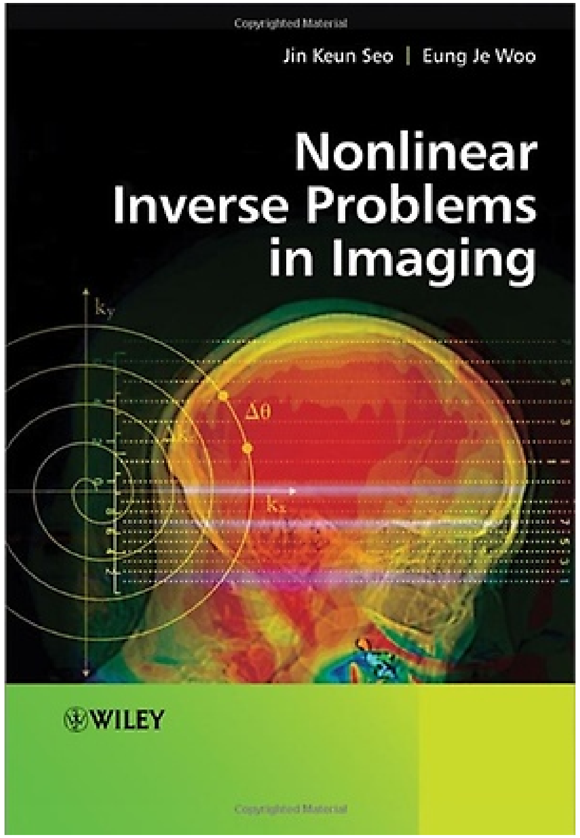
Partial Differential Equations

for Computational Science & Engineering



Lecture 2. Representations of solutions of linear PDEs

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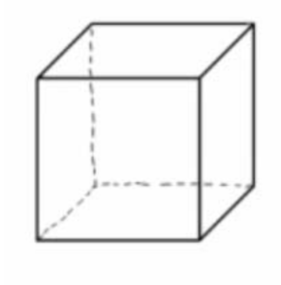
Derivation of Heat Equation

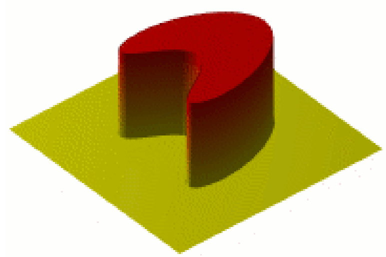
Suppose $u(\mathbf{r}, t)$ measures the temperature at time t and position $\mathbf{r} = (x, y, z) \in \Omega$ in a three-dimensional domain $\Omega \subset \mathbb{R}^3$.



According to Fourier's law, the heat flow $\mathbf{J} = (J_x, J_y, J_z)$ satisfies

$$\mathbf{J}(\mathbf{r}, t) = -k(\mathbf{r})\nabla u(\mathbf{r}, t) \qquad (\mathbf{r} \in \Omega,\ t > 0)$$

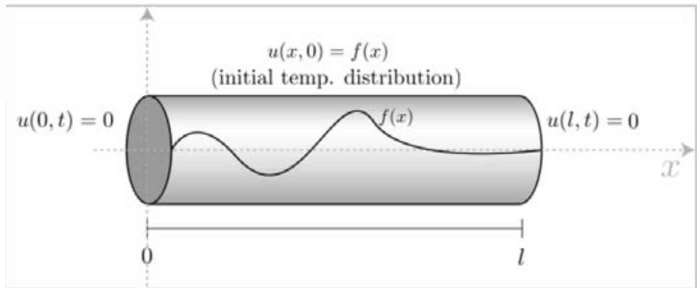
where k is the thermal conductivity (that is a measure of its ability to conduct of the material) and ∇u is the temperature gradient.



For any domain $D \subset \Omega$, the law of conservation of energy leads to

$$\underbrace{\int_D \rho c \frac{\partial u}{\partial t} d\mathbf{r}}_{A} = \underbrace{\int_D \nabla \cdot (k\nabla u) d\mathbf{r}}_{B} + \underbrace{\int_D f(\mathbf{r}) d\mathbf{r}}_{C}.$$

where ρ is the density and c is the specific heat representing the amount of heat required to raise the temperature of one unit mass by 1°. ✓ A=the change of the total amount of heat per unit time in D. ✓ B=the amount of heat per unit time flowing into D. ✓ C=the total amount of heat produced in D per unit time



Since D is arbitrary, u satisfies

$$\frac{\partial}{\partial t} u(\mathbf{r}, t) - \frac{1}{\rho(\mathbf{r})c(\mathbf{r})} \nabla \cdot (k(\mathbf{r})\nabla u(\mathbf{r}, t)) = \frac{1}{\rho(\mathbf{r})c(\mathbf{r})} f(\mathbf{r}, t).$$

Image credit: Wikipedia

Theorem (One-dimensional Heat Equation)

For $\phi \in C_0(\mathbb{R})$, we define

$$u(x,t) = \int_{-\infty}^{\infty} \underbrace{\frac{1}{\sqrt{4\pi kt}} e^{-\frac{|x-x'|^2}{4kt}}}_{K(x-x',t)} \phi(x')dx' \qquad (\forall\, x \in \mathbb{R}, \quad t > 0)$$

Then, u satisfies the heat equation with the initial condition ϕ:

$$\begin{cases} \left[\frac{\partial}{\partial t} - k\frac{\partial^2}{\partial x^2}\right] u(x,t) = 0 & (\forall\, x \in \mathbb{R}, \quad t > 0) \\ u(x,0) = \phi(x) & (\forall\, x \in \mathbb{R}). \end{cases}$$

Proof.

