Lecture 11

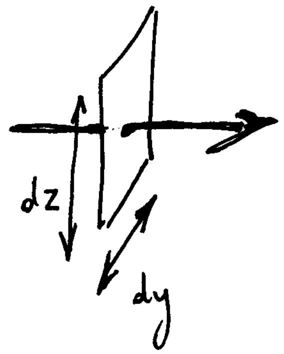
Heat and Diffusion Equation in Space and Time

References

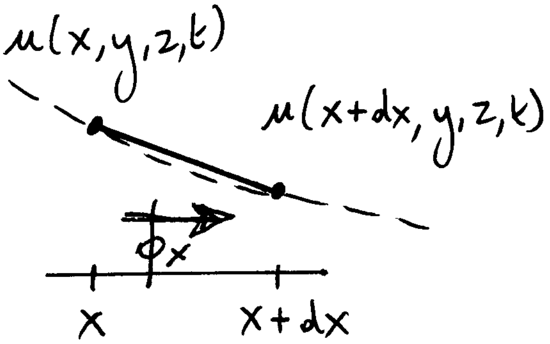
Haberman APDE, Sec. 11.3.
http://en.wikipedia.org/wiki/Heat_equation
http://en.wikipedia.org/wiki/Diffusion_equation

HEAT AND DIFFUSION IN 3-D SPACE AND TIME

Flux in space:



ϕ_x : Flux through surface in (y,z) plane, per unit area $dy\,dz$ and time dt, in the positive x-direction



Flux is opposite and proportional to the gradient of u in x

- Fourier's law (heat, temperature)
- Fick's law (diffusion, concentration)
- Ohm's law (current, voltage)

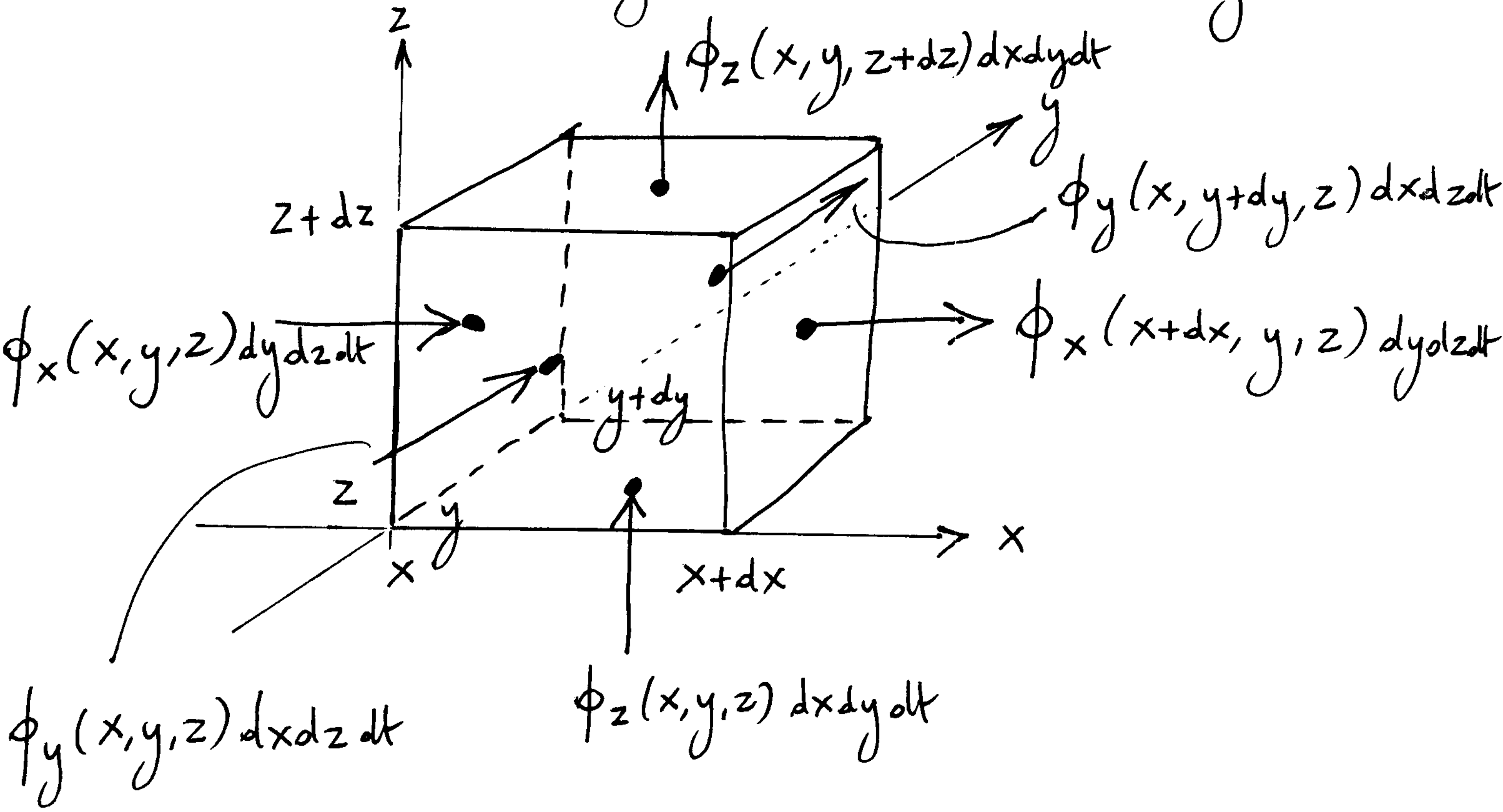
$ \phi \qquad u$

$$\Rightarrow \quad \phi_x = -K_0 \frac{\partial u}{\partial x}, \text{ and similarly:}$$

