Contents

I Introduction to Partial Differential Eq'ns

I.A Examples of PDE's

eq'n that is func of more than one independent variable and contains at least one partial derivaive

1. The order of a PDE - determined by highest order of partial derivative
2. Linear and Non-Linear PDE's - linear if dependent vars and derivatives appear in terms with degrees at most one
3. Well-posed problems - satisfies 3 conditions
   - solution exists
   - solution is unique
   - solution depends continusously on problem data
4. Boundary and initial conditions
   - Dirichlet boundary conditions - solution value is specified on boundary of the region
   - Newman boundary condition - normal derivative of solution is specified on boundary of region
   - Cauchy boundary condition - combination of solution and normal derivative specified on boundary of region

I.B First Order PDE's

I.B.1 The method of characteristics

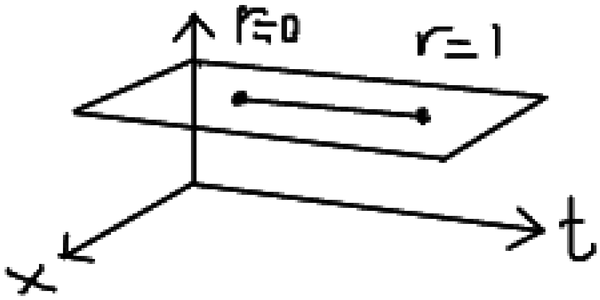
1. Move terms containing dervitives to the LHS and rest to RHS
2. Parameterize contour on the solution whose tangent is always equal to the RHS $(characteristic * askcharleyaboutword*)$
3. Use chain rule on curve and compare to the original PDE to get set of ODE's
4. Solve this set and apply boundary and/or initial conditions

I.B.2 Example

find general solution of u (x, t) of PDE

$\frac{di(x,t)}{\partial t} + \frac{di(x,t)}{\partial x} = 0$

find particular solution when u(x,0) = x^2



$\frac{di(x,t)}{\partial t} + \frac{di(x,t)}{\partial x} = 0 \qquad x = x(r) \quad t = t(r) \quad \frac{\partial u}{\partial r} = 0$

$\frac{\partial u}{\partial r} = \frac{\partial u}{\partial t}\frac{\partial t}{\partial r} + \frac{\partial u}{\partial x}\frac{\partial x}{\partial r} = 0\ , \quad \frac{\partial t}{\partial r} = 1 \quad \& \quad \frac{\partial x}{\partial r} = 1 \qquad \therefore t = r \quad \& \quad x = r + c \qquad t\,(r=0) = 0$

$(x,t) \to (r,c) \quad \Rightarrow \quad \frac{\partial u}{\partial r} = 0 \quad , \quad \frac{\partial u(r,c)}{\partial r} = 0 \quad \Rightarrow \quad u\,(r,c) = f\,(c) \to f\,(x-t) \quad \therefore \quad c = x - r = x - t$

$u\,(x,0) = x^2 = f(x) \quad \therefore \quad f\,(x-t) = x^2$

I.B.3 Example

solve $x\frac{\partial z(x,y)}{\partial x} + y\frac{\partial(x,y)}{\partial y} = xy$ with conditions $z = f\,(S)$ when $x = s$ and $y = 1 - s$

$x\frac{\partial z(x,y)}{\partial x} + y\frac{\partial(x,y)}{\partial y} = xy \quad \Rightarrow \quad \frac{\partial z(r)}{\partial r} = xy \qquad x = x\,(r)\ ,\ y = y\,(r)$

$\frac{\partial z}{\partial r} = \frac{\partial z}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial z}{\partial y}\frac{\partial y}{\partial r} = xy \qquad \to \frac{\partial x}{\partial r} = x\ ,\ \frac{\partial y}{\partial r} = y$

rearrange and integrate $\Rightarrow lnx = r + c \quad \& \quad lny = r \quad \Rightarrow \quad e^c x = e^r$

$x = \underbrace{e^{-c}}_{A} e^r = Ae^r \quad \& \quad y = e^r \qquad \therefore x = Ay$

$\frac{\partial z}{\partial r} = xy = Ae^{2r} \quad \Rightarrow \quad \int \partial z = A \int e^{2r} \partial r \quad \Rightarrow \quad z + c = \frac{A}{2}e^{2r} \quad = \quad \frac{A}{2}\left(\frac{x}{A}\right)^2 = \frac{x^2}{2A}$

$Az + cA = \frac{x^2}{2} \quad \Rightarrow \quad Az + B = \frac{x^2}{2}$

$z = f\,(s)\ ,\ x = s\ ,\ y = 1 - s \quad \Rightarrow \quad x = Ay \quad \therefore A = \frac{x}{y} = \frac{s}{1-s}$

$B = \frac{x^2}{2} - Az \quad = \quad \frac{s^2}{2} - \frac{s}{1-s}f\,(s)\ ,\ s = \frac{x}{x+y}$

$B = \frac{1}{2}\left(\frac{x}{x+y}\right)^2 - \frac{\frac{x}{x+y}}{1-\frac{x}{x+y}}f\left(\frac{x}{x+y}\right) \quad = \quad \frac{1}{2}\left(\frac{x}{x+y}\right)^2 - \frac{x}{y}f\left(\frac{x}{x+y}\right) \quad \therefore \quad z = \frac{1}{A}\frac{x^2}{z} - \frac{B}{A}$

$z = \frac{y}{x}\frac{x^2}{2} - \frac{y}{x}\left[\frac{1}{2}\left(\frac{x}{x+y}\right)^2 - \frac{x}{y}f\left(\frac{x}{x+y}\right)\right] \quad \Rightarrow \quad \frac{1}{2}xy - \frac{1}{2}\frac{xy}{x+y}^2 + f\left(\frac{x}{x+y}\right)$

I.C Second Order Linear PDEs

1. Types
   - mainly linear and second order
   - generally must be solved numerically
   - three types:
     (a) Parabolic - e.g. diffusion equation
     (b) Hyperbolic - e.g. wave equation
     (c) Elliptic - e.g. Laplace equation
2. Why these names
   - In Cartisian coordinates, the graph of a quadratic equation in two variables is always a conic section
     $Ax^2 + 2Bxy + Cy^2 + Dx + Ey + F = 0$
   - The discriminant, $AC - B^2$ determines the type of conic
     - $AC - B^2 = 0$ is a parabola
     - $AC - B^2 < 0$ is a hyperbola
     - $AC - B^2 > 0$ is a ellipse
   - The most general 2nd order linear PDE for two variables can be written in Cartesian coordinates as
     $A\frac{\partial^2 u(x,y)}{\partial x^2} + 2B\frac{\partial^2 u(x,y)}{\partial x \partial y} + C\frac{\partial^2 u(x,y)}{\partial y^2} + D\frac{\partial^u (x,y)}{\partial x} + E\frac{\partial u(x,y)}{\partial y} + Fu\,(x,y) + G = 0$
   - The discriminant, $AC - B^2$ determines the type of conic
     - $AC - B^2 = 0$ is a parabola
     - $AC - B^2 < 0$ is a hyperbola
     - $AC - B^2 > 0$ is a ellipse

For higher dimensionality, or in other coordinate systems, the explanation becomes more complicatied. In the coming sections, we will look at examples of each of these three types of linear, second order, equations. We will consider how to solve them analytically and numerically.