- A direct computation gives

$$\left[\frac{\partial}{\partial t} - k\frac{\partial^2}{\partial x^2}\right] K(x,t) = 0 \qquad (\forall x \in \mathbb{R}, \quad t > 0).$$

  Hence, for $t > 0$, we have

$$\left[\frac{\partial}{\partial t} - k\frac{\partial^2}{\partial x^2}\right] u(x,t) = \int_{-\infty}^{\infty} \left(\left[\frac{\partial}{\partial t} - k\frac{\partial^2}{\partial x^2}\right] K(x-x',t) \right) \phi(x')dx' = 0.$$

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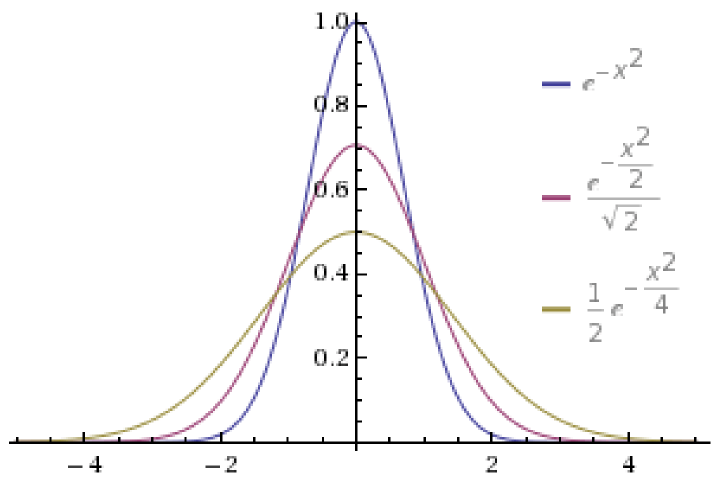
It remains to prove the initial condition

$$\lim_{t\to 0^+} \underbrace{\int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi kt}} e^{-\frac{|x-x'|^2}{4kt}} \phi(x')dx}_{u(x,t)} = \phi(x) \qquad (\forall x \in \mathbb{R}).$$

This comes from the fact that

$$\lim_{t\to 0^+} \underbrace{\frac{1}{\sqrt{4\pi kt}} e^{-\frac{|x|^2}{4kt}}}_{K(x,t)} = \delta(x) \qquad (\forall x \in \mathbb{R}).$$



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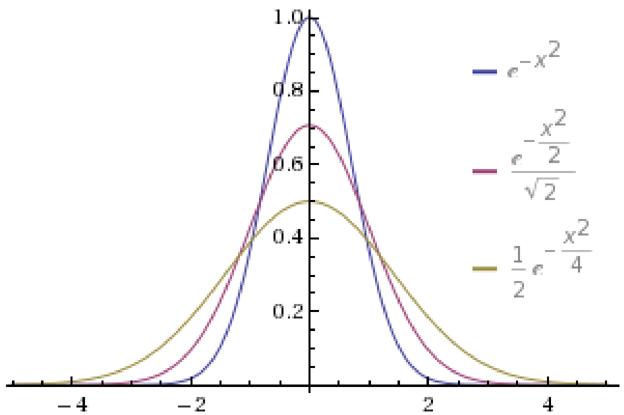
Proof of $$\lim_{t\to 0^+} \underbrace{\frac{1}{\sqrt{4\pi kt}} e^{-\frac{|x|^2}{4kt}}}_{K(x,t)} = \delta(x) \qquad (\forall x \in \mathbb{R}).$$

Proof

- Application of the change of variable $y = x/\sqrt{4kt}$ yields

$$\int_{-\infty}^{\infty} K(x,t)dx = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-|y|^2} dy = 1 \qquad (t>0)$$

- Clearly, $\lim_{t\to 0^+} K(x,t) = 0 \qquad (\forall x \neq 0)$.



Theorem (Maximum principle (1D Heat))

If a non-constant function $u(x,t)$ satisfies

$$\left[\frac{\partial}{\partial t} - k\frac{\partial^2}{\partial x^2}\right] u(x,t) = 0 \qquad (\forall\ 0 < x < L,\ \ 0 < t < T),$$

then $u(x,t)$ cannot attain its maximum anywhere in the rectangle $(0,L) \times (0,T]$. In other words, u attains its maximum on the bottom $[0,L] \times \{t = 0\}$ or the lateral side $\{0,L\} \times [0,T]$.

