

**Last Time****Fundamental Solutions of Co-dimension 1, 2, and 3**


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**Method of Images**


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**Finite Domains: Separation of Variables**


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**3.21 Spring 2001: Lecture 11****Periodic or Finite Domains: Separation of Variables**

Consider the diffusion equation on the finite one-dimensional domain,  $0 < x < L$ , with Dirichlet BCs:

$$c(x = 0, t) = 0 = c(x = L, t) \quad (11-1)$$

and ICs

$$c(x, t = 0) = c_0 \quad (11-2)$$

Assuming that  $c(x, t) = X(x)T(t)$  and inserting into the diffusion equation resulted in a pair of separated ordinary differential equations each of which was equal to the same constant,  $-\lambda$ .

The possible solutions are:

$$X(x) = \begin{cases} A \sin(\sqrt{\lambda}x) + B \cos(\sqrt{\lambda}x) & (\lambda > 0) \\ A'e^{\sqrt{-\lambda}x} + B'e^{-\sqrt{-\lambda}x} & (\lambda < 0) \\ A''x + B'' & (\lambda = 0) \end{cases} \quad (11-3)$$

for  $X(x)$  and for  $T(t)$ ,

$$T(t) = \tau e^{-\lambda Dt} \quad (11-4)$$

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The BCs cannot be solved simultaneously with a non-trivial solution unless  $\lambda > 0$ .

Applying the BCs to Eq. 10-7,  $B = 0$ , but there are an infinite number of other values that will satisfy the boundary conditions:

$$\lambda_n = \frac{n^2\pi^2}{L^2} \quad (11-5)$$

where  $n$  is any integer.

The general solutions (for the BCs and ICs given above) are:

$$\begin{aligned} X_n(x) &= A_n \sin\left(\frac{n\pi x}{L}\right) \\ T_n(t) &= \tau_n e^{-\left(\frac{Dn^2\pi^2 t}{L^2}\right)} \end{aligned} \quad (11-6)$$

However, to satisfy the initial conditions the general solution must be taken as a linear superposition of each possible solution—and with the weighting factor at  $t = 0$  chosen to satisfy the initial conditions. Therefore, seek  $a_n$  such that:

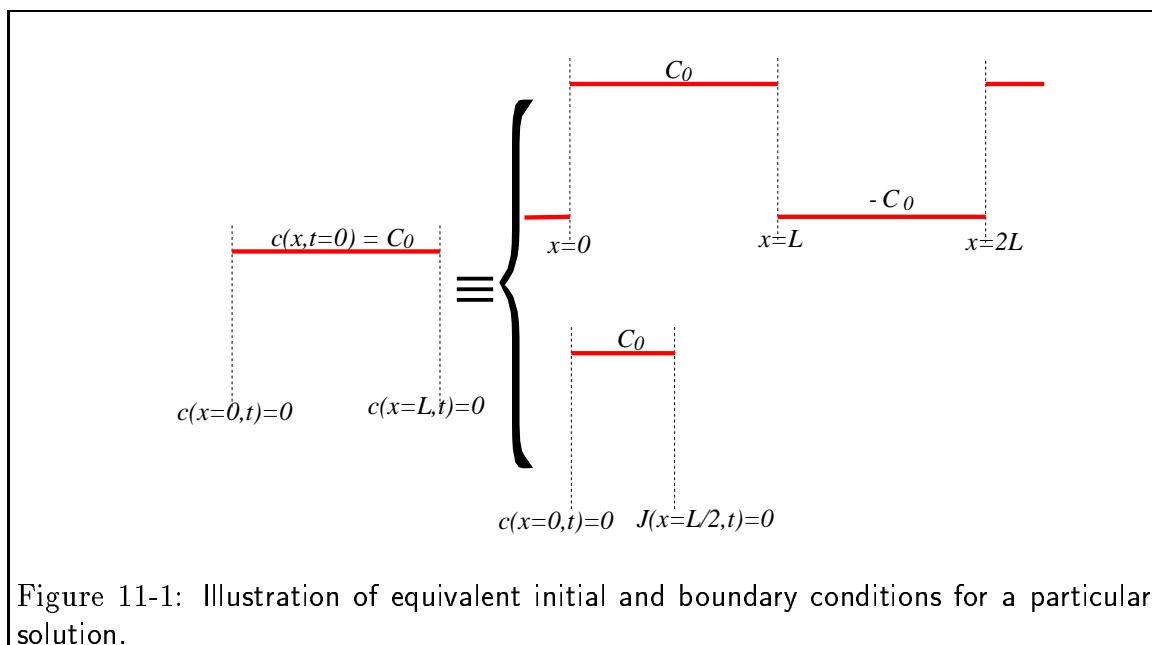
$$c_o = \sum_{n=1}^{\infty} a_n \sin(n\pi \frac{x}{L}) \quad (11-7)$$

which is a Fourier sine series representation of  $c_o$ .<sup>24</sup>

## Remarks on the Fourier Method of Solution

(A)