$$\phi_y = -K_0 \frac{\partial u}{\partial y} \quad \text{in } y \text{ through } (x,z) \text{ plane,}$$

$$\phi_z = -K_0 \frac{\partial u}{\partial z} \quad \text{in } z \text{ through } (x,y) \text{ plane.}$$

Flux balance over infinitesimal volume $dx\,dy\,dz$:



$$\Rightarrow \underbrace{c\rho\,dx\,dy\,dz\;u(x,y,z,t+dt)}_{\text{"INSIDE ENERGY AFTER"}} - \underbrace{c\rho\,dx\,dy\,dz\;u(x,y,z,t)}_{\text{"INSIDE ENERGY BEFORE"}} =$$

$$Q(x,y,z,t)\,dx\,dy\,dz\,dt \qquad \text{"HEAT GENERATED"}$$

$$+\ \phi_x(x,y,z,t)\,dy\,dz\,dt - \phi_x(x+dx,y,z,t)\,dy\,dz\,dt$$
$$+\ \phi_y(x,y,z,t)\,dx\,dz\,dt - \phi_y(x,y+dy,z,t)\,dx\,dz\,dt$$
$$+\ \phi_z(x,y,z,t)\,dx\,dy\,dt - \phi_z(x,y,z+dz,t)\,dx\,dy\,dt$$

"NET FLUX ENTERING IN x, y, z"

Flux balance, per unit $dx\,dy\,dz\,dt$ (volume & time):

$$c\rho \lim_{dt\to 0} \frac{u(x,y,z,t+dt) - u(x,y,z,t)}{dt} =$$

$$Q(x,y,z,t)$$

$$- \lim_{dx\to 0} \frac{\phi_x(x+dx,y,z,t) - \phi_x(x,y,z,t)}{dx}$$

$$- \lim_{dy\to 0} \frac{\phi_y(x,y+dy,z,t) - \phi_y(x,y,z,t)}{dy}$$

$$- \lim_{dz\to 0} \frac{\phi_z(x,y,z+dz,t) - \phi_z(x,y,z,t)}{dz}$$

, or:

$$c\rho \frac{\partial u}{\partial t} = Q(x,y,z,t) - \left(\frac{\partial \phi_x}{\partial x} + \frac{\partial \phi_y}{\partial y} + \frac{\partial \phi_z}{\partial z} \right)$$

$$\underset{\substack{\text{Fick's}\\ \text{Fourier's}\\ \text{Ohm's}}}{=} Q(x,y,z,t) + K_0\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$

$$\Rightarrow \frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + \frac{Q(x,y,z,t)}{c\rho} \; ; \; D = \frac{K_0}{c\rho}$$

General case (for uniform K_0, c, ρ):

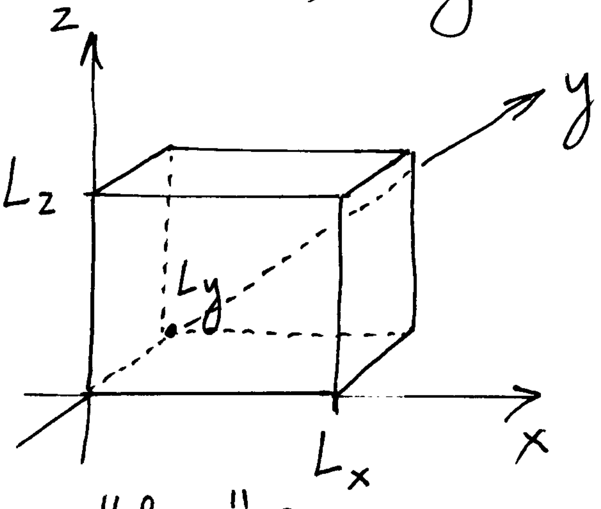
$u = u(x,y,z,t)$ with:

$$\begin{cases} \bullet \ \dfrac{\partial u}{\partial t} = D\left(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} + \dfrac{\partial^2 u}{\partial z^2}\right) + q(x,y,z,t) \\ \bullet \ \text{I.C.} \quad u_0(x,y,z) = u(x,y,z,0) \\ \bullet \ \text{B.C. on } u(x,y,z,t) \text{ over the SURFACE of the boundary of the domain, for all } t. \end{cases}$$

$$D = \frac{K_0}{c\rho} \qquad q = \frac{Q}{c\rho}$$

All the complexity in the solution is in the geometry of the boundary surface!