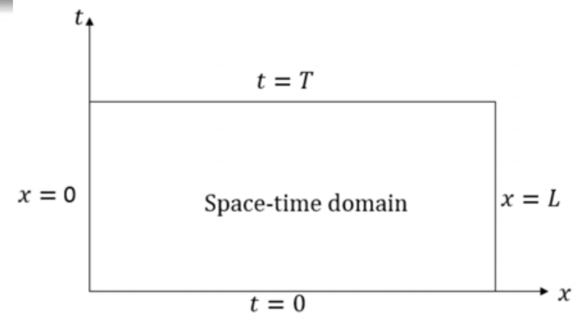
- For $\epsilon > 0$, $v_\epsilon(x,t) := u(x,t) + \epsilon x^2$ satisfies

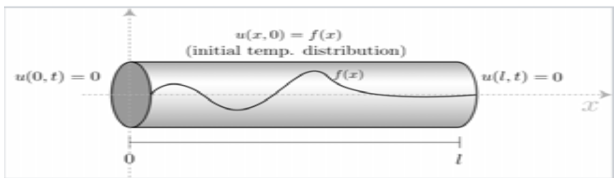
$$\left[\frac{\partial}{\partial t} - k\frac{\partial^2}{\partial x^2}\right] v_\epsilon = -2k\epsilon < 0 \quad (\forall\ (x,t) \in [0,L] \times [0,T]).$$

- v_ϵ cannot attain its maximum anywhere inside the rectangle $(0,L) \times (0,T]$. Why? If v_ϵ attains its maximum at $(x_0,t_0) \in (0,L) \times (0,T]$, then

$$k\frac{\partial^2}{\partial x^2} v_\epsilon(x_0,t_0) = \frac{\partial}{\partial t} v_\epsilon(x_0,t_0) + 2k\epsilon \geq 0 + 2k\epsilon > 0 \quad (\text{Not possible})$$

- The proof follows from $\lim_{\epsilon \to 0} v_\epsilon = u$.





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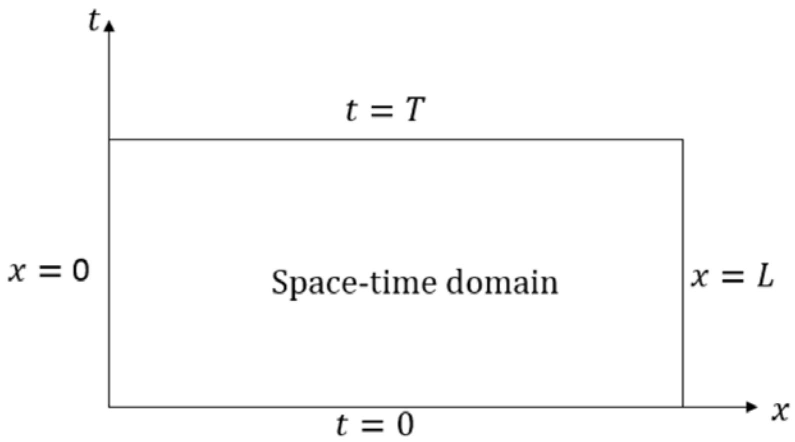


Theorem (Uniqueness; 1D Heat)

There is at most one solution of

$$\begin{cases} \left[\dfrac{\partial}{\partial t} - k\dfrac{\partial^2}{\partial x^2}\right] u(x,t) = f(x,t) & ((\forall\ (x,t) \in (0,L) \times (0,T]) \\ u(x,0) = \phi(x) & (\forall\ x \in [0,L]) \\ u(0,t) = g_0(t), \quad u(L,t) = g_1(t) & (0 < t < T) \end{cases}$$

where f, ϕ, g and h are smooth functions. If u_1 and u_2 are two solutions of the above problem, then $u_1 = u_2$.

- The difference $w = u_1 - u_2$ satisfies

$$\begin{cases} \left[\dfrac{\partial}{\partial t} - k\dfrac{\partial^2}{\partial x^2}\right] w(x,t) = 0 & (\forall\ (x,t) \in [0,L] \times [0,T]) \\ w(x,0) = 0 & (\forall\ x \in [0,L]) \\ w(0,t) = 0, \quad w(L,t) = 0 & (0 < t < T). \end{cases}$$

- By the maximum principle, $w = 0$.

Theorem (Two-dimensional Heat Equation)

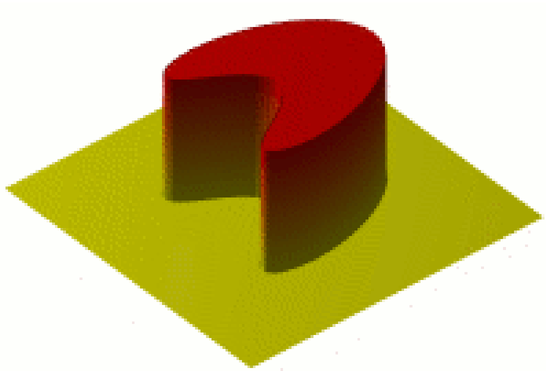
Let $\phi \in C_0(\mathbb{R}^2)$. If $u(\mathbf{r}, t)$ is a solution of the two-dimensional heat equation

$$\begin{cases} \left[\dfrac{\partial}{\partial t} - \nabla^2\right] u(\mathbf{r}, t) = 0 & (\mathbf{r} \in \mathbb{R}^2, \quad t > 0) \\ u(\mathbf{r}, 0) = \phi(\mathbf{r}), & \end{cases}$$

then u can be expressed by

$$u(\mathbf{r}, t) = \int_{\mathbb{R}^2} K(\mathbf{r} - \mathbf{r}', t)\, \phi(\mathbf{r}')\, d\mathbf{r}'$$

where $K(\mathbf{r}, t) = \frac{1}{4\pi t} e^{-\frac{|\mathbf{r}|^2}{4t}}$ is the heat kernel in the two dimension.



