Lecture 7
Derivation of the Diffusion Equation

In this lecture, we give two very different techniques for deriving the diffusion equation. The first is based upoon a Galerkin method in angle, and the second is based upon an asymptotic expansion.

1 A Galerkin Method

We begin with the differential transport equation:

$$\mu\frac{\partial\psi}{\partial x} + \sigma_t\psi = \frac{\sigma_s}{4\pi}\,\phi + \frac{Q_o}{4\pi}\,. \tag{1}$$

We propose a Galerkin approximation to Eq. (1) based upon a linear trial space of the following form:

$$\psi(x,\mu) = \frac{a(x)}{4\pi} + \frac{3b(x)\mu}{4\pi}\,, \tag{2}$$

with the weighting space equal to the trial space. Note that

$$2\pi\int_{-1}^{+1}\psi(x,\mu)\,d\mu = \phi(x) = a(x)\,, \tag{3a}$$

$$2\pi\int_{-1}^{+1}\psi(x,\mu)\mu\,d\mu = J(x) = b(x)\,. \tag{3b}$$

Thus Eq. (2) can be rewritten as

$$\psi(x,\mu) = \frac{\phi(x)}{4\pi} + \frac{3J(x)\mu}{4\pi}\,. \tag{4}$$

Substituting from Eq. (4) into Eq. (1) and integrating over all directions, we get the zero'th moment or balance equation:

$$\frac{\partial J}{\partial x} + \sigma_a = Q_0\,. \tag{5}$$

Substituting from (4) into (1) multiplying by μ, and integrating over all directions we get the the first-moment equation:

$$\frac{1}{3}\frac{\partial \phi}{\partial x} + \sigma_t J = 0\,. \tag{6}$$

Using Eq. (6) to solve for J, we get Fick's law:

$$J = -D\frac{\partial \phi}{\partial x}\,, \tag{7}$$

where

$$D = \frac{1}{3\sigma_t}\,. \tag{8}$$

Substituting from Eq. (7) into Eq. (5) we get the diffusion equation:

$$-\frac{\partial}{\partial x}D\frac{\partial \phi}{\partial x} + \sigma_a\phi = Q_0\,. \tag{9}$$

Thus we see from the derivation that the diffusion equation is exact whenever the flux is either isotropic or linearly anisotropic. However, the derivation gives no hint as to when one would expect the transport solution to be linear in angle. Furthermore, if the Galerkin approximation is made for the time-dependent transport equation rather than the steady-state equation, one does not obtain the diffusion equation unless one also assumes that $\frac{\partial J}{\partial t} = 0$.

1.1 Asymptotic Derivation

We next use asymptotics to obtain the time-dependent diffusion equation. Unlike the Galerkin derivation, this derivation does give insight into the conditions under which one would expect the transport solution to be linear in μ and hence diffusive. The central theme of our asymptotic expansion is to first use a "small" dimensionless parameter, ϵ, to scale parameters in a non-dimensional form of the transport equation, and thereby establish the relative sizes of these parameters in the limit as $\epsilon \to 0$. The transport solution is then expanded in a power series in ϵ, and substituted into the scaled transport equation. The terms of that equation that multiply each power of ϵ are grouped together to obtain a hierarchical system of equations for the solution. Our purpose here is to define an asymptotic expansion of the transport equation with a leading-order solution that satisfies the diffusion equation, thereby defining a formal mathematical limit in which transport theory becomes equivalent to diffusion theory.

We begin with the time-dependent transport equation:

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \mu \frac{\partial \psi}{\partial x} + \sigma_t \psi = \frac{\sigma_s}{4\pi}\phi + \frac{Q_0}{4\pi} \,. \tag{10}$$

The following quantities are defined as follows for the purpose of putting this equation in a non-dimensional form.

$\bar{\psi}$: a constant value of ψ that is characteristic of the solution for ψ.

Δt: a constant time interval that characterizes the temporal scale length of the solution for ψ.

Δx: a constant length that characterizes the spatial scale length of the solution for ψ.