II The Diffusion Equations

II.A Some First Order PDEs

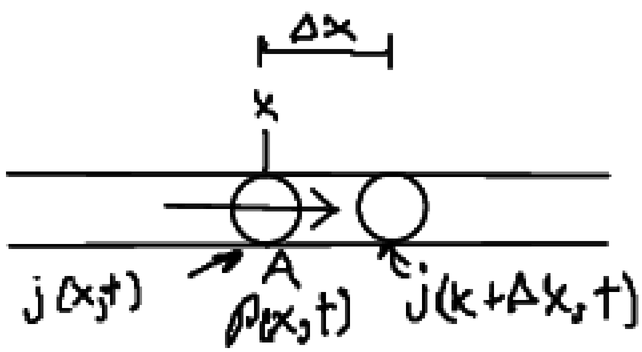
II.A.1 The Equation of Continuity

- The equation of continuity states that the change in the amount of "stuff" in a region is that same as the amount of "stuff" flowing into or out of that region

Example

$$\underbrace{\frac{\partial \rho(x,t)}{\partial t}}_{\text{density } \Delta} + \underbrace{\frac{\partial j(x,t)}{\partial x}}_{\text{change of stuff in region}} = 0 \quad \leftarrow \quad \text{One Dimensional Continuity Equation}$$

Total change in mass per unit area per time $= \Delta j \quad \rightarrow \quad j(x,t) - j(x+\Delta x, t)$



$\frac{\partial \rho}{\partial t}\Delta x = -\left[j(x+\Delta x,t) - j(x,t)\right] \qquad \frac{\partial \rho}{\partial t}(x,t) = -\lim_{x\to 0} \frac{j(x+\Delta x,t)-j(x,t)}{\Delta x}$

$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x} \quad \Rightarrow \quad \frac{\partial \rho(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0$

$\tilde{\rho} \Rightarrow c\rho T \ , \ j \Rightarrow Q$

$\frac{c\rho \partial T(x,t)}{\partial t} + \frac{\partial Q(x,t)}{\partial x} = 0$

$\frac{\partial \rho(x,y,z,t)}{\partial t} = -\frac{\partial j_x(x,y,z,t)}{\partial x} - \frac{\partial j_y}{\partial y} - \frac{\partial j_z}{\partial z}$

$\frac{\partial \rho(x,y,z,t)}{\partial t} = -\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \cdot (j_x, j_y, j_z)$

$\frac{\partial \rho(x,y,z,t)}{\partial t} = \nabla \cdot \vec{j}(\vec{r},t) = 0$ In three dimensions, this would be

$\frac{\partial \rho(r,t)}{\partial t} + \nabla \cdot j(r,t) = 0 \quad \leftarrow \quad$ Three Dimensional Continuity Equation

Where $\quad \nabla \equiv \left(\frac{\partial}{\partial x}\frac{\partial}{\partial y}\frac{\partial}{\partial z}\right) \quad \leftarrow \quad$ *"nabla" or "del"*

II.A.2 Fick's First Law and Fourier's Law

- This law is an empirical relationship stating the proportionality between the spatial change of the density and the current density

Example

$j\left(x,t\right)=-D\frac{\partial\rho(x,t)}{\partial x}$ $\leftarrow$ Fick's First Law in one dimension

$Q\left(x,t\right)=-\kappa\frac{\partial T(x,t)}{\partial x}$ $\leftarrow$ Fourier's Law in one dimension

N-particles of mass M

$\frac{N(x)}{2}-\frac{n(x+\Delta x)}{2}$

$j=\frac{d}{2}\left[\frac{N(x+\Delta x)-N(x)}{A\Delta t}\right]$ Mass density$\rho=\frac{N}{\Delta xA}\Rightarrow\frac{N}{A}=\rho\Delta x$

$j=\frac{-1}{2}\frac{\Delta x^2}{\Delta t}\left[\frac{\rho(x+\Delta x)-\rho(x)}{\Delta x}\right]$, $D\equiv\frac{\Delta x^2}{2\Delta t}$ $\left(\frac{area}{time}\right)$

$\lim_{x\to 0}\Rightarrow j=-D\frac{\partial\rho(x,t)}{\partial x}$

$\kappa=\frac{watts}{mK}$ $j_x=-D\frac{\partial\rho}{\partial x}\Rightarrow\vec{j}=-D\nabla\rho\ \Rightarrow\ \vec{j}\left(\vec{r},t\right)=-D\nabla\rho\left(\vec{r},t\right)$

$\nabla\rho=\frac{\partial\rho}{\partial x}\hat{i}+\frac{\partial\rho}{\partial y}\hat{j}+\frac{\partial\rho}{\partial\ z}\hat{k}=\left(\frac{\partial\rho}{\partial x},\frac{\partial\rho}{\partial y},\frac{\partial\rho}{\partial z}\right)$

$\vec{j}\left(\vec{r},t\right)=-\kappa\Delta T\left(\vec{r},t\right)$ (Fouriers law in 3-D)

In three dimensions these would be:

$j\left(r,t\right)=-D\underbrace{\nabla\rho}_{\text{“gradient”}}\left(r,t\right)$ $j\left(r,t\right)=-\kappa\nabla T\left(r,t\right)$

II.B Analytical Methods

II.B.1 Derivation

- Combining the equation of continuity with Fick's first law give

Example

$\frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2}$ $\leftarrow$ One Dimensional Diffusion Equation (Fick's Second Law, Heat Conduction Equation)

Substitute $j = -D\frac{\partial \rho}{\partial x}$ into $\frac{\partial \rho}{\partial t} + \frac{\partial j(x)}{\partial x} = 0$

Substitute $\vec{j} = -D\nabla\rho$ into $\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0$

$\frac{\partial \rho}{\partial t} + \nabla \cdot (-D\nabla\rho) = 0 \quad \Rightarrow \frac{\partial \rho}{\partial t} = D\nabla^2\rho$ 3-D

$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ In three dimensions, this would be

$\frac{\partial \rho(r,t)}{\partial t} = D\nabla^2\rho(r,t)$ $\leftarrow$ Three Dimensional Diffusion Equation

Where $\nabla^2 \equiv \left(\frac{\partial}{\partial x}\frac{\partial}{\partial y}\frac{\partial}{\partial z}\right) \cdot \left(\frac{\partial}{\partial x}\frac{\partial}{\partial y}\frac{\partial}{\partial z}\right) = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ $\leftarrow$ "Laplacian"

II.B.2 Applications

- Heat conduction
- Random walks
- Brownian motion
- Polymer science
- Self-Assemby
- Time dependent Schrodinger Equation
  - (add a complex "j" and a potential term)

II.B.3 Seperation of Variables

The diffusion equaion can sometimes be solved analytically using speration of variables

1. Assume the solution is seperable in the form $\rho(x, y, z, t) = X(x)\,Y(y)\,Z(z)\,T(t)$
2. Divide the PDE by $\rho(x, y, z, t) = X(x)\,Y(y)\,Z(z)\,T(t)$ and set equal to a constant to find a set of ODEsl one for each variable
3. Find the general solution to the ODEs: $X(x)\,Y(y)\,Z(z)\,T(t)$
4. Recombine these to get general solutions to $\rho(x, y, z, t) = X(x)\,Y(y)\,Z(z)\,T(t)$ (There might be more than one solution)
5. Apply the boundary conditions and the initial condition to get the solution to the problem, summing over the solutions if needed.

II.B.4 Example

Solve the 1D diffusion equation subject to the boundary conditions:

- $u(0,t) = 0 \qquad (t \geq 0)$
- $u(l,t) = 0 \qquad (t \geq 0)$
- $u(x,0) = u_0\left(\frac{1}{2} - \frac{x}{l}\right) \qquad (0 < x < l)$

This is solving a problem of heat conduction in a bar that is held at zero temperature at its ends and with a given intial temperature profile

Solution:
$\frac{\partial u(x,t)}{\partial t} = \kappa \frac{\partial^2 u(x,t)}{\partial x^2}$

1. Assume $u(x,t) = X(x)\,T(t)$

2. Substitute and separate $\frac{\partial XT}{\partial t} = \kappa \frac{\partial^2 XT}{\partial x^2}$

$\frac{X\partial T}{\partial t} = \kappa T \frac{\partial^2 X}{\partial x^2}$, divide by XT

$\frac{1}{T}\frac{\partial T}{\partial t} = \frac{\kappa}{X}\frac{\partial^2 X}{\partial x^2}$ = constant=$-\alpha$

$g(t) = h(x)$ only if both are constant

3. Solve ODEs

$T(t) = Ce^{-\alpha t} \qquad \frac{\partial^2 X}{\partial x^2} = -\lambda^2 X\ ,\ \lambda = \frac{\alpha}{\kappa}$

$X(x) = Asin\lambda x + Bcos\lambda x$

4. Combine $u(x,t) = X(x)\,T(t)$

$$= e^{-\alpha t}\left(\underbrace{AC}_{D}\,sin\lambda x + \underbrace{BC}_{E}\,cos\lambda x\right)$$