- The proof is exactly same as that of the one-dimensional case.
- Indeed, the proof comes from the following facts:

$$\left[\frac{\partial}{\partial t} - \nabla^2\right] K(\mathbf{r}, t) = 0 \qquad (\forall \mathbf{r} \in \mathbb{R}^2, \quad t > 0)$$

and

$$\lim_{t \to 0^+} K(\mathbf{r}, t) = \delta(\mathbf{r}) \qquad (\forall \mathbf{r} \in \mathbb{R}^2).$$

Image credit: Wikipedia

Gaussian filter & Denoising

Recall the solution of the heat equation:

$$u(\mathbf{r}, t) = \int_{\mathbb{R}^2} \frac{1}{4\pi t} e^{-\frac{|\mathbf{r}-\mathbf{r}'|^2}{4t}} \phi(\mathbf{r}')\, d\mathbf{r}'$$

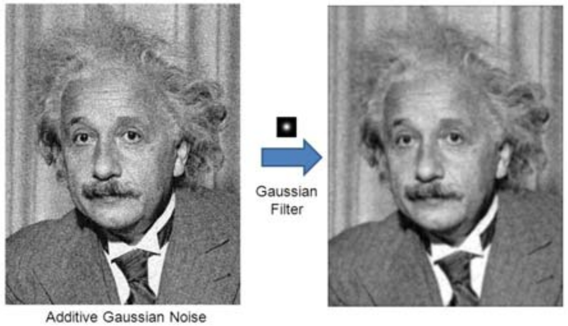
- With $t = \frac{\sigma^2}{2}$,

$$u(\mathbf{r}, \frac{\sigma^2}{2}) = G_\sigma * \phi(\mathbf{r}) = \int_{\mathbb{R}^2} G_\sigma(\mathbf{r}-\mathbf{r}')\phi(\mathbf{r}')\, d\mathbf{r}'$$

where G_σ is the Gaussian filter defined by

$$G_\sigma(\mathbf{r}) = \frac{1}{2\pi\sigma^2} e^{-\frac{|\mathbf{r}|^2}{2\sigma^2}}.$$

Denoising



- When ϕ is an observed image containing noise, we can view $G_\sigma * \phi$ as a denoised image.
- For a small σ, $G_\sigma * \phi \approx \phi$ and, therefore, details in the image are kept.The larger σ results in a blurred image $G_\sigma * \phi$ with reduced noise.
- Hence, σ determines the local scale of the Gaussian filter which reduces noise while eliminating details of the image ϕ.

Summery: Heat Equation

We assume a three-dimensional domain Ω occupying a solid object where heat conduction occurs. If there is no heat source inside Ω, then the temperature $u(\mathbf{r}, t)$ satisfies

$$\underbrace{c(\mathbf{r})\rho(\mathbf{r})\partial_t u(\mathbf{r}, t)}_{\text{the rate of change of heat energy}} = \underbrace{\operatorname{div}(k\nabla u)}_{\text{the heat flux into voxel region through its boundary}}.$$

- To predict future temperature, we need to know the **initial temperature distribution**

$$u(\mathbf{r}, 0) = u_0(\mathbf{r}),$$

- and some boundary conditions which usually will be one of the followings:

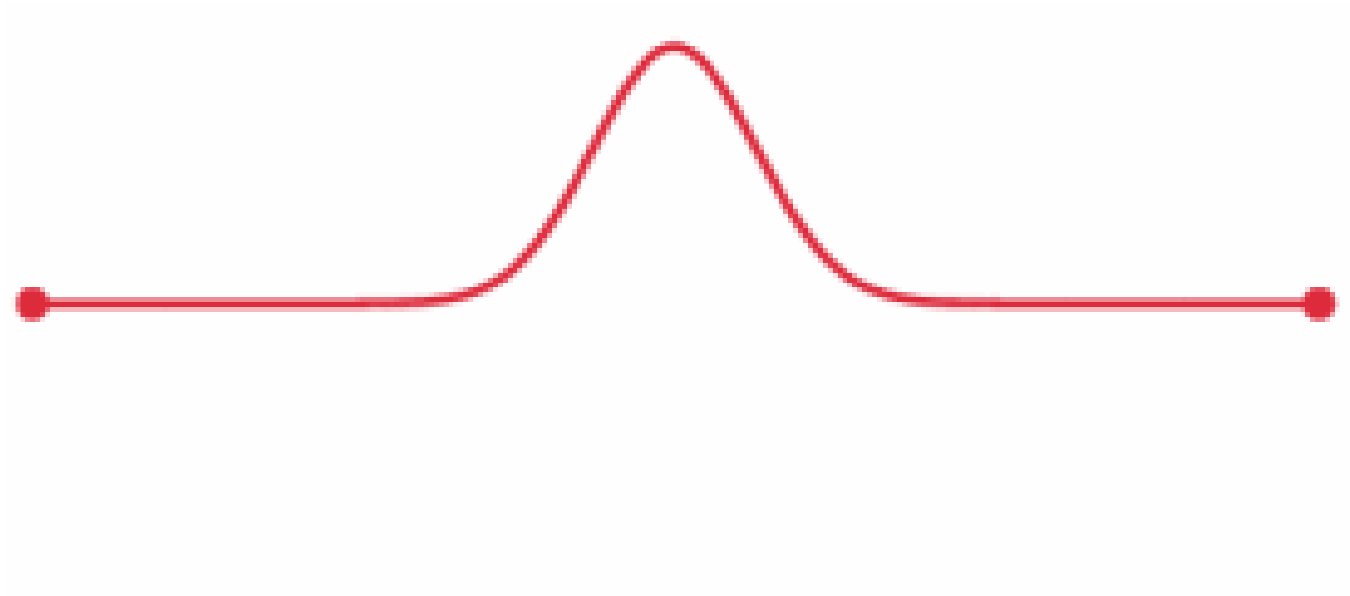
$$\begin{aligned}
&\text{Dirichlet boundary condition:} && u(\cdot, t)|_{\partial\Omega} = f \quad \text{(prescribed temperature)},\\
&\text{Neumann boundary condition:} && k\mathbf{n}\cdot\nabla u(\cdot, t)|_{\partial\Omega} = g \quad \text{(prescribed flux)},\\
&\text{Robin boundary condition:} && k\mathbf{n}\cdot\nabla u(\cdot, t)|_{\partial\Omega} = -H(u(\cdot, t) - f(\cdot, t))|_{\partial\Omega}.
\end{aligned}$$