From the solution above, a periodic solution in  $-\infty < x < \infty$  can be constructed for  $c(x = NL, t) = 0$  and  $c(x, t = 0) = \pm c_0$  for all integer  $N$  (use the  $-c_0$  in  $-L < x < 0$ , etc).

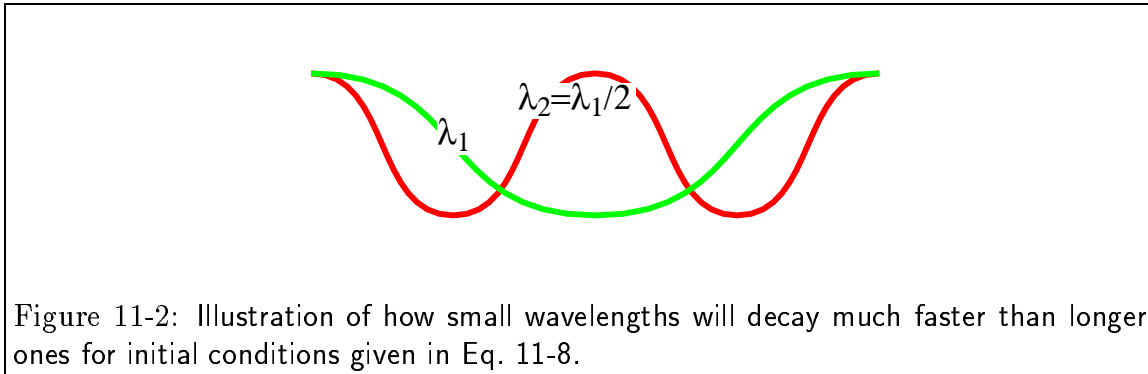


<sup>24</sup>The student should review the section in the book on Fourier series if this is unfamiliar.

**(B)**

Note how each term in the Fourier series decays much faster than the previous term—the rate at which amplitudes get smaller is exponential with smaller wavelengths.

This dependence on wavelengths is a useful intuitive device for understanding the diffusion equation.



For example, consider two different initial conditions on the infinite domain  $-\infty < x < \infty$ :

$$\begin{aligned} c_1(x, t = 0) &= a \left[ 1 - \sin \left( \frac{2\pi x}{\lambda} \right) \right] \\ c_2(x, t = 0) &= a \left[ 1 - \sin \left( \frac{4\pi x}{\lambda} \right) \right] \end{aligned} \quad (11-8)$$

The solutions  $c_1(x, t)$  and  $c_2(x, t)$  are obviously,

$$\begin{aligned} c_1(x, t) &= a \left[ 1 - \sin \left( \frac{2\pi x}{\lambda} \right) e^{-\frac{(2\pi)^2 t}{D\lambda^2}} \right] \\ c_2(x, t) &= a \left[ 1 - \sin \left( \frac{4\pi x}{\lambda} \right) e^{-\frac{(4\pi)^2 t}{D\lambda^2}} \right] \end{aligned} \quad (11-9)$$

Therefore shorter wavelengths,  $\lambda_{short}$ , decay  $e^{\left(\frac{\lambda_{long}}{\lambda_{short}}\right)^2}$  times faster than longer wavelengths  $\lambda_{long}$ .

## **Time Dependent Boundary Conditions, Semi-Infinite Domains**

The final analytic method for obtaining an analytic solution to the diffusion equation is the method of Laplace transforms. This method is applicable to semi-infinite domains and is especially effective for problems with time-dependent boundary conditions.

The method of Laplace transforms is an example of operator calculus. In this case, the operator is a transformation of time derivatives to algebraic expressions in a transformation variable. The transformed diffusion equation becomes an inhomogeneous ordinary differential

equation in the spatial variable. The ordinary differential equation is solved for the transformed boundary conditions and then the transformation is reversed—usually through a table of Laplace transform pairs.