5. Apply Boundary Conditions

$u(0,t) = e^{-\alpha t}(E) = 0 \qquad \therefore E = 0$

$u(l,t) = e^{-\alpha t}(Dsin\lambda l) = 0 \qquad \therefore sin\lambda l = 0$

$\lambda l = n\pi \rightarrow \lambda = \frac{n\pi}{l} \rightarrow \lambda^2 = \frac{\alpha}{\kappa} = \frac{n^2\pi^2}{l^2}$

$u(l,t) = e^{\frac{-n^2\pi^2\kappa t}{l}} sin\left(\frac{n\pi x}{l}\right)$

$u(x,0) = Dsin\left(\frac{n\pi x}{l}\right) = u_0\left(\frac{1}{2} - \frac{x}{l}\right)$

Using linear superposition of n's:

$u(x,t) = \sum_{n=1}^{\infty} u_n(x,t) = \sum_{n=1}^{\infty} D_n e^{\frac{-n^2\pi^2\kappa t}{l^2}} sin\left(\frac{n\pi x}{l}\right)$

$u(x,0) = \sum_{n=1}^{\infty} D_n sin\left(\frac{n\pi x}{l}\right) = u_0\left(\frac{1}{2} - \frac{x}{l}\right)$

Fourier

$D_n = \frac{2}{l}\int_0^l \left(\frac{1}{2} - \frac{x}{l}\right) sin\left(\frac{\pi x}{l}\right) dx$

Expand, and let $z = \frac{n\pi x}{l}$ $\quad \therefore dx = \frac{l}{n\pi dz}$ 1. $= \frac{l}{2n\pi}\int_0^{n\pi} sin\ z\ dz = -cos\ z|_0^{n\pi} x \frac{l}{2n\pi} = \frac{-l}{2n\pi}\left(cos\ n\pi - 1\right) \ \rightarrow = \frac{-l}{2n\pi}\left((-1)^n - 1\right) = \frac{l}{2n\pi}\left(1 - (-1)^n\right)$

2. $= \frac{-1}{l}\int_0^l xsin\frac{n\pi x}{l}dx = \frac{-l^2}{n^2\pi^2}\int_0^{n\pi} zsin\ z\ dz$

u=z , du = dz , dv = sinz dz , v = -cos z

$= \frac{-l^2}{ln^2\pi^2}\left[-zcosz|_0^{n\pi} + \int_0^{n\pi} cosz\ dz\right] = \frac{l}{n\pi}\left(-1\right)^n$

Overall,

$D_n = \frac{2u_0}{l}\left[\frac{l}{2n\pi}\left[1 - (-1)^n\right] + \frac{l}{n\pi}\left(-1\right)^n\right] = \frac{2u_0}{n\pi}\left[\frac{1}{2} + \frac{1}{2}\left(-1\right)^2\right]$

Finally,

$u\left(x,t\right) = \frac{u_0}{\pi}\sum_{m=1}^{\infty}\frac{1}{m}e^{\frac{-4m^2\pi^2\kappa t}{l}^2} \sin\left(\frac{2m\pi x}{l}\right)$ or

$u\left(x,t\right) = \frac{u_0}{\pi}\left[e^{\frac{-4m^2\pi^2\kappa t}{l}^2} \sin\left(\frac{2m\pi x}{l}\right) + \frac{1}{2}e^{\frac{-16m^2\pi^2\kappa t}{l}^2} \sin\left(\frac{4m\pi x}{l}\right) + \frac{1}{3}e^{\frac{-36m^2\pi^2\kappa t}{l}^2} \sin\left(\frac{6m\pi x}{l}\right) + ...\right]$

II.B.5 Transform Methods

The diffusion equation can sometimes be solvd analytically using Fourier or Laplace tansforms.

1. Transform both sides of the PDE and simplify
2. Find the solution to the transformed equation and apply boundary and inital conditions - some conditions will be built into the transform
3. Inverse transform (this might be the tricky part) to get the solution of the PDE

II.B.6 Example

A very long and narrow pipe is filled with water. At time t=0 a quantity of salt (M grams) is introduced into the pipe at some point x_0 (remote from both ends of the pipe). What is the concentration of salt at any later time?

Solution

- Assume an infinitely long one dimensional pipe of cross section A and solve the diffusion equation for $\rho\left(x,t\right)$
- The initial condition will be given by a Dirac delta function
- The boundary conditions should be zero at plus and minus infiinity

$\frac{\partial\rho}{\partial t} = D\frac{\partial^2\rho}{\partial x^2}$, $\rho\left(x,0\right) = 0$ everywhere except $x = x_0$, $\frac{M}{A}S\left(x - x_0\right)$, $\int_{-\infty}^{\infty} f\left(x\right)S\left(x - x_0\right)dx = f\left(x_0\right)$

$\lim_{x\to\pm\infty}\rho\left(x,t\right) = 0$

$\mathcal{F}\{\frac{\partial\rho}{\partial t}\} = \mathcal{F}\{D\frac{\partial^2\rho}{\partial x^2}\} \quad \to \quad \frac{\partial}{\partial t}\mathcal{F}\{\rho\} = D\mathcal{F}\{\frac{\partial^2\rho}{\partial x^2}\}$

$\frac{\partial}{\partial t}\mathcal{F}\{\rho\} = Dj^2k^2\mathcal{F}\{\rho\}$, Let $R\left(k,t\right) = \mathcal{F}\{\rho\}\left(x,t\right)$

$\frac{\partial}{\partial t}R\left(k,t\right) = -k^2DR\left(k,t\right) \quad \Rightarrow \quad R\left(k,t\right) = c\left(k\right)e^{-k^2Dt}$

$R\left(k,0\right) = c\left(k\right)$, $R\left(k,t\right) = R\left(k,0\right)e^{-k^2Dt}$, $R\left(k,0\right) = \mathcal{F}\{\rho\left(x,0\right)\} = \mathcal{F}\{\frac{M}{A}S\left(x - x_0\right)\} = \frac{M}{A}\int_{-\infty}^{\infty} S\left(x - x_0\right)e^{jkx}dx = \frac{M}{A}e^{SK-x_0}$

$R\left(k,t\right) = \frac{M}{A}e^{-Dk^2t}e^{jkx_0} \quad \rho\left(x,t\right) = \mathcal{F}^-1\{R\left(k,t\right)\} = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{M}{A}e^{-Dk^2t}e^{jkx_0}e^{jkx}dk$

$\frac{1}{2\pi}\frac{M}{A}\int_{-\infty}^{\infty} e^{-Dk^2t-jk(x-x_0)}dk \quad \to \quad$ Complete the square

$\int_{-\infty}^{\infty} e^{-\alpha x^2-jkx}dx \Rightarrow ...$

$\rho\left(x,t\right) = \frac{1}{2\pi}\frac{M}{A}\sqrt{\frac{\pi}{DT}}e^{\frac{-(x-x_0)^2}{4DT}}$

$\rho\left(x,t\right) = \frac{M}{A}\frac{1}{\sqrt{4\pi Dt}}e^{\frac{-(x-x_0)^2}{4Dt}}$

II.C Numerical Methods

II.C.1 Finite Difference

- For numerical solution, functions can be discretized and solved approximately
- For the diffusion equation, we can discretize x and t as $x_i = x_0 + i\Delta x$ and $t_n = t_0 + n\Delta t$ where i and n are positive integers
- As a shorthand, we can write $u(x_i, t_n)$ as $u(i, n)$ or u_i^n
- The intervals Δx and Δt
  can be used in Taylor series expansions to express the derivatives of $u(x,t)$ in terms of finite differences.
  $u(x_i + \Delta x, t_n) = u(x_i, t_n) + \Delta x \frac{\partial u}{\partial x}|_{x_i,t_n} \quad \Rightarrow \quad \frac{\partial u}{\partial x}|_{x_i,t_n} = \frac{u(x_i+\Delta x,t_n)-u(x_i,t_n)}{\Delta x} \quad \Rightarrow \quad \frac{\partial u}{\partial x} = \frac{u_{i+1}^n - u_i^n}{\Delta x}$
- Truncation error results from the truncation of the Taylor series
  Forward Difference - 1st order(local error of order Δx)

