.

Notes

Discretizing the heat equation

Let us use a finite difference scheme to evaluate the heat equation numerically in one spatial dimension.

$$T_t = \kappa T_{xx} \qquad (21)$$

Again, assume open boundaries with initial condition:

$$T(x, t=0) = \Phi(x)$$

Apply forward difference to T_t and second centered difference to T_{xx}:

$$\frac{T_j^{n+1} - T_j^n}{\Delta t} = \kappa \frac{T_{j+1}^n - 2T_j^n + T_{j-1}^n}{(\Delta x)^2} \qquad (22)$$

where $T_j^n = T(j\Delta x, n\Delta t)$.

Notes

Discretizing the heat equation - errors

There are two types of errors in this finite difference scheme:

- *Truncation errors:* The **local** truncation error for the second centered difference is Δx^2 and for the time derivative Δt. These errors may accumulate and given an overall **global** truncation error that may be bigger than the local one.
- *Round off error:* This occurs in real computations, since the computer only retains a certain number of digits for floating point numbers. e.g. in C, *float* variables have 8 digit and *double* have 16 digit precision. These round off errors also accumulate. Always use *double* variables for finite difference schemes!

Notes

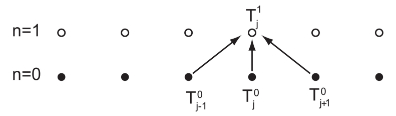
Discretizing the heat equation

Solving for T_j^{n+1} we obtain

$$T_j^{n+1} = (1-2s)T_j^n + s(T_{j+1}^n + T_{j-1}^n) \tag{23}$$

where $s = \frac{\kappa \Delta t}{(\Delta x)^2}$.

This is an **explicit** difference scheme, since the values of the $(n+1)$th time step are explicitly given in terms of the value at earlier times.



Notes

Example 1

Let's look at a simple example. For simplicity, set $s = 1$. Then the difference scheme simplifies to

$$T_j^{n+1} = T_{j+1}^n - T_j^n + T_{j-1}^n \tag{24}$$

Suppose $\Phi(x_j)$ is a simple impulse: $T_j^{n=0} = 1$ for a particular point j in space and zero everywhere else.
Can integrate this by "marching in time":

$n=4$	1	-4	10	-16	19	-16	10	-4	1	
$n=3$	0	1	-3	6	-7	6	-3	1	0	
$n=2$	0	0	1	-2	3	-2	1	0	0	
$n=1$	0	0	0	1	-1	1	0	0	0	
$n=0$	0	0	0	0	1	0	0	0	0	$\rightarrow x$

Notes

Example 1

Something has gone wrong ! Expect the impulse to diffuse away.

According to the *maximum principle* of diffusion PDE's, the maximum of $T(x,t)$ occurs either at the initial conditions $t = 0$ or at the boundaries. In our example, this means that $T(x,t) < 1$ for $t > 0$.

Instead the difference equations has given us an approximation where the central point is 19 and growing.

It turns out that for this particular difference scheme Δt and Δx cannot be chosen arbitrarily.

Notes

Example 2

Let's consider another example of the heat equation with the following boundary conditions:

$$\begin{aligned} T_t &= T_{xx} \quad \text{for } 0 < x < \pi, t > 0 \\ T &= 0 \quad \text{at } x = 0, \pi \end{aligned}$$

The initial condition is

$$T(x,0) = \Phi(x) = \begin{cases} x & \text{for } 0 < x \le \pi/2 \\ \pi - x & \text{for } \pi/2 < x < \pi \end{cases} \tag{25}$$

First, let's solve this analytically using separation of variables.

Notes

Example 2

If the PDE is *separable*, then its solution can be expressed as

$$T(x,t) = A(x)B(t)$$

This allows us to turn the PDE into two ordinary differential equations (ODE's). Substitution yields

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2} \tag{26}$$

$$A(x)\frac{\partial B(t)}{\partial t} = \kappa B(t)\frac{\partial^2 A(x)}{\partial x^2} \tag{27}$$

Dividing by $(A(t)B(x)\kappa)$ we obtain

$$\frac{1}{\kappa B(t)}\frac{\partial B(t)}{\partial t} = -k^2 = \frac{1}{A(x)}\frac{\partial^2 A(x)}{\partial x^2}$$

where $-k^2$ is the *constant of separation*. LHS and RHS are equal for all x and t, which are independent of each other.

Notes

Example 2

The two ODE's are

$$\frac{1}{\kappa B(t)}\frac{\partial B(t)}{\partial t} = -k^2 \tag{28}$$

$$\frac{1}{A(x)}\frac{\partial^2 A(x)}{\partial x^2} = -k^2 \tag{29}$$

The solutions are

$$A(x) = a\cos(kx) + b\sin(kx) \tag{30}$$

$$B(t) = ce^{-\kappa k^2 t} \tag{31}$$

where a, b, c are constants of integration.
The boundary conditions $T(x=0,t) = T(x=\pi,t) = 0$, require $a = 0$ and k to be an integer.

Notes

Example 2

Therefore,

$$T(x,t) = b_k \sin(kx)e^{-\kappa k^2 t} \tag{32}$$

where k is an integer.