The temporal and spatial scale lengths are used to define a non-dimensional time variable,

$$t' = \frac{t}{\Delta t} \,, \tag{11}$$

and a non-dimensional spatial variable,

$$x' = \frac{x}{\Delta x} \tag{12}$$

respectively. Finally, we obtain the desired non-dimensional form of the transport equation by dividing Eq. (10) by $\hat{\psi}\sigma_t\bar{\psi}$, transforming to the non-dimensional time and space variables, and expressing σ_s as $\sigma_t - \sigma_a$:

$$\alpha \frac{\partial \hat{\psi}}{\partial t'} + \beta\mu \frac{\partial \hat{\psi}}{\partial x'} + \hat{\psi} = \frac{\sigma_t - \sigma_a}{\sigma_t}\frac{1}{4\pi}\hat{\phi} + \frac{\hat{Q}_0}{4\pi} \,, \tag{13}$$

where

$$\alpha = \frac{1}{\sigma_t v \Delta t} \,, \tag{14}$$

$$\hat{\psi} = \frac{\psi}{\bar{\psi}} \,, \tag{15}$$

$$\beta = \frac{1}{\sigma_t \Delta x} \,, \tag{16}$$

$$\hat{\phi} = \frac{\phi}{\bar{\psi}} \,, \tag{17}$$

$$\hat{Q}_0 = \frac{Q_0}{\sigma_t \bar{\psi}} \,. \tag{18}$$

The parameter, α, represents the mean time between particle collisions divided by the temporal scale length of the solution, and the quantity, β, represents the mean-free-path divided by the spatial scale length of the solution. To obtain a diffusion solution to leading-order, we assume that $\bar{\psi}$ is order one, scale α by ϵ^2, scale β by ϵ, and scale σ_a by ϵ^2, and scale $\hat{Q}_0$ by ϵ^2. This means that the diffusion limit is characterized by time scales that are "very much smaller" than the mean time between particle collisions, spatial scales that are "much smaller" than a mean-free-path, an absorption cross-section that is "very much smaller" than the total cross-section, and a source that is "very much smaller" than $\sigma_t \bar{\psi}$. The source scaling simply arises from the fact that we have assumed that $\bar{\psi}$ is order one, i.e., that the first term in the expansion with respect to ϵ is ϵ^0. If the source is order one, the first term in the expansion must be ϵ^{-2}. If the appropriate source scaling is not performed, the asymptotic analysis indicates that the source must be zero. The appropriate scaling is recognized by the fact that it eliminates this unacceptable result.

Applying the scaling to Eq. (13), we get

$$\epsilon^2 \alpha \frac{\partial \hat{\psi}}{\partial t'} + \epsilon \beta \mu \frac{\partial \hat{\psi}}{\partial x'} + \hat{\psi} = \frac{\sigma_t - \sigma_a \epsilon^2}{\sigma_t} \frac{1}{4\pi} \hat{\phi} + \epsilon^2 \frac{\hat{Q}_0}{4\pi} \,, \tag{19}$$

We next expand the solution to Eq. (19) in powers of ϵ:

$$\psi(x,\mu) = \sum_{n=0}^{\infty} \psi^{(n)}(x,\mu)\ \epsilon^n \,. \tag{20}$$

Substituting from Eq. (20) into Eq. (19), we collect terms associated with each order of ϵ. The following equations are obtained.

The equation for order ϵ^0:

$$\hat{\psi}^{(0)} = \frac{1}{4\pi} \hat{\phi}^{(0)} \,. \tag{21}$$

This equation states that the leading order solution is isotropic in angle.

The equation for order ϵ^1:

$$\beta \mu \frac{\partial \psi^{(0)}}{\partial x'} + \hat{\psi}^{(1)} = \frac{1}{4\pi} \phi^{(1)} \,. \tag{22}$$

Integrating Eq. (22) over all directions, and recognizing that the integral of $\hat{\psi}^{(1)}$ is $\hat{\phi}^{(1)}$, we get what is called a solvability condition:

$$2\pi \int_{-1}^{+1} \beta \mu \frac{\partial \psi^{(0)}}{\partial x'} \, d\mu = 0 \,. \tag{23}$$

Taking Eq. (21) into account, we find that Eq. (23) is indeed satisfied. Rearranging Eq. (22), and taking Eq. (21) into account, we get

$$\hat{\psi}^{(1)} = \hat{\phi}^{(1)} - \beta \frac{\mu}{4\pi} \frac{\partial \phi^{(0)}}{\partial x'} \,. \tag{24}$$

Equation (24) states that the first-order component of the solution is linearly anisotropic in μ. The equation for order ϵ^2:

$$\alpha \frac{\partial \hat{\psi}^{(0)}}{\partial t'} + \beta \mu \frac{\partial \hat{\psi}^{(1)}}{\partial x'} + \hat{\psi}^{(2)} = \frac{1}{4\pi} \hat{\phi}^{(2)} - \frac{\sigma_a}{\sigma_t} \frac{1}{4\pi} \hat{\phi}^{(0)} + \frac{\hat{Q}_0}{4\pi} \,. \tag{25}$$