"Simple" case: CARTESIAN (or Manhattan) boundary conditions, e.g.:



"box" B.C.

$$\begin{cases} u(0,y,z) = 0 & \text{VALUE @ } x=0 \\ u(L_x,y,z) = 0 & \text{VALUE @ } x=L_x \\ u(x,0,z) = 0 & \text{VALUE @ } y=0 \\ u(x,L_y,z) = 0 & \text{VALUE @ } y=L_y \\ u(x,y,0) = 0 & \text{VALUE @ } z=0 \\ u(x,y,L_z) = 0 & \text{VALUE @ } z=L_z \end{cases}$$

SEPARATION OF VARIABLES IN SPACE & TIME

"Box" B.C. allow for separation of variables in SPACE, in addition to TIME:

Homogeneous heat/diffusion PDE with box B.C.:

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial^2 z}\right) \quad \text{with} \quad \begin{cases} u(x,y,z,0) = u_0(x,y,z) & \text{I.C.} \\ u(0,y,z,t) = 0 & \\ u(L_x,y,z,t) = 0 & \\ u(x,0,z,t) = 0 & \text{VALUE} \\ u(x,L_y,z,t) = 0 & \text{B.C.} \\ u(x,y,0,t) = 0 & \\ u(x,y,L_z,t) = 0 & \end{cases}$$

Separation of variables: Try:

$$u(x,y,z,t) = \phi_x(x)\cdot\phi_y(y)\cdot\phi_z(z)\cdot G(t)$$

with $\begin{cases} \phi_x(0) = 0 \\ \phi_x(L_x) = 0 \end{cases}$, $\begin{cases} \phi_y(0) = 0 \\ \phi_y(L_y) = 0 \end{cases}$, and $\begin{cases} \phi_z(0) = 0 \\ \phi_z(L_z) = 0 \end{cases}$

As before:

$$\phi_x \phi_y \phi_z \frac{dG}{dt} = D\left(\frac{d^2\phi_x}{dx^2}\phi_y\phi_z + \phi_x \frac{d^2\phi_y}{dy^2}\phi_z + \phi_x\phi_y \frac{d^2\phi_z}{dz^2} \right) G$$

or:

$$\underbrace{\frac{\frac{dG(t)}{dt}}{G(t)}}_{\substack{\text{FUNCTION OF} \\ t \text{ ONLY} \\ = \text{CONSTANT} \\ -D(\lambda_x+\lambda_y+\lambda_z)}} = D\left(\underbrace{\frac{\frac{d^2\phi_x(x)}{dx^2}}{\phi_x(x)}}_{\substack{\text{FUNCTION OF} \\ x \text{ ONLY} \\ = \text{CONSTANT} \\ -\lambda_x}} + \underbrace{\frac{\frac{d^2\phi_y(y)}{dy^2}}{\phi_y(y)}}_{\substack{\text{FUNCTION OF} \\ y \text{ ONLY} \\ = \text{CONSTANT} \\ -\lambda_y}} + \underbrace{\frac{\frac{d^2\phi_z(z)}{dz^2}}{\phi_z(z)}}_{\substack{\text{FUNCTION OF} \\ z \text{ ONLY} \\ = \text{CONSTANT} \\ -\lambda_z}} \right)$$

- $\frac{dG}{dt} = -D(\lambda_x+\lambda_y+\lambda_z)G \Rightarrow G(t) = G(0)\cdot e^{-D(\lambda_x+\lambda_y+\lambda_z)t}$
- $\frac{d^2\phi_x}{dx^2} = -\lambda_x\phi_x$ and $\left.\begin{matrix}\phi_x(0)=0 \\ \phi_x(L_x)=0\end{matrix}\right\} \Rightarrow \phi_x = A_x \sin(\sqrt{\lambda_x}\,x)$; $\sqrt{\lambda_x} = \frac{k\pi}{L_x}$
- $\frac{d^2\phi_y}{dy^2} = -\lambda_y\phi_y$ and $\left.\begin{matrix}\phi_y(0)=0 \\ \phi_y(L_y)=0\end{matrix}\right\} \Rightarrow \phi_y = A_y \sin(\sqrt{\lambda_y}\,y)$; $\sqrt{\lambda_y} = \frac{l\pi}{L_y}$
- $\frac{d^2\phi_z}{dz^2} = -\lambda_z\phi_z$ and $\left.\begin{matrix}\phi_z(0)=0 \\ \phi_z(L_z)=0\end{matrix}\right\} \Rightarrow \phi_z = A_z \sin(\sqrt{\lambda_z}\,z)$; $\sqrt{\lambda_z} = \frac{m\pi}{L_z}$

$$\Rightarrow u(x,y,z,t) = \sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\sum_{m=1}^{\infty} A_{klm} \underbrace{\sin\left(\frac{k\pi}{L_x}x\right)\sin\left(\frac{l\pi}{L_y}y\right)\sin\left(\frac{m\pi}{L_z}z\right)}_{\phi_{klm}(x,y,z)} e^{-D\left(\left(\frac{k\pi}{L_x}\right)^2+\left(\frac{l\pi}{L_y}\right)^2+\left(\frac{m\pi}{L_z}\right)^2\right)t}$$