Fourier analysis allows us to obtain the solution for our specified initial condition:

$$T(x,t) = \sum_{k=1}^{\infty} b_k \sin(kx)e^{-\kappa k^2 t} \tag{33}$$

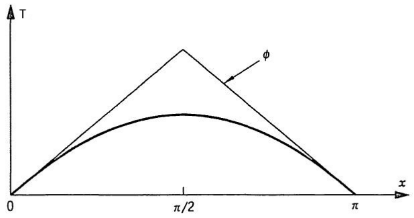
where

$$b_k = \begin{cases} \frac{(-1)^{(k+1)/2}}{\pi k^2} & \text{for odd } k \\ 0 & \text{for even } k \end{cases} \tag{34}$$

Notes

Example 2

This plot shows the initial temperature distribution $\Phi(x)$ and $T(x,t)$ for $t = 3\pi^2/80$.



As $t \to \infty$, $T \to 0$ everywhere.

Notes

Numerically solving example 2

Now solve numerically using our difference scheme

$$T_j^{n+1} = (1-2s)T_j^n + s(T_{j+1}^n + T_{j-1}^n) \tag{35}$$

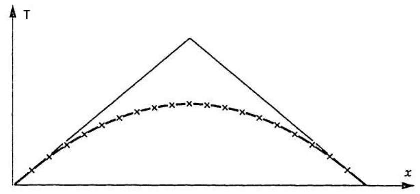
with $s = \frac{\kappa \Delta t}{(\Delta x)^2} = 5/11 = 0.45$ and $\Delta x = \pi/20$, where we have discretized space with $J+1 = 21$ points.
The discrete boundary and initial conditions are

$$u_0^n = u_J^n = 0 \text{ and } u_j^0 = \Phi(j\Delta x)$$

where $j = 0, 1, 2, \ldots J$.

Notes

Numerically solving example 2

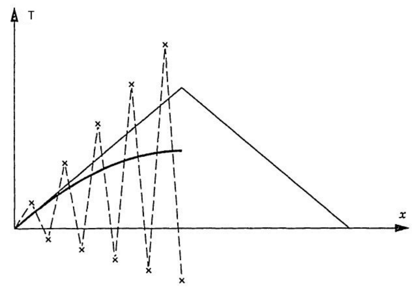


Agrees very well with analytical solution.

Notes

Numerically solving example 2

However, if we choose $s = 5/9 = 0.55$, the finite difference scheme yields wild oscillations similar to what we obtained for the impulse IC earlier.



Notes

Stability of finite difference scheme

In the following we will derive the stability criterion for this difference scheme:
Let's solve the difference scheme by separation of variables:

$$T_j^n = A_j B_n \tag{36}$$

Substitution in the difference scheme (eq. (35)) yields

$$A_j B_{n+1} = (1-2s) A_j B_n + s(A_{j+1} B_n + A_{j-1} B_n) \tag{37}$$

Dividing by $A_j B_n$ we get

$$\frac{B_{n+1}}{B_n} = \xi = 1 - 2s + s\frac{A_{j+1} + A_{j-1}}{A_j} \tag{38}$$

where ξ is the constant of separation.

Notes

Stability of finite difference scheme

Thus,

$$\frac{B_{n+1}}{B_n} = \xi \tag{39}$$

which has the solution

$$B_n = \xi^n B_0 \tag{40}$$

where B_0 is some constant.
Now solve the spatial part:

$$1 - 2s + s\frac{A_{j+1} + A_{j-1}}{A_j} = \xi \tag{41}$$

We wish to investigate the eigenmodes of the solution. Therefore, assume a plane wave solution with wave number k (ignore boundary conditions for this analysis):

$$A_j = e^{ikj\Delta x} \tag{42}$$

Notes

Stability of finite difference scheme

Substituting yields

$$\begin{aligned}
1 - 2s + s\frac{e^{ik(j+1)\Delta x} + e^{ik(j-1)\Delta x}}{e^{ikj\Delta x}} &= \xi \\
1 - 2s + s(e^{ik\Delta x} + e^{-ik\Delta x}) &= \xi \\
1 - 2s + 2s\cos(k\Delta x) &= \xi \\
1 - 2s(1 - \cos(k\Delta x)) &= \xi \\
1 - 4s\left(\sin\left(\frac{k\Delta x}{2}\right)\right)^2 &= \xi
\end{aligned}$$

For the difference scheme to be stable, require

$$|\xi(k)| \leq 1 \text{ for all } k \tag{43}$$

since the amplitude grows as $\propto \xi^n$ (eq. (40))

Notes

Stability of finite difference scheme

Therefore,

$$\left|1 - 4s\left(\sin\left(\frac{k\Delta x}{2}\right)\right)^2\right| \leq 1$$

for all k. This leads to the following stability criterion:

$$\begin{aligned}
4s &\leq 2 \\
\frac{2\kappa\Delta t}{(\Delta x)^2} &\leq 1
\end{aligned}$$

Physically, this means that the maximum allowed time step Δt is the diffusion time across a cell of size Δx (up to a numerical factor). The diffusion time across some length λ goes as $t_\lambda \sim \frac{\lambda^2}{\kappa}$

Notes

von Neumann stability analysis

This is the von Neumann stability analysis:

- The von Neumann analysis looks at the evolution of the eigenmodes of the solution by substituting

$$u_j^n = \xi^n e^{ikj\Delta x}$$

into the difference equation, where $\xi(k)$ is the *amplification factor*

- For the difference scheme to be stable, require

$$|\xi(k)| \leq 1 + O(\Delta t) \text{ for all } k$$

Otherwise, eigenmodes grow exponentially in time.

Notes

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