  $u(x_i + \Delta x, t_n) = u(x_i, t_n) + \Delta x \frac{\partial u}{\partial x}|_{x_i,t_n} \quad \Rightarrow \quad \frac{\partial u}{\partial x} = \frac{u_{i+1}^n - u_i^n}{\Delta x}$

  Backward Difference - 1st order(local error of order Δx)

  $u(x_i - \Delta x, t_n) = u(x_i, t_n) - \Delta x \frac{\partial u}{\partial x}|_{x_i,t_n} \quad \Rightarrow \quad \frac{\partial u}{\partial x} = \frac{u_i^n - u_{i-1}^n}{\Delta x}$

  Centre Difference - 2nd order (local error of order Δx^2)

  $u(x_i + \Delta x, t_n) - u(x_i - \Delta x, t_n) = 2\Delta x \frac{\partial u}{\partial x}|_{x_i,t_n} + \mathcal{O}(\Delta x^3) \quad \Rightarrow \quad \frac{\partial u}{\partial x} = \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}$

	Forward	Backward	Centre
Order	1st	1st	2nd
∂x	$\frac{\partial u}{\partial x} = \frac{u_{i+1}^n - u_i^n}{\Delta x}$	$\frac{\partial u}{\partial x} = \frac{u_i^n - u_{i-1}^n}{\Delta x}$	$\frac{\partial u}{\partial x} = \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}$
∂t	$\frac{\partial u}{\partial t} = \frac{u_i^{n+1} - u_i^n}{\Delta t}$	$\frac{\partial u}{\partial t} = \frac{u_i^n - u_i^{n-1}}{\Delta t}$	$\frac{\partial u}{\partial t} = \frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t}$

- We also will need an expression for the second derivative
- For ODEs, we turned higher order equations into sets of first order equations
- That's not helpful for the diffusion equation because the time derivative (the time stepping variable) is already of first order
  Centre Differnce - 2nd order (local error of order Δx^3) $u(x_i + \Delta x, t_n) + u(x_i - \Delta x, t_n) = 2u(x_i, t_n) + \frac{\partial^2 u}{\partial x^2}|_{x_i,t_n} + \mathcal{O}(\Delta x^3) \quad \Rightarrow \quad \frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$
- In principle, we could use this finite difference expression for the second derivative of ODEs too. But that would be more complicated than just making sets of first order ODEs

II.C.2 Numerical Schemes for the Diffusion Equation

$\frac{u_i^{n+1} - u_i^{n+1}}{2\Delta t} \quad \rightarrow \quad \frac{\partial u(x,t)}{\partial t} = D \frac{\partial^2 u(x,t)}{\partial x^2} \quad \leftarrow \quad \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$

This gives the scheme:

$u_i^{n+1} = \frac{2D\Delta t}{(\Delta x)}^2 \left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right) + u_i^{n-1}$

- Time derivative time levels (n+1 and n-1) "leapfrog" the spatial time levels(n)

- This makes the scheme more complicated to analyze. The scheme is also unstable
  $\frac{u_i^{n+1}-u_i^n}{2\Delta x} \quad \rightarrow \quad \frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} \quad \leftarrow \quad \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$

  This gives the scheme: FTCS [Forward Time Centre Space]

  $u_i^{n+1} = \alpha u_{i+1}^n - (2\alpha - 1)\, u_i^n + \alpha u_{i-1}^n \qquad \text{where } \alpha \equiv \frac{2D\Delta t}{(\Delta x)}^2$

- This is an explicit method. FTCS is 1st order in time and 2nd order in space
  $\frac{u_i^n - u_i^{n-1}}{\Delta t} \quad \rightarrow \quad \frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} \quad \leftarrow \quad \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$

  This gives the scheme: BTCS [Backward Time Centre Space]

  $u_i^n = -\alpha u_{i+1}^{n+1} - (2\alpha - 1)\, u_i^{n+1} + \alpha u_{i-1}^{n+1} \qquad \text{where } \alpha \equiv \frac{2D\Delta t}{(\Delta x)}^2$

- This is an implicit method. BTCS is 1st order in time and 2nd order in space
- This implicit BTCS method needs to be solved using matrix methods.
- Why would we ever use BTCS instead of the easier to code FTCS?
- In fact, why would we ever even use the scheme (CTCS) that is second order in both time and space?
- The answer is stability

II.C.3 Fourier Analysis

- Round-off error is a part of all numerical calculations because digital computers cannot represent all numbers exactly.
- Due to round-off error, some algorithms propogate error cumulatively over iterations so that the algorithm is said to be unstable.
- This means, in a time-stepping finite difference method, that the error will swamp the solution as we continue to step forward in time.
- Eventually, the result will blow up and we will not have a valid solution to the PDE
- Von Neumann stability analysis (also called Fourier analysis) provides a way to estimate the stability condidtions for a numerical finite difference scheme
  1. Assume the error to be of the form $\epsilon_i^n = A^n e^i jk\Delta x$
  2. Substitute this into the discreteized scheme for the PDE
  3. Solve for the amplitude factor A (in general, A is complex)
  4. Determine under what conditions $|A|^2 \leq 1$
     (a) $|A|^2 \leq 1$ for a stable scheme
     (b) $|A|^2 > 1$ for an unstable scheme

Example

$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$, $u = \tilde{u} + \epsilon$

$\frac{\partial \tilde{u}}{\partial t} + \frac{\partial \epsilon}{\partial t} = D\frac{\partial^2 \tilde{u}}{\partial x^2} + D\frac{\partial^2 \epsilon}{\partial x^2} \therefore \frac{\partial \epsilon}{\partial t} = D\frac{\partial^2 \epsilon}{\partial x^2}$

$\epsilon \Rightarrow \epsilon\left(x,t\right)$

$\epsilon\left(x,t\right) = \sum_{m=-\infty}^{\infty} A_m\left(t\right)e^{jmkx}, k = \frac{2\pi}{L}, km = \frac{2\pi m}{L}$

$= \sum_{m=-\infty}^{\infty} A_m\left(t\right)e^{jkmx}, x = i\Delta x$

$\epsilon\left(x_i, t_n\right) = \epsilon E_i^n = \sum_{m=-\infty}^{\infty} A_m\left(n\right)e^{jkmi\Delta x}$

Take only one mode: $\epsilon_i^n \tilde{A}_m\left(n\right)e^{jkmi\Delta x} = A\left(n\right)e^{jki\Delta x}$

After 1 iteration, error amplitude is A, after 2, A^2... $\therefore A\left(n\right) = A^n \quad \rightarrow \quad \epsilon_i^n = A^n e^{jki\Delta x}$

II.C.4 Example

Find the amplification factor and the stability condition for the 1D diffusion equation FTCS scheme

$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \quad \underbrace{\rightarrow}_{FTCS} \quad \underbrace{u_i^{n+1}}_{\epsilon_i^{n+1}} = \alpha\underbrace{u_{i+1}^n}_{\epsilon_{i+1}^n} - \left(2\alpha - 1\right)u_i^n + \alpha u_{i-1}^n$

$A^{n+1}e^{jki\Delta x} = \alpha A^n e^{jki+1\Delta x} - \left(2\alpha - 1\right)A^n e^{jki\Delta x} + \alpha A^n e^{jki-1\Delta x}$

Divide by $A^{n+1}e^{jki\Delta x}$

$A = \alpha e^{jk\Delta x} - \left(2\alpha - 1\right) + \alpha e^{-jk\Delta x} = 2\alpha\frac{e^{jk\Delta x} + e^{-jk\Delta x}2}{-}\left(2\alpha - 1\right)$

$= 2\alpha cos\left(k\Delta x\right) - 2\alpha + 1 = 1 - 2\alpha\left[1 - cos\left(k\Delta x\right)\right], sin\frac{\theta}{2} = \sqrt{\frac{1 - cos\theta}{2}}$

$A = 1 - 4\alpha sin^2\left(\frac{k\Delta x}{2}\right)$

$|A|^2 = 1 - 8\alpha sin^2\left(\frac{k\Delta x}{2}\right) + 16\alpha^2 sin^4\left(\frac{k\Delta x}{2}\right) \leq 1$