Here, H is called the heat transfer coefficient.

Wave Equation

$$\left[\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2}\right] u(x, t) = 0$$

The wave equation describes how waves propagate.
This 1D wave propagates at the speed of c .



1D Wave Equation: flexible, elastic homogeneous string

- Assume that the string (that is stretched between two points $x = 0$ and $x = L$) undergoes relatively small transverse vibrations and its displacement $u(x, t)$ at time t and position x is perpendicular to the direction of wave propagation.
- Assuming that the tension T and the density ρ are constants over the string, the vertical component of the force acting on the string at $[x, x + \Delta x]$ is

$$T\frac{u_x(x+\Delta x,t)}{\sqrt{1+u_x^2}} - T\frac{u_x(x,t)}{\sqrt{1+u_x^2}} \approx \underbrace{T\left(u_x(x+\Delta x,t) - u_x(x,t)\right)}_{T\int_x^{x+\Delta x} u_{xx}(s,t)\ \ ds}.$$

- Since force = mass $\times$ acceleration = $\int_x^{x+\Delta x} \rho u_{tt}(s,t)\ \ ds$ over the interval $[x, x + \Delta x]$, we obtain

$$\int_x^{x+\Delta x} \rho u_{tt}(s,t)\ \ ds = T\int_x^{x+\Delta x} u_{xx}(s,t)\ \ ds.$$

- Letting $\Delta x \to 0$, we have $\boldsymbol{\rho u_{tt} - T u_{xx} = 0}$.
- If the string is released from the initial configuration described by the curve $y = f(x), 0 \leq x \leq L$ and it is at rest when released from this configuration,

$$u(x,0) = f(x) \quad \& \quad u_t(x,0) = 0, \qquad x \in (0, L)$$

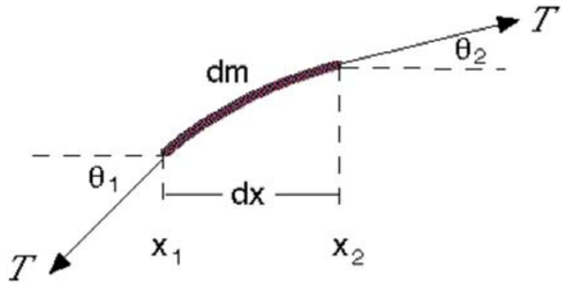


Image credit: Wikipedia

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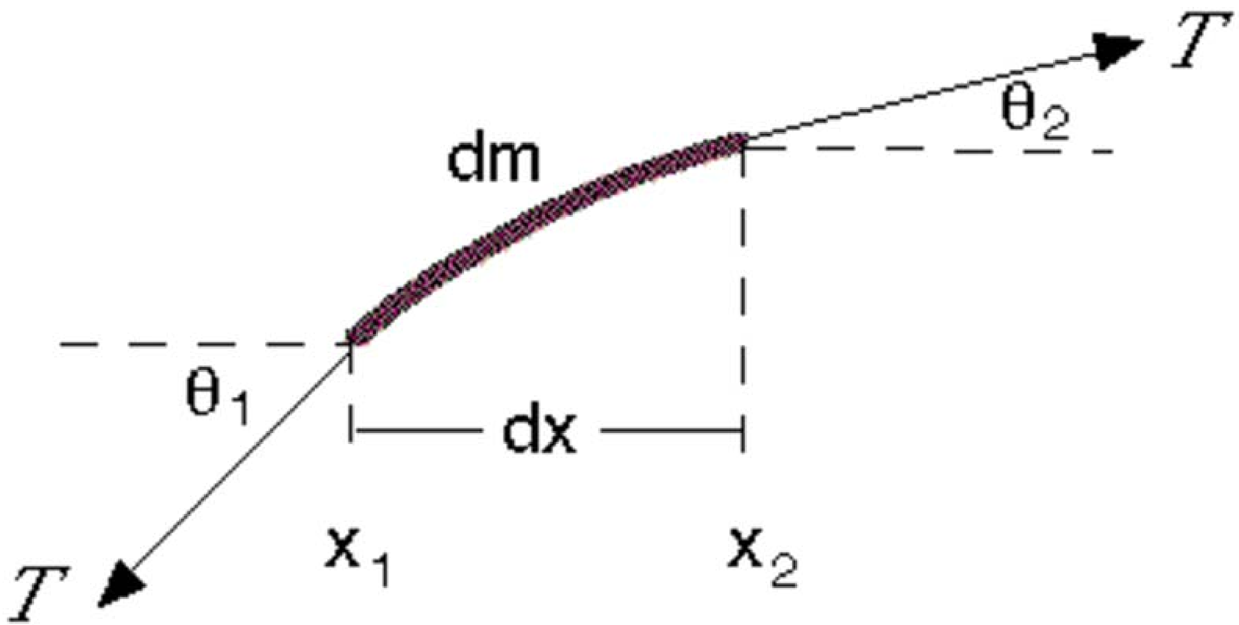