Substituting from Eqs. (21) and (24) into Eq. (25), and integrating over all directions, and recognizing that the integral of $\hat{\psi}^{(2)}$ is $\hat{\phi}^{(2)}$, we get

$$\alpha \frac{\partial \hat{\phi}^{(0)}}{\partial t'} - \beta \frac{\partial}{\partial x'} \frac{\beta}{3} \frac{\partial \hat{\phi}^{(0)}}{\partial x'} + \frac{\sigma_a}{\sigma_t} \hat{\phi}^{(0)} = \hat{Q}_0 \,. \tag{26}$$

Multiplying Eq. (26) by $\sigma_t \bar{\psi}$ and transforming back to the dimensional time and space variables, we obtain

$$\frac{1}{v} \frac{\partial \phi^{(0)}}{\partial t} - \frac{\partial}{\partial x} \frac{1}{3\sigma_t} \frac{\partial \phi^{(0)}}{\partial x} + \sigma_a \phi^{(0)} = Q_0 \,. \tag{27}$$

Equation (27) states that the leading-order solution to the asymptotic expansion satisfies the diffusion equation. It is in this sense that the transport equation becomes equivalent to the diffusion equation in the asymptotic limit defined here. The asymptotic expansion associated with the diffusion limit is necessarily valid only in regions several mean-free-paths from boundaries, material interfaces, or source discontinutities. Sufficiently rapid variations in cross-sections or sources can render the scale length assumptions associated with the expansion invalid. The transport solution can be diffusive at the boundaries of diffusive regions, depending upon the incident angular flux shape, but it more often is not. The region of transition from a non-diffusive transport solution to a diffusive solution is only a few mean-free-paths thick and the solution within it generally varies quite rapidly. Such a region is referred to as a boundary layer.

1.2 Diffusion Boundary Conditions

We cannot meet vacuum boundary conditions exactly with our linear trial space. Thus we must meet them approximately. One of the most common approximations is the Marshak boundary condition. For instance, the exact vacuum boundary condition at $x = x_L$ is

$$\psi(x_L, \mu) = 0 \quad , \mu \geq 0, \tag{28}$$

The Marshak approximation to Eq. (9) preserves the rate of particle inflow:

$$2\pi \int_0^1 \psi(x_L, \mu)\mu \, d\mu = 0 \, . \tag{29}$$

Substituting from Eq. (4) into Eq. (29), and evaluating the integral, we get

$$\frac{\phi}{4} + \frac{J}{2} = 0 \, . \tag{30}$$

Using Eqs. (7) and (8), Eq. (30) can rewritten as

$$\phi - \left(\frac{2}{3} \lambda \frac{\partial \phi}{\partial x} \right) = 0 \, , \tag{31}$$

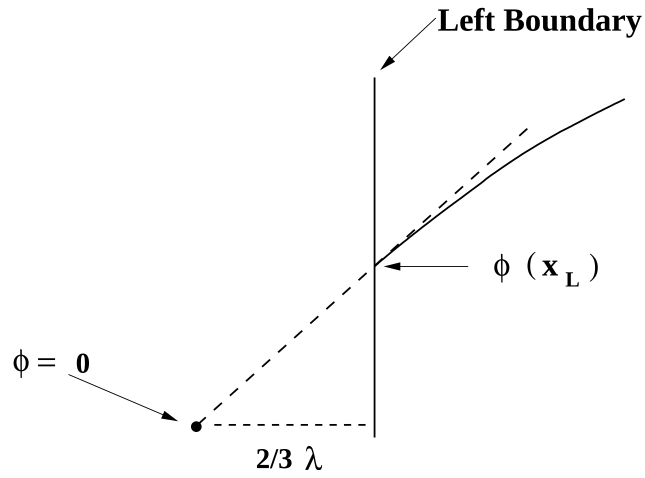

Figure 1: Solution extrapolation at boundary with vacuum condition.

where $\lambda \equiv 1/\sigma_t$ is the mean-free-path. Equation (31) shows that the Marshak vacuum condition is equivalent to making the flux extrapolate to zero at a distance of 2/3 of a mean-free-path from the boundary, as illustrated in Fig. 1.

Let us suppose that we have a non-zero angular flux, $f(\mu)$, incident at the left boundary. Then the exact boundary condition is the

$$\psi(x_L, \mu) = f(\mu) \quad , \mu \geq 0. \tag{32}$$

As in the vacuum case, the Marshak condition simply preserves the rate of particle inflow:

$$2\pi \int_0^1 \psi(x_L, \mu)\mu \, d\mu = 2\pi \int_0^1 f(\mu)\mu \, d\mu \, . \tag{33}$$

Substituting from Eq. (4) into Eq. (33), and evaluating the integral, we get

$$\frac{\phi}{4} + \frac{J}{2} = 2\pi \int_0^1 f(\mu)\mu \, d\mu \equiv j^+ \, , \tag{34}$$