$-8\alpha sin^2\left(\frac{k\Delta x}{2}\right) + 16\alpha^2 sin^4\left(\frac{k\Delta x}{2}\right) \leq 0$

$-1 + 2\alpha sin^2\left(\frac{k\Delta x}{2}\right) \leq 0 \ \Rightarrow \ 2\alpha\underbrace{sin^2\left(\frac{k\Delta x}{2}\right)}_{1} \leq 1$

$2\alpha \leq 1$ where $\alpha = \frac{D\Delta t}{(\Delta x)^2} \ \Rightarrow \ \frac{2D\Delta t}{(\Delta x)^2}$ For stability

Solution:

$A = 1 - \frac{4D\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right) \quad \Rightarrow \quad \frac{2D\Delta t}{\Delta x}^2 \leq 1$

- A similar analysis of the CTCS scheme for the diffusion equation shows that it is unconditionally unstable

- For the BTCS diffusion equation scheme, the amplification factor is found to be:
  $A = \frac{1}{1+4\alpha\sin^2\left(\frac{k\Delta x}{2}\right)}$
- Therefore, the BTCS implicit scheme is unconditionally stable

II.C.5 The Crank-Nicolson Scheme

- The CTCS scheme is second order in both space and time, but is unconditionally unstable
  Crank-Nicolson scheme - 2nd order in space and time $\frac{u_i^{n+1}-u_j^n}{\Delta t} = \frac{D}{2}\left[\frac{\left(u_{i+1}^{n+1}-2u_i^n+1+u_{i-1}^{n+1}\right)+\left(u_{i+1}^n-2u_i^n+u_{i-1}^n\right)}{(\Delta x)^2}\right]$
- A Taylor series expansion can be used to prove that this is 2nd order in x and t, but we will not show this.
- The Crank-Nicolson algorithm (and the FTCS and BTCS schemes) can be re-derived in higher spatial dimensions
- One can, for example, use operator splitting to deal with higher dimensions
- This involves subdividing each time step into multiple steps in which the system diffuses slightly in one direction at a time
- The Crank-Nicolson method can also be used to solve the time-dependent Schrodinger equation
- See the lab for more computational information

II.C.6 Consistency, Stability, and Convergence

- There are three aspects to consider when using a time stepping finite difference scheme
  1. Consistency: truncation error from the Taylor series $\to 0$ as $\Delta t, \Delta x$, etc. $\to 0$
  2. Stability: roundoff error is not amplified
  3. Convergence: numerical solution $\to$ real solution as $\Delta t, \Delta x$,etc. $\to 0$
- Consistency + stability $\Leftrightarrow$ convergence

  Lax Equivalence Theorem: a consistent finit difference formula is convergent if and only if it is stable

II.C.7 Accuracy

- A convergent numerical formulation (consistent and stable) still may not be practical if it takes a very long time to run
- For fixed $\Delta t, \Delta x$, etc., a higher order scheme will converge to a given accuracy in fewer iterations than a lower order scheme
- Therefore we want
  - a scheme that is convergent (consistent and stable)

    We'll always need this, with a least conditional stability
  - a scheme that is of high order

    We may have to accept a lower order scheme to achieve stability, or for quick coding
  - a scheme that is not too difficult to implement

    We will often use packaged software in order to avoud complicating programming

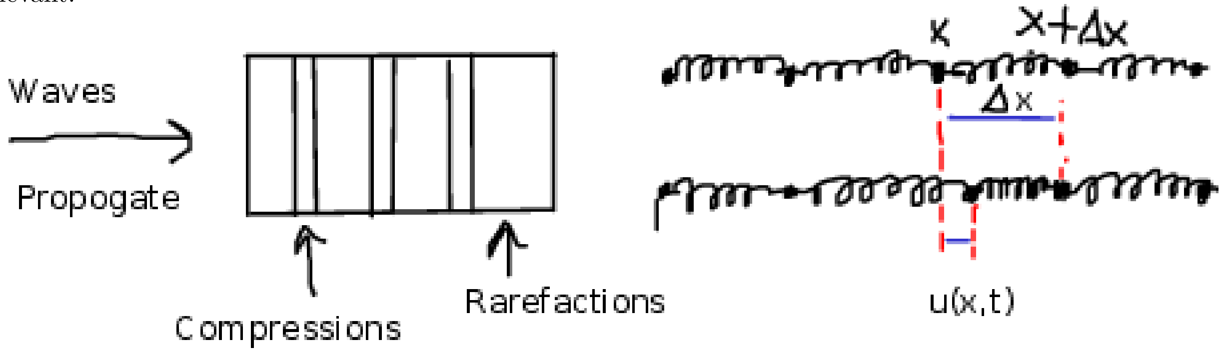
III The Wave Equation

III.A Derivation

III.A.1 Matter Waves

AMEM derives the one dimensional wave equation considering transverse waves on a string.

For nanotechnology, longitudinal waves in a material,which form the basis of phonon theory, are more relevant.



Using Newton's second law for the sum of the forces, the equation of motion for a mass m is found to be the wave equation.

Example

Matter Wave

$\sum F_x = ma_x \quad Hooke'sLaw = F = -kd$

$-ku(x,t) - ku(x,t) + ku(x+\Delta x,t) + ku(x-\Delta x,t) = \frac{m\partial^2 u}{\partial t^2}(x,t)$

$\frac{m\partial^2 u}{\partial t^2}(x,t) = ku(x-\Delta x,t) - 2ku(x,t) + ku(x+\Delta x,t)$

$\frac{\partial^2 u}{\partial t^2}(x,t) = \frac{k}{m}\left[u(x-\Delta x,t) - 2u(x,t) + u(x+\Delta x,t)\right]$

N masses, $L = N\Delta x$, $K = \frac{k}{N}$, $\frac{1}{K} = \frac{1}{K_1} + \frac{1}{K_2}...$, $M = Nm$

$k = KN$, $m = \frac{M}{N}$, $\frac{k}{m} = \frac{KN^2}{M}$, $N = \frac{L}{\Delta x}$, $N^2 = \frac{L^2}{\Delta x^2}$

$\frac{k}{m} = \frac{KL^2}{M\Delta x^2}$

$\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{KL^2}{M}\left[\frac{u(x-\Delta x,t) - 2u(x,t) + u(x+\Delta x,t)}{\Delta x^2}\right]$

As $x \to 0$, $\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{KL^2}{M}\frac{\partial^2 u(x,t)}{\partial x^2}$

$\frac{KL^2}{M} = \frac{\frac{mass}{time^2}\ length^2}{mass^2} = speed^2 = c^2$

$\frac{\partial^2 u(x,t)}{\partial t^2} = c^2\frac{\partial^2 u(x,t)}{\partial x^2} \leftarrow$ 1-D wave equation

Example

$F = -k_1x_1 = -k_2x_2 \;\rightarrow\; \frac{x_1}{x_2} = \frac{k_2}{k_1} \Rightarrow F = -k_{eff}$... Missing

$k_2 = k_{eff}\left(\frac{x_1}{x_2}+1\right) = k_eff = \left(\frac{x_2}{x_1}+1\right) -$

$\frac{1}{k_{eff}} = \frac{1}{k_2}\left(\frac{k_2}{k_1}+1\right) or \frac{1}{k_{eff}} = \frac{1}{k_1} + \frac{-1}{k_2}$

This procedure can be repeated in three dimensions to give the three dimensional wave equation $\frac{\partial^2 u(r,t)}{\partial t^2} = c^2\nabla^2 u(r,t) \leftarrow$ 3-D wave equation

III.A.2 Electromagnetic Waves

- Electromagnetic radiation also obeys the wave equation.
- Electric and magnetic fields form transverse waves from Maxwell's equation in source-free regions