Again, the $\phi_{klm}(x,y,z)$ form an orthogonal basis, now over the volume $L_xL_yL_z$:

$$\int_0^{L_x}\int_0^{L_y}\int_0^{L_z} \phi_{klm}(x,y,z)\,\phi_{uvw}(x,y,z)\,dx\,dy\,dz = \delta_{ku}\,\delta_{lv}\,\delta_{mw} \cdot \frac{L_xL_yL_z}{8}$$

$$\Rightarrow A_{klm} = \frac{8}{L_xL_yL_z}\int_0^{L_x}\int_0^{L_y}\int_0^{L_z} \underbrace{u_0(x,y,z)}_{\text{I.C.}} \cdot \phi_{klm}(x,y,z)\,dx\,dy\,dz$$

$$\Rightarrow G(x,y,z,t;\,x_0,y_0,z_0,t_0) =$$

$$\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\sum_{m=1}^{\infty} \frac{8}{L_xL_yL_z}\,\phi_{klm}(x_0,y_0,z_0)\,\phi_{klm}(x,y,z)\,e^{-D\left(\left(\frac{k\pi}{L_x}\right)^2+\left(\frac{l\pi}{L_y}\right)^2+\left(\frac{m\pi}{L_z}\right)^2\right)(t-t_0)}$$

More generally: SEPARATION OF GREEN'S FUNCTION:

$$G(x,y,z,t;\, x_0,y_0,z_0,t_0) =$$

$$\sum_k \sum_l \sum_m g_{xk}(x,t;x_0,t_0) \cdot g_{yl}(y,t;y_0,t_0) \cdot g_{zm}(z,t;z_0,t_0)$$

INTO GREEN'S COMPONENTS g_{xk}, g_{yl}, g_{zm},

AS LONG AS THE B.C. ARE CARTESIAN ("Manhattan") SEPARABLE IN x, y, and z.

e.g.:

- Bounded domain in x: $\begin{cases} u(0,y,z,t)=0 \\ u(L_x,y,z,t)=0 \end{cases}$

$$\Rightarrow g_{xk}(x,t;x_0,t_0) = \frac{2}{L_x}\sin\left(\frac{k\pi}{L_x}x_0\right)\sin\left(\frac{k\pi}{L_x}x\right)\cdot e^{-D\left(\frac{k\pi}{L_x}\right)^2(t-t_0)}, \quad k=1,2,\ldots\infty$$

(+ flux and value-flux variations)

- Unbounded (infinite) domain in x: $\begin{cases} u(-\infty,y,z,t)=0 \\ u(+\infty,y,z,t)=0 \end{cases}$

$$\Rightarrow g_{xk}(x,t;x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}}\, e^{-\frac{(x-x_0)^2}{4D(t-t_0)}}, \quad k=1 \text{ only}$$

- Half-bounded (semi-infinite) domain in x: $\begin{cases} u(0,y,z,t)=0 \\ u(+\infty,y,z,t)=0 \end{cases}$

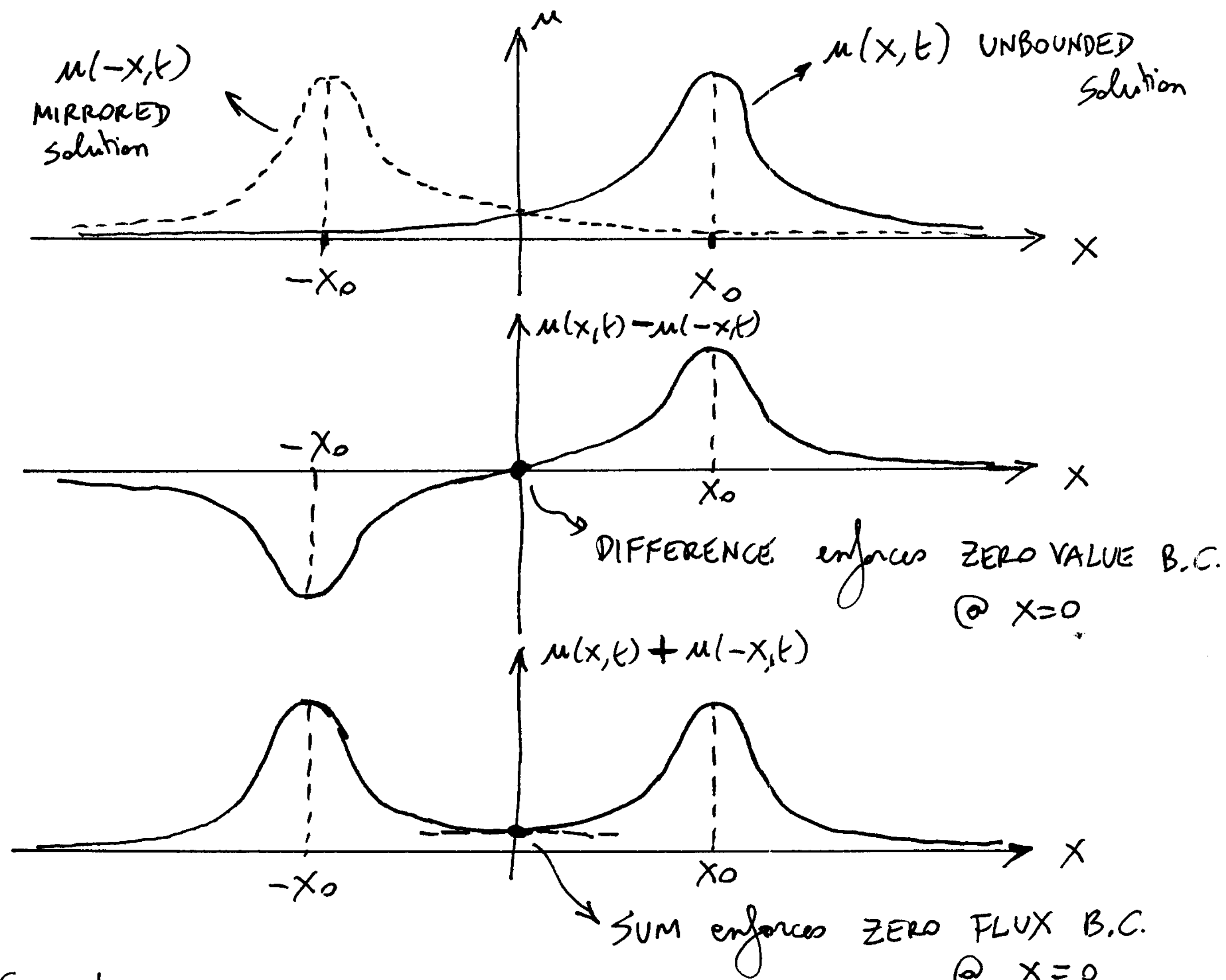
$$\Rightarrow g_{xk}(x,t;x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}}\left(e^{-\frac{(x-x_0)^2}{4D(t-t_0)}} - e^{-\frac{(x+x_0)^2}{4D(t-t_0)}}\right), \quad k=1$$