Simple Wave Equation

The wave equation describes wave propagation in the medium. We begin with understanding the structure of the general solution of the simple wave equation:

$$a(x, y)\frac{\partial u}{\partial x} + b(x, y)\frac{\partial u}{\partial y} = 0.$$

- When $a = 1, b = 0$, it becomes $\frac{\partial u}{\partial x} = 0$ which means that u does not depend on x. Hence, the general solution is

  $$u = f(y) \quad \text{for an arbitarly function } f.$$

  For example, $u = y^2 - 5y$ and $u = e^y$ could be solutions of $\frac{\partial u}{\partial x} = 0$.

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- When a and b are constant, it becomes $au_x + bu_y = 0$ or $(a, b) \cdot \nabla u = 0$, which means that u does not change in the direction (a, b). That is, u is constant on any line $bx - ay = constant$, called the characteristic line. We should note that the characteristic line $bx - ay = constant$ satisfies $\frac{dy}{dx} = \frac{b}{a}$. Hence, the general solution is

$$u = f(bx - ay) \quad \text{for an arbitarly function } f.$$

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- Consider $2u_x + yu_y = 0$ or $(2, y) \cdot \nabla u = 0$. Then, u is constant on *any characteristic curve satisfying* $\frac{dy}{dx} = \frac{y}{2}$. This means that $u = \textit{constant}$ for any *characteristic curve* $ye^{-x/2} = C$, which is a solution of $\frac{dy}{dx} = \frac{y}{2}$. Hence, the general solution is

$$u = f\left(e^{-x/2}y\right) \qquad \text{for an arbitarly function } f.$$

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- Consider $2u_x + 4xy^2 u_y = 0$. Then u is constant along the characteristic curves satisfying
$$\frac{dy}{dx} = \frac{4xy^2}{2} = 2xy^2.$$
Since the characteristic curves are $y = (C - x^2)^{-1}$ or $x^2 + \frac{1}{y} = C$, the general solution is
$$u = f\left(x^2 + \frac{1}{y}\right) \qquad \text{for an arbitarly function } f.$$

Theorem

The general solution of the wave equation

$$\left[\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right]u(x,t) = 0 \quad on \quad -\infty < x < \infty$$

is

$$u(x,t) = f(x+ct) + g(x-ct)$$

where f and g are two arbitrary functions of a single variable.

- We can decompose the wave operator into
$$\left[\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right] = \left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right).$$
- Writing $v(x,t) = \left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)u(x,t)$, v satisfies
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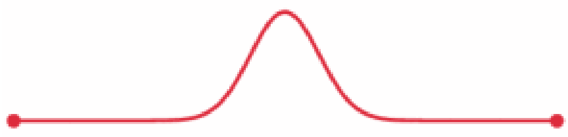

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- The general solution of v is $v(x,t) = h(x+ct)$ for $\forall h \in C^1(\mathbb{R})$.
- Then, u satisfies
$$\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)u(x,t) = v(x,t) = h(x+ct) \quad \forall h \in C(\mathbb{R})$$

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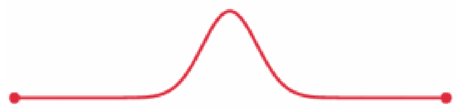
- Writing $v(x,t) = \left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)u(x,t)$, v satisfies

$$\left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right)v = 0 \quad \text{in} \quad -\infty < x < \infty.$$



$$\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)u(x,t) = v(x,t) = h(x+ct) \quad \forall h \in C(\mathbb{R})$$

- We can express the general solution as

$$u(x,t) = g(x-ct) \; + \; \text{particular solution}$$

  where $g(x-ct)$ is the general solution of $u_t + cu_x = 0$.
- To determine the particular solution, we substituting $f(x+ct)$ into it to get

$$\left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right)f(x+ct) = 2cf'(x+ct) = h(x+ct).$$

  Hence, f satisfying $2cf' = h$ is a particular solution.
- The solution is

$$u(x,t) = f(x+ct) + g(x-ct)$$

Theorem

For a given initial displacement $\phi \in C^1(\mathbb{R})$ and initial velocity $\psi \in C^1(\mathbb{R})$, the solution of the initial value problem

$$\begin{cases} u_{tt} = c^2 u_{xx} & (-\infty < x < \infty, \quad t > 0) \\ u(x,0) = \phi(x) & (-\infty < x < \infty) \\ u_t(x,0) = \psi(x) & (-\infty < x < \infty) \end{cases}$$

can be expressed as

$$u(x,t) = \frac{1}{2}\Big[\phi(x+ct) + \phi(x-ct)\Big] + \frac{1}{2c}\int_{x-ct}^{x+ct} \psi(s)\,ds.$$