The Laplace Transform is defined as the linear operator:

$$\mathcal{L}\{f(x, t)\} \equiv \hat{f}(x, p) = \int_0^{\infty} e^{-pt} f(x, t) dt \quad (11-10)$$

that maps  $f(x)$  to another function  $\hat{f}(p)$ .

The essential property of the Laplace transform is its operation on time derivatives:

$$\mathcal{L}\left\{\frac{\partial f}{\partial t}\right\} = \int_0^{\infty} e^{-pt} \frac{\partial f(x, t)}{\partial t} dt \quad (11-11)$$

which can be integrated by parts,

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$$\mathcal{L}\left\{\frac{\partial f}{\partial t}\right\} = p\mathcal{L}\{f\} - f(x, t=0) = p\hat{f}(p) - f(x, t=0) \quad (11-12)$$

so the initial condition gets integrated into the the transformed derivative.

The transform has no effect on spatial derivatives, therefore the transformed diffusion equation becomes:

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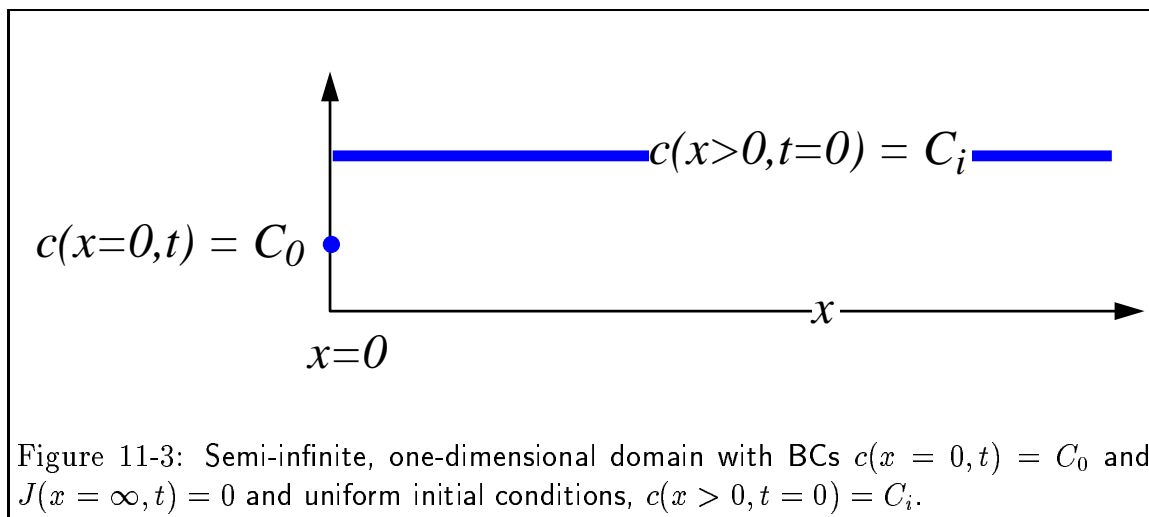


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$$p\hat{c}(x, p) - c(x, t=0) = D \frac{\partial^2 \hat{c}(x, p)}{\partial x^2} \quad (11-13)$$

which is an ordinary differential equations since there are only derivatives with respect to  $x$ .

### Two Examples of the Laplace Transform Method



For this initial condition, the transformed diffusion equation, Eq. 11-13, becomes

$$D \frac{\partial^2 \hat{c}(x, p)}{\partial x^2} - p \hat{c}(x, p) = -c(x, t = 0) = -C_i \quad (11-14)$$

The general solution,  $\hat{c}$ , to this differential equation is the sum of two different kinds of solutions. The first kind of solution is the one that satisfies Eq. 11-14 for a finite value of the right-hand-side ( $C_i \neq 0$ , called the *particular solution*). Secondly, a sum of the *particular solution* and any solution for which the right-hand-side is zero (called the *homogeneous solution*) is also a solution to Eq. 11-14.