(+ flux variation)

and SAME in y & z.

HEAT / DIFFUSION EQUATION ON SEMI-INFINITE DOMAINS:

→ MIRRORING METHOD: Construct a SUM or DIFFERENCE of the UNBOUNDED solution and its MIRRORED ($x \leftarrow -x$) version to arrive at a HALF-BOUNDED solution with FLUX or VALUE homogeneous B.C. at the center ($x=0$):



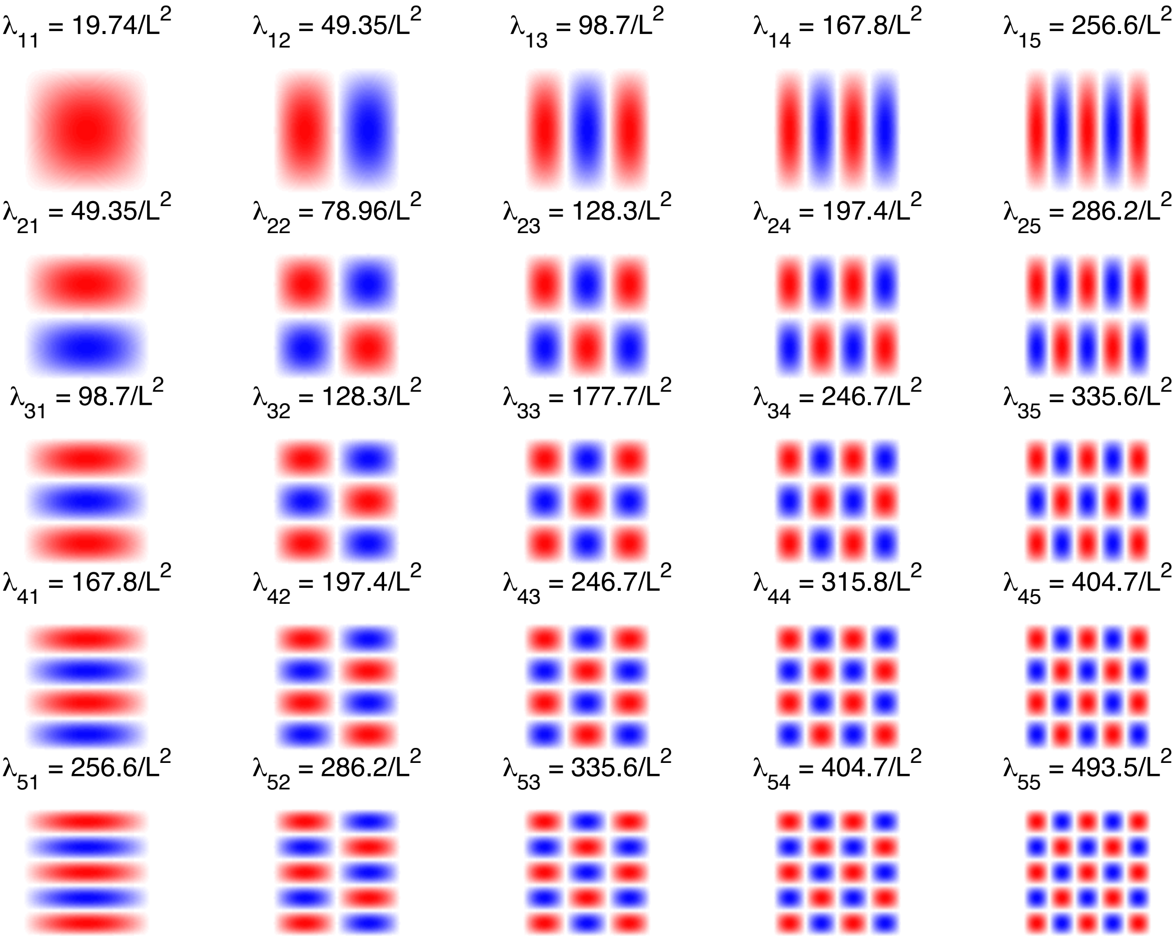
⇒ Green's component is:

$$g_x(x,t;x_0,t_0) - g_x(-x,t;x_0,t_0) \quad \text{for } u(0,t)=0 \text{ VALUE B.C.}$$

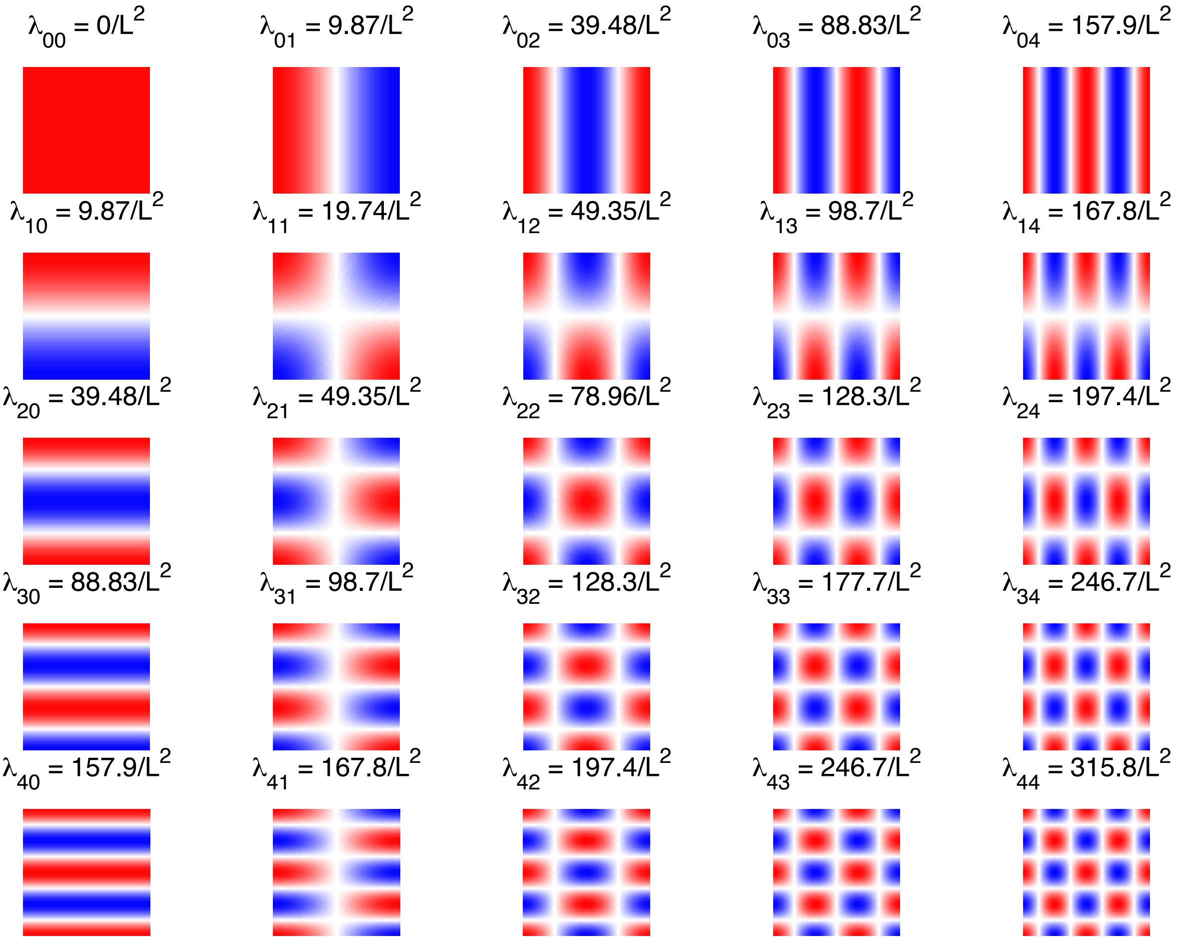
$$g_x(x,t;x_0,t_0) + g_x(-x,t;x_0,t_0) \quad \text{for } \frac{\partial u}{\partial x}(0,t)=0 \text{ FLUX B.C.}$$

where $g_x(x,t;x_0,t_0)$ is the UNBOUNDED Green's component.