  $\nabla \cdot E(r,t) = \underbrace{\frac{\rho}{\epsilon_0}}_{\rho=0}$ Gauss' Law

  $\nabla x E(r,t) = \frac{-\partial B(r,t)}{\partial t}$ Faraday's Law

  $\nabla \cdot B(r,t) = 0$ No magnetic monopoles

  $\underbrace{\nabla x}_{\text{“}Curl''} \; B(r,t) = \mu_0\left[\underbrace{J(r,t)}_{J=0} + \epsilon_0\frac{\partial E(r,t)}{\partial t}\right]$ Ampere's Law ... with Maxwell's addition

  Example

  $\vec{\nabla} \times \vec{B} = \epsilon_0\mu_0\frac{\partial \vec{E}}{\partial t}$

  $\underbrace{\vec{\nabla} \times \vec{\nabla} \times \vec{B}}_{\text{vector identity}} = \epsilon_0\mu_0\frac{\partial}{\partial t}(\vec{\nabla} \times \vec{E}) \leftarrow$ Faraday's Law

  $\vec{\nabla} \times \vec{\nabla} \times \vec{V} = \vec{\nabla}(\vec{\nabla} \cdot \vec{V}) - \vec{\nabla}^2\vec{V}$

  $\vec{\nabla}(\underbrace{\vec{\nabla}}_{0}) - \vec{\nabla}^2\vec{B} = \epsilon_0\mu_0\frac{\partial}{\partial t}\left(-\frac{\partial \vec{B}}{\partial t}\right)$

  $\vec{\nabla}^2\vec{B} = \epsilon_0\mu_0\frac{\partial^2 \vec{B}}{\partial t^2}$

  $\frac{\partial^2 \vec{B}}{\partial t^2} = c^2\vec{\nabla}^2\vec{B} \qquad$ similarly $\frac{\partial^2 \vec{E}}{\partial t^2} = c^2\vec{\nabla}^2\vec{E}$

  $\vec{\nabla} \times \vec{B} = \mu_0(\vec{J} + \epsilon_0\frac{\partial \vec{E}}{\partial t})$

  $\vec{\nabla} \cdot \vec{\nabla} \times \vec{B} = \mu_0(\vec{\nabla} \cdot \vec{J} + \epsilon_0\frac{\partial}{\partial t}(\vec{\nabla} \cdot \vec{E}))\;,\; \vec{\nabla} \cdot \vec{\nabla} \times \vec{V} = 0$

  $0 = \mu_0(\vec{\nabla} \cdot \vec{J} + \epsilon_0\frac{\partial}{\partial t}(\frac{\rho}{\epsilon_0}) \quad\rightarrow\quad \vec{\nabla}^2 \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0$

Example

Vector Identities

$\vec{\nabla} \times \vec{\nabla} \times \vec{V} = \vec{\nabla}(\vec{\nabla} \cdot \vec{V}) - \vec{\nabla}^2 \vec{V}$

(i) $\vec{\nabla} \times \vec{V} = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}) x (V_x, V_y, V_z)$

$|\vec{A} \times \vec{B}| = ABsin\theta$

The gradient operator $\vec{\nabla}$ measure the slope of a vector $\vec{V}$, so $\vec{\nabla} x \vec{V}$ acts on the slope perpendicular to the vector $\vec{V}$

(ii)

$$\vec{\nabla} \times \vec{V} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \partial x & \partial y & \partial z \\ V_x & V_y & V_z \end{vmatrix}$$

$\hat{i}(\partial y V_z - \partial z V_y) - \hat{j}(\partial x V_z - \partial z V_x) + \hat{k}(\partial x V_y - \partial y V_x)$

$(\vec{\nabla} \times \vec{\nabla} \times \vec{V})_x = \partial x \partial y V_y - \partial^2 y V_x - \partial^2 z V_x + \partial x \partial z V_z = L.H.S$

$\left[\vec{\nabla}(\vec{\nabla} \cdot \vec{V}) - \vec{\nabla}^2 \vec{V}\right]_x = \partial x(\partial x V_x + \partial y v_y + \partial z V_z) - (\partial x^2 V_x + \partial^2 y V_y + \partial^2 z V_z)$

$\vec{\nabla}^2 \vec{V} = (\vec{\nabla}^2 V_x, \vec{\nabla}^2 V_y, \vec{\nabla}^2 V_z) = \partial^2 x V_x + \partial x \partial y V_y + \partial x \partial z V_z - \partial^2 x V_x - \partial^2 y V_x - \partial^2 z V_x$

$\partial x \partial y V_y - \partial^2 y V_x - \partial^2 z V_x + \partial x \partial z V_z = L.H.S$

(iii) $\vec{\nabla} \cdot \vec{\nabla} \times \vec{V} = 0$ See assignment 3

- Combine source-free Ampere's law with Maxwell's addition and Faraday's law
  - Use the magnetic monopole equation to get the B wave equation and the source-free Gauss' law to get the E wave equation.

III.B Analytical Methods

III.B.1 D'Alembert Solution

- The one dimensional wave equation can be simplified by making the coordinate transformation r=x+ct and s =x-ct $\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2} \qquad \frac{\partial^2 u}{\partial r \partial s} = 0$ (1)
- Integraction with respect to r and s gives the general solution $u(x,t) = f(x+ct) + g(x-ct)$ where f and g are arbitrary functions
- For the initial conditions $u(x,0) = F(x) and \frac{\partial u(x,0)}{\partial t} = G(x)$ a particular solution is possible

  Example

  $\frac{\partial u}{\partial x} = \frac{\partial u}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial u}{\partial s}\frac{\partial s}{\partial x} = \frac{\partial u}{\partial r} + \frac{\partial u}{\partial s}$

  $\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x}(\frac{\partial u}{\partial x}) = \frac{\partial}{\partial r}(\frac{\partial u}{\partial x})\frac{\partial r}{\partial x} + \frac{\partial}{\partial s}(\frac{\partial u}{\partial x})\frac{\partial s}{\partial x}$

  $= \frac{\partial}{\partial r}(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial s}) + \frac{\partial}{\partial s}(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial s})$

  $= \frac{\partial^2 u}{\partial r^2} + \frac{\partial^2 u}{\partial r \partial s} + \frac{\partial^2 u}{\partial r \partial s} + \frac{\partial^2 u}{\partial r^2}$

  $= \frac{\partial^2 u}{\partial r^2} + 2\frac{\partial^2 u}{\partial r \partial s} + \frac{\partial^2 u}{\partial r^2}$

  $\frac{\partial u}{\partial t} = \frac{\partial u}{\partial r}\frac{\partial r}{\partial t} + \frac{\partial u}{\partial s}\frac{\partial s}{\partial t} = c\left(\frac{\partial u}{\partial r} - \frac{\partial u}{\partial s}\right)$

  $\frac{\partial^2 u}{\partial t^2} = c^2\left(\frac{\partial^2 u}{\partial r^2} - 2\frac{\partial^2 u}{\partial r \partial s} + \frac{\partial^2 u}{\partial s^2}\right) = c^2\left(\frac{\partial^2 u}{\partial r^2} + 2\frac{\partial^2 u}{\partial r \partial s} + \frac{\partial^2 u}{\partial s^2}\right)$

  Substitute in for $\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2} \qquad \frac{\partial^2 u}{\partial r \partial s} = 0$

  $\frac{\partial^2 u}{\partial r \partial s} = 0$

  Integrate wrt s $\frac{\partial u}{\partial r} = \theta(r)$, then wrt r, $u = f(r) + g(s)$

  $\therefore u(x,t) = f(r) + g(s) = f(x+ct) + g(x-ct)$

  $u(x,0) = f(x) + g(x) = F(x)$ (2)

  $\frac{\partial u(x,0)}{\partial t} = cf'(x) - cg'(x) = G(x)$ (3) Divide both sides by c, and integrate

  $f(x) - g(x) = \frac{1}{c}\int G(x)dx + \kappa = \frac{H(x)}{c} + \kappa(4)$

  Add 2 and 4, divide by 2 $f(x) = \frac{1}{2}F(x) + \frac{1}{2c}H(x) + \frac{\kappa}{2}$

  from other math $g(x) = \frac{1}{2}F(x) - \frac{1}{2c}H(x) - \frac{\kappa}{2}$

  $u(x,t) = \frac{1}{2}\left[F(x+ct) + F(x-ct)\right] + \frac{1}{2c}\left[H(x+ct) - H(x-ct)\right]$