For this problem, the homogeneous solution is:

$$\hat{c}(x, p) = a_1 e^{qx} + a_2 e^{-qx} \quad (11-15)$$

where

$$q \equiv \sqrt{\frac{p}{D}} \quad (11-16)$$

The particular solution is:

$$\hat{c}(x, p) = \frac{C_i}{p} \quad (11-17)$$

so the general solution is given by:

$$\hat{c}(x, p) = a_1 e^{qx} + a_2 e^{-qx} + \frac{C_i}{p} \quad (11-18)$$

The transformed boundary conditions become

$$\hat{c}(x = 0, p) = \int_0^\infty C_0 e^{-pt} dt = \frac{C_0}{p} \quad (11-19)$$

and

$$\frac{\partial \hat{c}}{\partial x}(x = \infty, p) = 0 \quad (11-20)$$

This equation immediately above implies that  $a_1 = 0$  and the other determines  $a_2$ ,

$$\hat{c}(x, p) = \frac{C_0 - C_i}{p} e^{-qx} + \frac{C_i}{p} \quad (11-21)$$

This equation requires transformation back to the variable  $t$  through the inverse of a Laplace transform. The inverses are usually much more difficult to find than the Laplace transforms. Fortunately, Laplace transforms and their inverses are usually tabulated in math handbooks. For example,

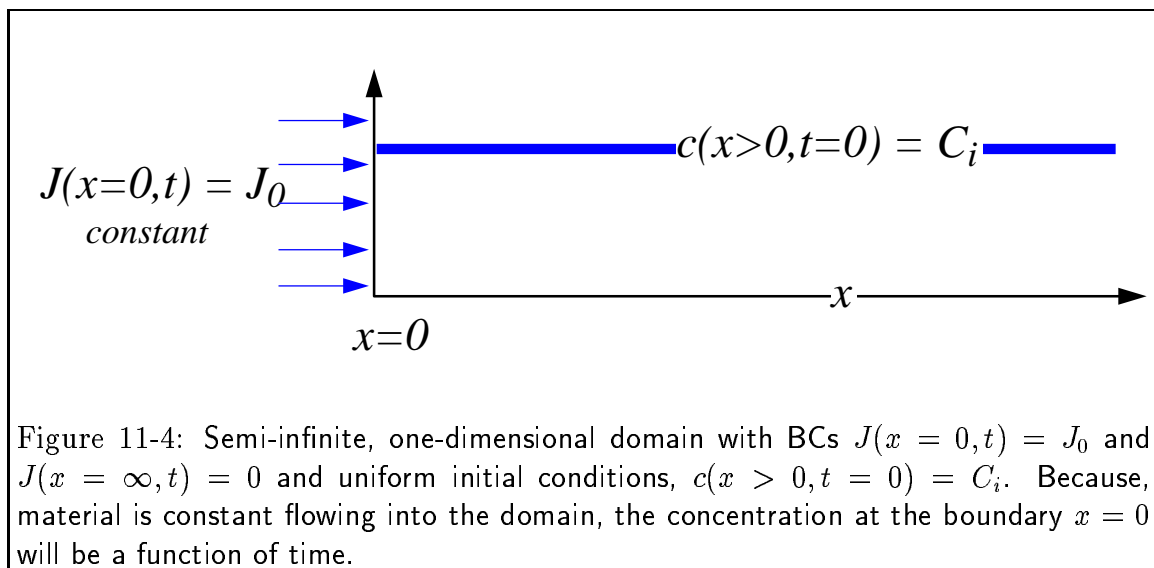
Selected Laplace Transform Pairs	
$\hat{c}(x, p) = \int_0^\infty e^{-pt} c(x, t) dt$	
$q \equiv \sqrt{(p/D)}$	
$\frac{1}{p}$	1
$\frac{1}{p^{\nu+1}}$ $\nu > -1$	$\frac{t^\nu}{\Gamma(\nu+1)}$
$\frac{1}{p+\alpha}$	$e^{-\alpha t}$
$\frac{\omega}{p^2+\omega^2}$	$\sin \omega t$
$\frac{p}{p^2+\omega^2}$	$\cos \omega t$
$e^{-qx}$	$\frac{x e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt^3}}$
$\frac{e^{-qx}}{q}$	$\sqrt{\frac{D}{\pi t}} e^{-\frac{x^2}{4Dt}}$
$\frac{e^{-qx}}{p}$	$\text{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)$
$\frac{e^{-qx}}{pq}$	$\sqrt{\frac{4Dt}{\pi}} e^{-\frac{x^2}{4Dt}} - x \text{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)$

So, the solution can be obtained through the use of the above table:

$$c(x, t) = (C_0 - C_i) \left[ 1 - \text{erf}\left(\frac{x}{\sqrt{4Dt}}\right) \right] + C_i \quad (11-22)$$

which could have been guessed from the symmetry of the infinite domain solution.