Cartesian Box Value Boundary Conditions



Cartesian Box Flux Boundary Conditions



BENG 221
M. Intaglietta
Lecture 9
Time dependent solution of the heat/diffusion equation

Derivation of the diffusion equation

The diffusion process is describe empirically from observations and measurements showing that the flux of the diffusing material F_x in the x direction is proportional to the negative gradient of the concentration C in the same direction, or:

$$F_x = -D\frac{dC}{dx} \qquad 1$$

where D, the diffusion constant, is a coefficient that may be constant, or a function of time, location and concentration.

With reference to **Figure 1**, the flux of material through the face of the element of volume at x, minus the flux through the face at $x + dx$ equals the rate at which the concentration changes in the volume, assuming that fluxes occur only in the x-direction, or:

$$F_x - (F_x + \frac{\partial F_x}{\partial x}dx) = \frac{\partial C}{\partial t} = -\frac{\partial F_x}{\partial x}$$

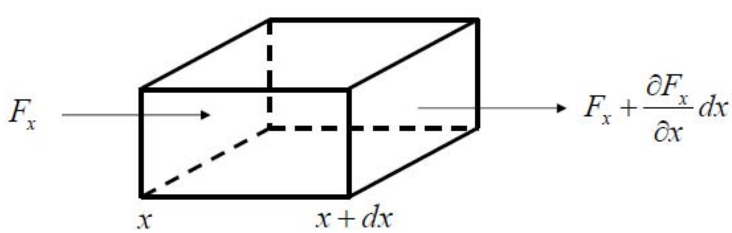


Figure 1. Flux balance along the x-direction in a region of space described in Cartesian coordinates.

This can be readily extended to effects in all directions yielding:

$$\frac{\partial C}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = 0$$

And applying (1) we obtain:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y}\left(D\frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z}\left(D\frac{\partial C}{\partial z} \right) \qquad 2$$

which in the nomenclature of vector analysis is expressed by:

$$\frac{\partial C}{\partial t} = div(D\, grad\, C) = D\nabla^2 C \quad \text{the Laplacian operator for } D = \text{constant}$$

Solution for constant diffusion coefficient from a plane source

Straight forward differentiation shows that:

$$C = At^{-\frac{1}{2}} e^{-\frac{x^2}{4Dt}} \qquad 3$$

is a solution of:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad 4$$

$$\frac{A}{2} t^{-3/2} e^{-\frac{x^2}{4Dt}} + \frac{Ax}{4Dt} t^{-5/2} = D\left(\frac{A}{2D} t^{-3/2} e^{-\frac{x^2}{4Dt}} + \frac{Ax}{4D^2 t} t^{-5/2} \right)$$

This solution for C is symmetrical relative to $x = 0$, tends to 0 as x tends to infinity, and is everywhere zero for $t = 0$, except for $x = 0$ where it is infinite. This solution shows the concentration of the diffusing material originating from a plane source with an amount of material M at zero time. The diffusing material is not consumed and the amount of material is constant at all times. To evaluate A we assume that material is diffusing in an infinite cylinder from a plane located at $x = 0$. Mass balance requires that for all times:

$$M = \int_{-\infty}^{\infty} C dx \qquad 5$$

Changing variables and substituting in 3 and 5:

$$\xi^2 = \frac{x^2}{4Dt}; \qquad 2\xi d\xi = \frac{2x}{4Dt} dx; \qquad \frac{x}{2\left(Dt\right)^{\frac{1}{2}}} d\xi = \frac{x}{4Dt} dx; \qquad dx = 2(Dt)^{\frac{1}{2}} d\xi$$

$$M = At^{-\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\xi^2} 2(Dt)^{\frac{1}{2}} d\xi = 2AD^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\xi^2} d\xi = 2A\left(\pi D\right)^{\frac{1}{2}}$$

and substituting *A* in 3 we obtain:

$$C = \frac{M}{\sqrt{4\pi Dt}} \exp(-\frac{x^2}{4Dt}) \qquad 5$$

In this solution half of the material diffuses in the positive *x* direction and the other half in the negative *x*. This solution is also valid for a semi infinite cylinder where diffusion takes place in the positive *x*-direction only from a plane located at $x = 0$. Clearly the concentration will be double of that of the infinite cylinder. In this case we indicate that the solution is reflected at the boundary and superposed. Note that the gradient of concentration at $x = 0$ is zero in both cases, indicating that in either case no material crosses the plane source (or boundary).

Diffusion from a finite region consisting of a volume source

The solution for the diffusion of material occupying a volume in space can be obtained by assuming that the region is composed of an infinite number of plane sources and superposing the infinite number of related solutions. This problem describes effects taking place in an infinite cylinder filled with water, where the concentration of a solute is $C = C_o$ for $x < 0$, $C = 0$ for $x > 0$, $t = 0$. Consider in the geometry of **Figure 2** a plane of unit surface area containing diffusible material in a quantity $C_o d\xi_i$ located at ξ_i according to 5 will produce a distribution of concentration at any time *t* given by:

$$C_i(x,t) = \frac{C_o d\xi_i}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-\xi_i)^2}{4Dt}\right) \qquad 6$$

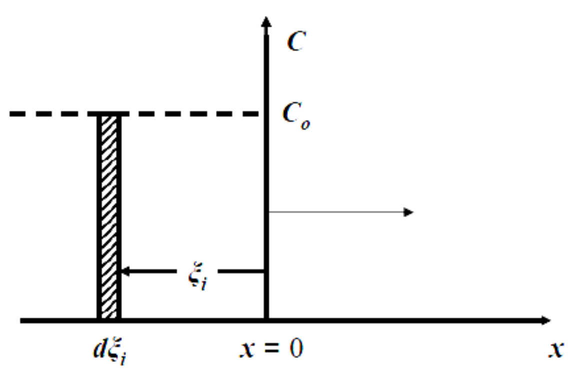


Figure 2. Material at a concentration C_o occupies the region along the negative *x*-axis.