  $u(x,t) = \frac{1}{2}\left[F(x+ct) + F(x-ct)\right] + \frac{1}{2c}\int_{x+ct}^{x-ct} G(z)dz$

III.B.2 Example

Solve the one dimensional wave equation subject to the conditions

(a) zero inital velocity, $\frac{\partial u(x,0)}{\partial t} = 0$ for all x

(b) initial displacement given by

$$u(x,0) = F(x) = \begin{cases} 1-x & (0 \leq x \leq 1) \\ 1+x & (-1 \leq x \leq 0) \\ 0 & otherwise \end{cases}$$

$u\left(x,t\right) = \frac{1}{2}\left[f\left(x+ct\right) + f\left(x-ct\right)\right]$

Where

$$F = \begin{cases} 1-x & 0 \leq x \leq 1 \\ 1+x & -1 \leq x \leq 0 \\ 0 & otherwise \end{cases}$$

$$F\left(x+ct\right) \begin{cases} 1-x-ct & 0 \leq x+ct \leq 1 \\ 1+x+ct & -1 \leq x+ct \leq 0 \\ 0 & otherwise \end{cases}$$

$$F\left(x-ct\right) = \begin{cases} 1-x+ct & 0 \leq x-ct \leq 1 \\ 1+x-ct & -1 \leq x-ct \leq 0 \\ 0 & otherwise \end{cases}$$

$|ct| > 1$

$$u\left(x,t\right) = \begin{cases} \frac{1}{2}\left(1+x+ct\right) & -1-ct \leq x \leq -ct \\ \frac{1}{2}\left(1-x-ct\right) & -ct \leq x \leq 1-ct \\ \frac{1}{2}\left(1+x-ct\right) & -1+ct \leq x \leq ct \\ \frac{1}{2}\left(1-x+ct\right) & ct \leq x \leq 1+ct \end{cases}$$

- Note the discontinuity is preserved in the waves, rather than being smoothed out as in the diffusion equation
- d'Alembert's solution only works for the one dimensional wave equation
- It is also only for an infinite interval, since we didn't apply any boundary conditions (only initial conditions)
- For different intervals, the boundary conditions start to complicate the solution
- For higher dimensions, it isn't valid

- Other analytical methods are better for most wave equation problems

III.B.3 Seperation of variables

- This method works for the wave equation following the same procedure as for the diffusion equation
  1. Assume the solution is seperable in the form $\rho(x,y,z,t) = X(x)Y(y)Z(z)T(t)$
  2. Divide the PDE by $\rho(x,y,z,t) = X(x)Y(y)Z(z)T(t)$ and set equal to a constant to find a set of ODEsl one for each variable
  3. Find the general solution to the ODEs: $X(x)Y(y)Z(z)T(t)$
  4. Recombine these to get general solutions to $\rho(x,y,z,t) = X(x)Y(y)Z(z)T(t)$ (There might be more than one solution)
  5. Apply the boundary conditions and the initial condition to get the solution to the problem, summing over the solutions if needed.

III.B.4 Example

Solve the one dimensional wave equation for vibrations in an organ pipe subject to the boundary conditions

1. $u(0,t) = 0 \quad (t \geq 0)$ (the end x=0 is closed)
2. $\frac{\partial u(l,t)}{\partial x} = 0 \quad (t \geq 0)$ (the end x=l is open)
3. $u(x,0) = 0 \quad (0 \leq x \leq l)$ the pipe is initially undisturbed)
4. $\frac{\partial u(x,0)}{\partial t} = v = constant \quad (0 \leq x \leq l)$ (the pipe is given an initial uniform blast of air)

$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad u(x,t) = X(x)T(t) \quad \to \quad X\frac{\partial^2 T}{\partial t^2} = c^2 T\frac{\partial^2 X}{\partial x^2}$

$\frac{1}{c^2 T}\frac{\partial^2 T}{\partial t^2} = \frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\lambda^2 \quad \to \frac{\partial^2 X}{\partial x^2} = -\lambda^2 \quad \to X(x) = A\cos(\lambda x) + B\sin(\lambda x) \quad T(t) = C\cos(c\lambda t) + D\sin(c\lambda t)$

$u(x,t) = (A\cos(\lambda x) + B\sin(\lambda x))\left[C\cos(c\lambda t) + D\sin(c\lambda t)\right]$

$u(x,t) = (A\cdot 1 + B\cdot 0)\left[C\cos(c\lambda t) + D\sin(c\lambda t)\right] \qquad \therefore A = 0$

$$u(x,t) = sin\lambda x\left[\underbrace{E}_{BC}\cos(c\lambda t) + \underbrace{F}_{BD}\sin(c\lambda t)\right]$$

$u(x,0) = 0$

$u(x,0) = sin\lambda x\left[E\cdot 1 + F\cdot 0\right] \qquad \therefore E = 0$

$u(x,t) = Fsin(\lambda x)\,sin(c\lambda t)$

$\frac{\partial u}{\partial x} = \lambda F sin(c\lambda t)\,cos(\lambda x)$

$\frac{\partial u}{\partial t}(l,t) = F\lambda sin(c\lambda t)\underbrace{cos(\lambda l)}_{0}$

$cos\lambda l = 0 \therefore \lambda = \frac{(n+\frac{1}{2})\pi}{l}$

$$u\left(x,t\right)=\sum_0^\infty F_n sin\left[\frac{c\left(n+\frac{1}{2}\right)\pi t}{l}\right]sin\left[\frac{\left(n+\frac{1}{2}\right)\pi x}{l}\right]$$

$$\frac{\partial u}{\partial t}=\sum_0^\infty F_n sin\left[\frac{\left(n+\frac{1}{2}\right)\pi x}{l}\right]cos\left[\frac{c\left(n+\frac{1}{2}\right)\pi t}{l}\right]*\left[\frac{c\left(n+\frac{1}{2}\right)\pi}{l}\right]$$

$$\frac{\partial u}{\partial t}\left(x,0\right)=\sum_0^\infty F_n\frac{c\left(n+\frac{1}{2}\right)\pi}{l}sin\left[\frac{\left(n+\frac{1}{2}\right)\pi x}{l}\right]=V$$

$$V=\sum_0^\infty F_n\frac{c(2n+1)\pi}{2l}sin\left[\frac{(2n+1)\pi x}{2l}\right]\qquad letm=2n+1$$

$$V=\sum_0^\infty F_{\frac{m-1}{2}}\frac{c\pi m}{2l}sin\left[\frac{m\pi x}{2l}\right]$$

$$\frac{c\pi m}{2l}F_{\frac{m-1}{2}}=\frac{2V}{2l}\int_0^{2l}sin\frac{m\pi x}{2l}dx\qquad F_{\frac{m-1}{2}}=\frac{4V}{m\pi}\frac{2l}{c\pi m}=\frac{8vl}{c\pi^2m^2}$$

$$u\left(x,t\right)=\frac{8lv}{c\pi^2}\sum_0^\infty\frac{1}{2n+1}^2sin\left[\frac{\left(n+\frac{1}{2}\right)\pi ct}{l}\right]sin\left[\frac{\left(n+\frac{1}{2}\right)\pi x}{l}\right]$$

Why does the constant have a negative?