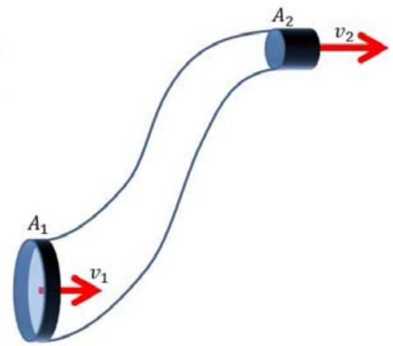
- The general solution is $u(x,t) = f(x+ct) + g(x-ct)$.
- We need to determine f and g using the two initial conditions:

$$f(x) + g(x) = u(x,0) = \phi(x) \qquad \& \qquad cf'(x) - cg'(x) = u_t(x,0) = \psi(x).$$

- Since $f' = \frac{1}{2}(\phi' + \psi/c)$ & $g' = \frac{1}{2}(\phi' - \psi/c)$,

$$f(x) = \frac{1}{2}\left[\phi(x) + \frac{1}{c}\int_0^x \psi(s)ds\right] + C_1 \quad \& \quad g(x) = \frac{1}{2}\left[\phi(x) - \frac{1}{c}\int_0^x \psi(s)ds\right] + C_2$$

Continuity equation



- Consider the flow of fluid with pressure $p(\mathbf{x}, t)$, density $\rho(\mathbf{x}, t)$ and the velocity of the particle of fluid $\mathbf{v}(\mathbf{x}, t)$.
- The conservation of mass in a unit time interval is expressed by the relation

$$\underbrace{\frac{d}{dt}\int_{\square}\rho(\mathbf{x}, t)d\mathbf{x}}_{\text{the rate of increase of mass in }\Omega} = \underbrace{-\int_{\partial\square}\rho\,\mathbf{v}\cdot\mathbf{n}dS}_{\text{the rate at which mass is flowing into }\partial\Omega}.$$

- From the divergence theorem,

$$\int_{\square}\left(\frac{\partial}{\partial t}\rho(\mathbf{x}, t) + \nabla\cdot(\rho\,\mathbf{v})\right)d\mathbf{x} = 0$$

which leads to the continuity equation of

$$\frac{\partial}{\partial t}\rho(\mathbf{x}, t) + \nabla\cdot(\rho\,\mathbf{v}) = 0.$$

How to prove $\iint_{\partial\Omega} \boldsymbol{n}\, p \; dS = \iiint_{\Omega} \nabla p \, dV$

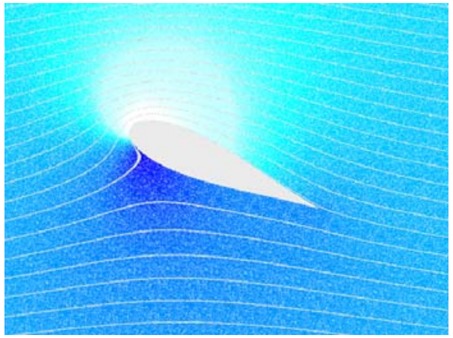
Key idea: $\boldsymbol{n} = (\boldsymbol{n}\cdot\mathbf{e}_x)\mathbf{e}_x + (\boldsymbol{n}\cdot\mathbf{e}_y)\mathbf{e}_y + (\boldsymbol{n}\cdot\mathbf{e}_z)\mathbf{e}_z$

$\boldsymbol{n} = (\boldsymbol{n}_x, \boldsymbol{n}_y, \boldsymbol{n}_z)$ $\quad \mathbf{e}_x = (\mathbf{1},\mathbf{0},\mathbf{0})$, $\quad \boldsymbol{e}_y = (\mathbf{0},\mathbf{1},\mathbf{0})$, $\quad \boldsymbol{e}_z = (\mathbf{0},\mathbf{0},\mathbf{1})$

$$\iint_{\partial\Omega} \boldsymbol{n}\cdot\mathbf{e}_x(\mathbf{e}_x\, p) \; dS = \mathbf{e}_x \iint_{\partial\Omega} \boldsymbol{n}\cdot(\mathbf{e}_x\, p) \; dS$$

$$= \mathbf{e}_x \iiint_{\Omega} \nabla\cdot(\mathbf{e}_x\, p) dV = \mathbf{e}_x \iiint_{\Omega} \mathbf{e}_x\cdot\nabla p \; dV$$

Similarly, we have $\iint_{\partial\Omega} \boldsymbol{n}\cdot\mathbf{e}_y(\mathbf{e}_y\, p) \; dS = \mathbf{e}_y \iiint_{\Omega} e_y\cdot\nabla p \; dV$ & $\iint_{\partial\Omega} \boldsymbol{n}\cdot\mathbf{e}_z(\mathbf{e}_z\, p) \; dS = \mathbf{e}_z \iiint_{\Omega} \mathbf{e}_z\cdot\nabla p \; dV$