Therefore the effect due to the infinite number of planes at any given time *t* is obtained by adding the effect of each plane solution from 0 to - ∞ or:

$$C(x,t) = \sum_{i=-\infty}^{0} C_i = \int_{-\infty}^{0} \frac{C_o}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x-\xi)^2}{4Dt}\right) d\xi \qquad 7$$

and making the substitution of variables:

$$\frac{x-\xi}{\sqrt{4Dt}} = \eta \qquad \text{and differentiating} \qquad d\xi = -\sqrt{4Dt}\,d\eta$$

Changing variables and limits of integration in 7 we obtain:

for $\xi = 0 \quad \eta = x/\sqrt{4Dt}$ and for $\xi = -\infty \quad \eta = \infty$

Substituting in 7 we obtain:

$$C(x,t) = -\frac{C_o}{\sqrt{\pi}} \int_{-\infty}^{x/\sqrt{4Dt}} \exp(-\eta^2)d\eta = -\frac{C_o}{\sqrt{\pi}} \int_{-\infty}^{0} \exp(-\eta^2)d\eta - \frac{C_o}{\sqrt{\pi}} \int_{0}^{x/\sqrt{4Dt}} \exp(-\eta^2)d\eta$$

$$= \frac{C_o}{\sqrt{\pi}} \int_{0}^{\infty} \exp(-\eta^2)d\eta - \frac{C_o}{\sqrt{\pi}} \int_{0}^{x/\sqrt{4Dt}} \exp(-\eta^2)d\eta$$

$$= \frac{C_o}{\sqrt{\pi}} \left(\frac{\sqrt{\pi}}{2} - \frac{\sqrt{\pi}}{2} erf\,\frac{x}{\sqrt{4Dt}} \right) = \frac{C_o}{2} \left(1 - erf\,\frac{x}{\sqrt{4Dt}} \right)$$

Note that:

$$erfx = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\eta^2} d\eta$$

Diffusion from and in confined regions

The methods described allow to describe diffusion from a substance confined between $-h < x < h$ along the x-axis. Solution of this problem gives the concentration in terms of:

$$C(x,t) = \frac{1}{2} C_0 \left(erf\,\frac{h-x}{\sqrt{4Dt}} + erf\,\frac{h+x}{\sqrt{4Dt}} \right)$$

This solution is symmetrical about $x = 0$ therefore the system can be cut in half, providing the solution for the semi-infinite system.

One dimensional diffusion from a finite system into a finite system that extends up to $x = l$ can be analyzed by the method of reflection and superposition, where in this case the reflection (and superposition) occurs at $x = l$ and $x = 0$. In this system the solution reflected at $x = l$ is reflected again at $x = 0$, at infinitum, resulting in an infinite series of error functions, namely:

$$C(x,t) = \frac{1}{2} C_0 \sum_{n=-\infty}^{\infty} \left(erf\, \frac{h + 2nl - x}{\sqrt{4Dt}} + erf\, \frac{h - 2nl + x}{\sqrt{4Dt}} \right)$$

This solution is useful for calculating the distribution of concentration at early times, when the series converges rapidly. A solution of this type can also be obtained using the Laplace transform.

Non-dimensionalization of the diffusion equation

Given the diffusion equation in one dimension (4) over a one dimensional region of total length L we introduce a non-dimensional spatial coordinate as the ratio x = $x'L$ so that the diffusion equation becomes:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial (Lx')^2} = \frac{D}{L^2} \frac{\partial^2 C}{\partial x'^2}$$

We can also define a non-dimensional time as $t = t' t_0$ where t_0 is an arbitrary time scale; the new equation is:

$$\frac{\partial C}{\partial (t_0 t')} = \frac{D}{L^2} \frac{\partial^2 C}{\partial x'^2} \qquad \therefore \qquad \frac{\partial C}{\partial (t')} = \frac{D t_0}{L^2} \frac{\partial^2 C}{\partial x'^2}$$

Therefore setting $t_0 = L^2/D$ the diffusion equation becomes:

$$\frac{\partial C}{\partial t'} = \frac{\partial^2 C}{\partial x'^2}$$

This result indicates that all diffusion problems are the same. This requires scaling the geometry so that the basic dimension ranges from zero to one. The combination of the size and the diffusivity yield the appropriate time unit. On the scaled domain and in the proper time units, problems of different size and diffusion constants will have the same solution. Thus solving the diffusion equation for one set of boundary conditions solves it for all cases. As an example the time that it takes for diffusion to change concentration by a given amount is directly proportional to the size of its principal dimension. Thus doubling its size quadruples the time.