$$\frac{1}{x}\frac{\partial^2X}{\partial x^2}=+\lambda^2=\frac{1}{c^2T}\frac{\partial^2T}{\partial t^2}$$

$$u(x,t)=(Ae^{\lambda x}+Be^{-\lambda x})(Ce^{c\lambda t}+De^{-c\lambda t})$$

$$u(0,t)=(A+B)(Ce^{c\lambda t}+De^{-c\lambda t})=0\qquad B=-A$$

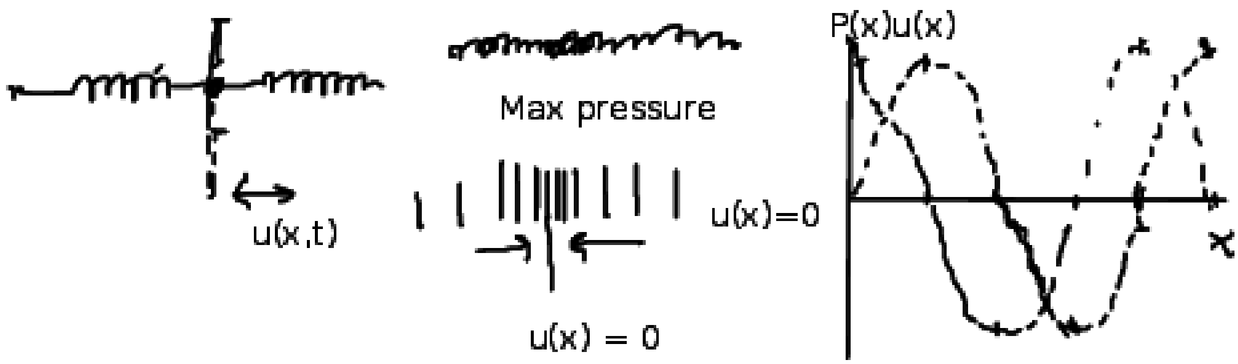
$$u(x,0)=(e^{\lambda x}-e^{-\lambda x})(AC+AD)=0\qquad F=-E$$

$$u(x,t)=E(e^{\lambda x}+e^{-\lambda x})(e^{c\lambda t}+e^{-c\lambda t})$$

$$\frac{\partial u}{\partial x}(l,t)=E\lambda(e^{\lambda}l)+e^{-\lambda l})(e^{c\lambda t}+e^{-c\lambda t})=0\qquad e^{\lambda l}=e^{-\lambda l}\ \therefore \text{ no solution for any real } \lambda$$

$$2\left(\frac{e^{j\lambda l}+e^{-j\lambda l}}{2}\right)=0\qquad cos(\lambda l)=0$$

Why does the second condition mean it is open?



III.B.5 Transform Solutions

This method works for the wave equation following the same procedure as for the diffusion equation:

1. Transform both sides of the PDE and simplify
2. Find the solution to the transformed equation and apply boundary and inital conditions *some conditions will be built into the transform*
3. Inverse transform (this might be the tricky part) to get the solution of the PDE

III.B.6 Example

Solve the one dimensional wave equation for a semi-infinite string using Laplace transforms given that

1. $u(x,0) = 0 \;\; (x \geq 0)$ (string initially undisturbed)
2. $\frac{\partial u(x,0)}{\partial t} = xe^{\frac{-x}{a}} \;\; (x \geq 0)$ (string given an initial velocity)
3. $u(0,t) = 0 \;\; (t \geq 0)$ (string held at x=0)
4. $u(x,t) \to 0$ as $x \to \infty$ for $t \geq 0$ (string held at infinity)

$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$

$U(x,s) \equiv \mathcal{L}\{u(x,t)\} = \int_0^\infty u(x,t)e^{-st}dt$

$\mathcal{L}\{\frac{\partial u}{\partial x}\} = \int_0^\infty \frac{\partial u}{\partial x} e^{-st}dt = \frac{\partial}{\partial x}\int_0^\infty u(x,t)e^{-st}dt = \frac{\partial}{\partial x}U(x,s)$

$\mathcal{L}\{\frac{\partial^2 u}{\partial x^2}\} = \frac{\partial^2}{\partial x^2}U(x,s)$

$\mathcal{L}\{\frac{\partial u}{\partial t}\} = \int_0^\infty \frac{\partial u}{\partial t} e^{-st}dt = sU(x,s) - u(x,0)$

$\mathcal{L}\{\frac{\partial^2 u}{\partial t^2}\} = s^2U(x,s) - \underbrace{\frac{\partial u}{\partial t}(x,0)}_{g(x)} - \underbrace{su(x,0)}_{f(x)}$

$c^2 \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial t^2}$ Laplace Transform $c\frac{\partial^2 U}{\partial x^2} = s^2U(x,s) - g(x) - sf(x)$

Use initial conditions

$f(x) = u(x,0) = 0 \quad g(x) = \frac{\partial u(x,0)}{\partial t} = xe^{\frac{-x}{a}}$

$c^2 \frac{\partial^2 u}{\partial x^2} - s^2U(x,s) = xe^{\frac{-x}{a}}$

Homogenous ODE

$\frac{\partial^2 U}{\partial x^2} - \frac{s^2}{c^2}U(x,s) = 0$

$m^2e^{mx} - \frac{s^2}{c^2}e^m x = 0$

$U = e^{mx} \quad \frac{\partial^2 U}{\partial x^2} = m^2e^{mx}$

$m = \pm \frac{s}{c}$

$U(x,s) = Ae^{\frac{s}{c}x} + Be^{-\frac{s}{c}x}$

Particular Solution

$U^* = \alpha x e^{-\frac{x}{a}} + \beta e^{-\frac{x}{a}}$

$\frac{\partial U^*}{\partial x} = \frac{-\alpha x}{a} e^{-\frac{x}{a}} + \alpha e^{\frac{-x}{a}} - \frac{\beta}{a} e^{-\frac{x}{a}}$

$\frac{\partial^2 U}{\partial x^2} = \frac{\alpha x}{a^2} e^{\frac{-x}{a}} - \frac{\alpha}{a} e^{-\frac{x}{a}} - \frac{\alpha}{a} e^{-\frac{x}{a}} + \frac{\beta}{a} e^{-\frac{x}{a}}$

$= e^{-\frac{x}{a}} \left(\frac{\alpha}{a^2} x - 2\frac{\alpha}{a} + \frac{\beta}{a}^2 \right)$

Substitute U^* and $\frac{\partial^2 U^*}{\partial x^2}$ into ODE:

$e^{-\frac{x}{a}} \left(\frac{\alpha}{a^2} x - 2\frac{\alpha}{a} + \frac{\beta}{a}^2 \right) - \frac{s^2}{c^2} \alpha x e^{\frac{-x}{a}} - \frac{s^2}{c^2} \beta e^{\frac{x}{a}} + \frac{x}{c^2} e^{\frac{-x}{a}}$

$\left(\frac{\alpha}{a^2} - \frac{s^2}{c^2}\alpha + \frac{1}{c^2} \right) x + \left(\frac{-2\alpha}{a} + \frac{\beta}{a^2} - \frac{s^2}{c^2}\beta \right) = 0$

$\frac{\alpha}{a^2} - \frac{s^2}{c^2}\alpha + \frac{1}{c^2} = 0 \qquad \therefore \alpha = \frac{-1}{\frac{c^2}{a^2} - s^2}$

$\frac{-2\alpha}{a} + \frac{\beta}{a^2} - \frac{s^2}{c^2}\beta = 0 \qquad \therefore \beta = \frac{-2\alpha^2 c^2}{a}$

$U^* = \alpha x e^{\frac{-x}{a}} - \frac{2\alpha^2 c^2}{a} e^{\frac{-x}{a}} = \alpha e^{\frac{-x}{a}} \left(x - \frac{2\alpha c^2}{a} \right)$

$U(x,s) = Ae^{\frac{sx}{c}} + Be^{\frac{-sx}{c}} + \alpha e^{\frac{-x}{a}} \left(x - \frac{2\alpha c^2}{a} \right)$

Boundary Conditions

$\lim_{x \to \infty} u(x,t) = u(\infty, t) = 0 \qquad U(\infty, s) = \int_0^\infty u(\infty, t) e^{-st} dt =$

$U(\infty, s) = \underbrace{A}_{0} e^{\infty} + Be^{-\infty} + \alpha e^{-\infty} \left(x - \frac{2\alpha c^2}{a} \right) = 0$

$u(0,t) \Rightarrow B = \frac{2\alpha^2 c^2}{a}$

Sol'n:

$u(x,t) = \frac{a}{c} \left[(ct - x) cosh\left(\frac{ct-x}{a}\right) H(ct-x) - cte^{\frac{-x}{a}} cosh\left(\frac{ct}{a}\right) \right] +$
$\frac{a}{c} \left[e^{\frac{-x}{a}} (x+a) sinh\left(\frac{ct}{a}\right) - asinh\left(\frac{ct-x}{a}\right) H(ct-x) \right]$ *H is Heaviside*

MIDTERM COVERS UP TO HERE