Euler's equation

- If we denote by $\mathbf{x}(t)$ the path followed by a fluid particle, then the velocity is $\mathbf{v}(\mathbf{x}(t), t) = \mathbf{x}'(t)$ and acceleration $\mathbf{a}$ satisfies

$$\underbrace{D_t\mathbf{v}(\mathbf{x}(t), t)}_{\mathbf{a}} = (\mathbf{v}\cdot\nabla)\mathbf{v}(\mathbf{x}, t) + \partial_t\mathbf{v}(\mathbf{x}, t).$$

- Newton's law gives

$$\underbrace{-\int_{\partial\Box} p(\mathbf{x}, t)\mathbf{n}(\mathbf{x})dS_{\mathbf{x}} + \int_{\Box}\rho\mathbf{g}\, d\mathbf{x}}_{\text{force of stress } + \text{ gravitational force}} = \underbrace{\int_{\Box}\rho D_t\mathbf{v}(\mathbf{x}, t)d\mathbf{x}}_{\text{mass}\times\text{acceleration}}.$$

- From the divergence theorem,

$$\int_{\Box}(\rho D_t\mathbf{v}(\mathbf{x}, t) + \nabla p(\mathbf{r}, t) - \rho\mathbf{g})\, dV = 0$$

which leads to Euler's equation of motion

$$\underbrace{\frac{\partial}{\partial t}\mathbf{v}(\mathbf{x}, t) + (\mathbf{v}\cdot\nabla)\mathbf{v}(\mathbf{x}, t)}_{D_t\mathbf{v}(\mathbf{x},t)} = -\frac{1}{\rho}\nabla p(\mathbf{x}, t) + \mathbf{g}(\mathbf{x}, t).$$

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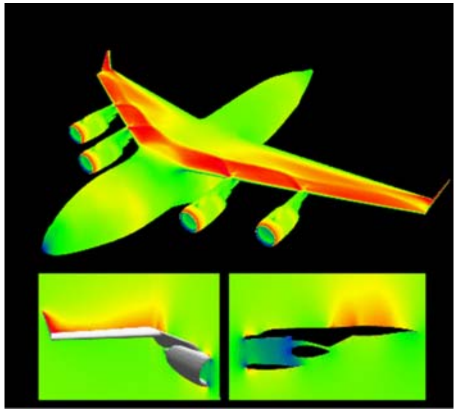

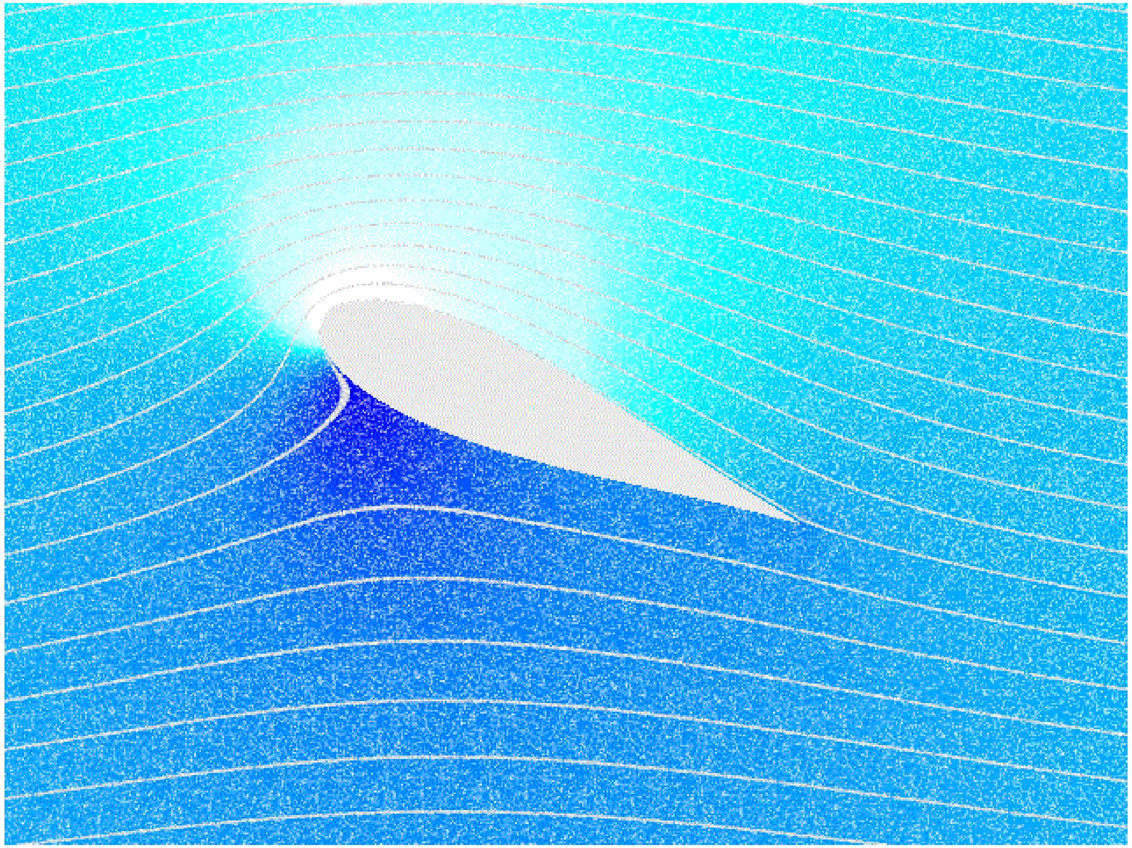

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