For a second example with time-dependent solutions,



For this case, the transformed diffusion equation is the same as that calculated in the previous example:

$$\hat{c}(x, p) = a_1 e^{qx} + a_2 e^{-qx} + \frac{C_i}{p} \quad (11-23)$$

and the zero-flux boundary condition at  $x = \infty$  again implies that  $a_1 = 0$ . The transformed constant flux boundary condition is:

$$\mathcal{L}\left\{\frac{\partial c}{\partial x}\right\} = \mathcal{L}\left\{-\frac{J_0}{D}\right\} = -\int_0^\infty e^{-pt} \frac{J_0}{D} dt = -\frac{J_0}{Dp} = \frac{\partial \hat{c}}{\partial x} \Big|_{x=0} = -a_2 q \quad (11-24)$$

Solving for the constant  $a_2$ ,

$$\hat{c}(x, p) = \frac{J_0}{Dpq} e^{-qx} + \frac{C_i}{p} \quad (11-25)$$

Using the table of Laplace transform pairs,

$$c(x, t) = C_i + \frac{J_0}{D} \left[ \sqrt{\frac{4Dt}{\pi}} e^{-\frac{x^2}{4Dt}} - x \operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right) \right] \quad (11-26)$$

Therefore, the surface concentration changes as  $\sqrt{t}$ :

$$c(0, t) = C_i + 2J_0 \sqrt{\frac{t}{\pi D}} \quad (11-27)$$

where  $J_0$  is the constant surface flux.

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## Anisotropic Diffusion Coefficients

The methods of solution that have been treated do not account for the general case of an anisotropic diffusion coefficient. However, a simple stratagem can be used to reconstruct the diffusion equation from its tensor form into the scalar form that is treated above.

Recall form of the the flux relationship in a particular frame of reference:

$$\begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix} = - \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix} \begin{pmatrix} \frac{\partial c}{\partial x} \\ \frac{\partial c}{\partial y} \\ \frac{\partial c}{\partial z} \end{pmatrix} = D_{ij} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} c \quad (11-28)$$


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The diffusion equation becomes:

$$\frac{\partial c}{\partial t} = \left( \frac{\partial}{\partial x} \frac{\partial}{\partial y} \frac{\partial}{\partial z} \right) \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} c \quad (11-29)$$

This would be difficult to solve in the general case. However, there is a trick for the case where the anisotropic diffusivity does not depend on  $c$ .

First, find the rotation  $a_{ij}$  which diagonalizes  $\underline{D}$ :

$$\underline{\hat{D}} = \begin{pmatrix} \hat{D}_{11} & 0 & 0 \\ 0 & \hat{D}_{22} & 0 \\ 0 & 0 & \hat{D}_{33} \end{pmatrix} \quad (11-30)$$


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The  $\hat{D}_{ii}$  are the eigenvalues of  $\underline{D}$  and the coordinate frame of reference of  $\underline{\hat{D}}$  have axes parallel to the eigenvalues of  $\underline{D}$ .

The diffusion equation is much simpler in the eigenframe:

$$\frac{\partial c}{\partial t} = \hat{D}_{11} \frac{\partial^2 c}{\partial \hat{x}_1^2} + \hat{D}_{22} \frac{\partial^2 c}{\partial \hat{x}_2^2} + \hat{D}_{33} \frac{\partial^2 c}{\partial \hat{x}_3^2} \quad (11-31)$$

Define an effective diffusivity  $D_{eff}$ :

$$D_{eff} = \det(\underline{D})^{1/3} = \det(\underline{\hat{D}})^{1/3} = (\hat{D}_{11}\hat{D}_{22}\hat{D}_{33})^{1/3} \quad (11-32)$$

and rescale the lengths of the coordinate axes with:

$$\hat{x}_i = \frac{\hat{D}_{ii}^{1/2}}{D_{eff}^{1/2}} \xi_i \quad (11-33)$$

Using the  $D_{eff}$  and the rescaled lengths,

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$$\frac{\partial c}{\partial t} = D_{eff} \nabla_{\xi}^2 \cdot c = D_{eff} \left( \frac{\partial^2 c}{\partial \xi_1^2} + \frac{\partial^2 c}{\partial \xi_2^2} + \frac{\partial^2 c}{\partial \xi_3^2} \right) \quad (11-34)$$

which is the simple scalar isotropic diffusion equation to which the solution methods (scaling, method of images, Fourier sum, and Laplace transform) were applied.