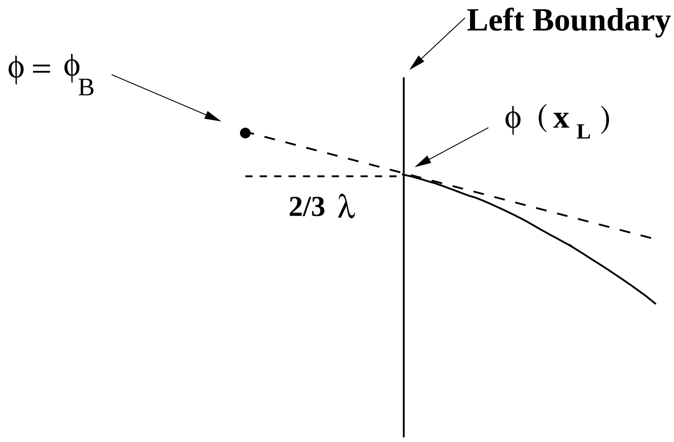

Figure 2: Solution extrapolation at boundary with source condition.

where j^+ is called the half-range incoming current. Equation (34) can rewritten as

$$\phi - \left(\frac{2}{3}\lambda\frac{\partial\phi}{\partial x}\right) = 4j^+ \equiv \phi_b\,, \tag{35}$$

where $\frac{\phi_b}{4\pi}$ represents an “equivalent” isotropic boundary flux in the sense that $\frac{\phi_b}{4\pi}$ has the same incoming half-range current as $f(\mu)$. Thus we see from Eq. (35) that the Marshak source condition is equivalent to making the scalar flux extrapolate to an equivalent boundary scalar flux value at a distance of 2/3 of a mean-free-path from the boundary. This is illustrated in Fig. 2.

Reflective (specular) boundary conditions must also be considered. Assuming such a condition at $x = x_L$, the exact transport boundary condition is

$$\psi(x_L, \mu) = \psi(x_L, -\mu) \quad , \mu \geq 0. \tag{36}$$

In this case, one simply sets $J = 0$ on the boundary. This is not unique to Marshak boundary conditions, but rather is the only physically correct choice.

Conditions at the interface between two dissimilar materials must also be considered. Let x_i denote the location of an interface. The transport angular flux solution must be continuous at a material interface. This implies that all angular moments of the angular flux must also be continuous. Thus the scalar flux and current must be continuous at a material interface. These are the interface conditions for the diffusion equation. As in the case of reflection, these conditions represent the only physically correct choice.

Marshak conditions are not the most accurate conditions for the diffusion equation, but they are the most accurate of the conditions that can be derived from simple physical considerations. More accurate conditions generally require information from exact transport solutions. For instance, asymptotic methods can be used to derive exact diffusion boundary conditions, but the associated boundary-layer analyses are very complicated and essentially require exact transport solutions.

2 An Example Diffusion Solution

We next solve the diffusion equation on $[0, x_0]$ with a constant isotropic distributed source, $\frac{Q_0}{4\pi}$, $\sigma_t = \sigma_s$, and vacuum boundary conditions. The equation to be solved is

$$-\frac{\partial}{\partial x} D \frac{\partial \phi}{\partial x} = Q_0 \quad , x \in [0, x_0], \tag{37}$$

with a left boundary condition given by

$$\frac{\phi}{4} + \frac{J}{2} = 0 \quad , x = 0, \tag{38a}$$

and a right boundary condition given by

$$-\frac{\phi}{4} + \frac{J}{2} = 0 \quad , x = x_0. \tag{38b}$$

The homogeneous solution to Eq. (37) is

$$\phi_h = a + bx \,, \tag{39}$$

and the particular solution is

$$\phi_p = -\frac{Q_0 x^2}{2D} \,. \tag{40}$$

Thus the total solution is

$$\phi = a + bx - \frac{Q_0 x^2}{2D} \,. \tag{41}$$

The constants a and b are determined by the boundary conditions. In particular, substituting from Eq. (41) into Eqs. (38a) and (38b), we respectively obtain

$$a - 2Db = 0 \,, \tag{42a}$$

and

$$a + bx_0 - \frac{Q_0 x_0^2}{2D} = 2D\left(b - \frac{2Q_0 x_0}{2D}\right) = 0 \,. \tag{42b}$$

Solving Eqs. (42a) and (42b), we get

$$a = Q_0 x_0 \,, \tag{43a}$$

$$b = \frac{Q_0 x_0}{2D} \,. \tag{43b}$$

Substituting from Eqs. (43a) and (43b) into Eq. (41), we obtain the following solution:

$$\phi = \frac{Q_0}{2D} \left(2D x_0 + x_0 x - x^2 \right) \,. \tag{44}$$