

Statics

TWO METHODS OF SPATIAL discretisation are introduced in order to obtain solutions the situations described by static reactor physics. The one dimensional cases are derived here, but generalization to three dimensional cases will be done in the context of space-time kinetics, which will be examined later.

As the initial conditions used in space-time kinetics usually correspond to the initially critical core, special care must be given to the techniques of static reactor physics.

First, the spatial mesh should be absolutely identical for the stationary reactor physics calculations which will serve as initial conditions in space-time kinetics. Otherwise, inconsistencies introduced will unmis-

takably produce non-zero temporal derivatives in some areas of the core, which will produce artificial transients.

The initial core will thus correspond to a critical reactor, which means that the K_{eff} will be equal to unity. The statics calculations will perform the evaluation of K_{eff} , and the $[\nu\Sigma_f]$ cross-sections will then all be divided by the K_{eff} before performing a kinetics calculation.

Static Diffusion Equations

We have introduced in chapter 4, *Energy Condensation*, page 37, the static equations in terms of energy groups. With the matrix notation and the definitions introduced in chapter 5, *Matrix Form of the Equations*, page 45, we have the following static equations

$$-\nabla \cdot [D]\vec{\nabla}[\phi] + [\Sigma][\phi] = \frac{1}{\gamma}[\chi][\nu\Sigma_f]^T[\phi] \quad (\text{EQ 21})$$

The problem in static physics consists in determining the flux $[\phi]$ and the corresponding K_{eff} (which we note here γ).

It is useless to try to find an analytic solution to the cases where more than one material type is present in two and three dimensions. In one dimension, it is possible to determine an analytic solution, but with two or more energy groups it becomes quite difficult.

This then induces the motivation to use numerical methods to find the solution of static neutron diffusion equations.

One Dimensional Formulation and Coordinate System

We will limit the derivation in this chapter to one dimensional cases. This has the advantage of simplicity, and the generalization to three dimensions will then not be so difficult. The complete derivation in three dimensions will be made in the context of space-time kinetics.

We introduce a cartesian coordinate system oriented along the x axis, as shown on Figure 7, “1D Coordinate System”, page 66, and by following the mesh “instructions” discussed in chapter 6, *Spatial Mesh Considerations*, page 49. We use the following numbering scheme for the regions:

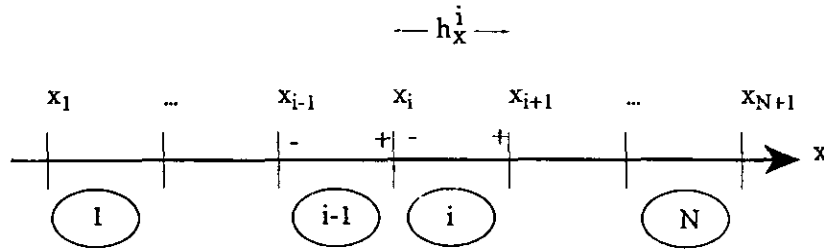
- the first coordinate is numbered x_1
- region number i extends from x_i to x_{i+1} . This number will serve to index the nuclear properties.
- the width of region i is denoted h_x^i
- the region number is used to label the cross-sections and the diffusion coefficients
- we will use the notation $[\phi]_i \equiv [\phi(x_i)]$

Reactor models in one dimension imply that it is infinite in the two other directions. This means that the flux will be constant in these directions, and therefore the corresponding partial derivatives. The net current will thus be zero in these directions. In such cases, the static equations reduce to

$$-\frac{d}{dx}[D]\frac{d}{dx}[\phi] + [\Sigma][\phi] = \frac{1}{K_{eff}}[\chi][\nu\Sigma_f]^T[\phi] \quad (EQ 22)$$

$$[J] = -[D]\frac{d}{dx}[\phi]$$

FIGURE 7. 1D Coordinate System



Classical Finite Differences

The classical finite differences consists in using the flux values at the boundary points between the regions, in other words at the coordinates x_i . Flux and current continuity must be enforced by taking into account the changes in nuclear cross-sections and diffusion coefficients from one region to the other.

Derivation

In region $i - 1$, at point x_i^+ , equation (22) becomes

$$-[D]_{i-1}\frac{d^2}{dx^2}[\phi]_i^+ + [\Sigma]_{i-1}[\phi]_i^+ = \frac{1}{\gamma}[\chi][\nu\Sigma_f]_{i-1}^T[\phi]_i^+ \quad (EQ 23)$$

while for region i at point x_i^- it becomes

$$-[D]_i \frac{d^2}{dx^2} [\phi]_i^- + [\Sigma]_i [\phi]_i^- = \frac{1}{\gamma} [\chi] [\nu \Sigma_f]_i^T [\phi]_i^- \quad (\text{EQ 24})$$

The second derivatives must be eliminated from each of these two equations; it probably suffers a discontinuity at region interfaces. To do this, we perform a Taylor series expansion of the flux starting from point x_i towards x_{i-1} and x_{i+1} respectively. We find

$$[\phi]_{i-1}^- = [\phi]_i^+ - h_x^{i-1} \frac{d}{dx} [\phi]_i^+ + \frac{(h_x^{i-1})^2}{2} \frac{d^2}{dx^2} [\phi]_i^+ \quad (\text{EQ 25})$$

$$[\phi]_{i+1}^+ = [\phi]_i^- + h_x^i \frac{d}{dx} [\phi]_i^- + \frac{(h_x^i)^2}{2} \frac{d^2}{dx^2} [\phi]_i^- \quad (\text{EQ 26})$$

Multiply (25) by $[D]_{i-1} / h_x^{i-1}$ and (26) by $[D]_i / h_x^i$, and add the two resulting expressions. Noting that current continuity implies that

$$[D]_{i-1} \frac{d}{dx} [\phi]_i^+ = [D]_i \frac{d}{dx} [\phi]_i^-$$

and that flux continuity implies that

$$[\phi]_i^+ = [\phi]_i^- = [\phi]_i$$

we find

$$\begin{aligned}
& \frac{[D]_{i-1}}{h_x^{i-1}}[\phi]_{i-1} - \left(\frac{[D]_{i-1}}{h_x^{i-1}} + \frac{[D]_i}{h_x^i} \right) [\phi]_i + \frac{[D]_i}{h_x^i} [\phi]_{i+1} \\
& = \left(\frac{[D]_{i-1} h_x^{i-1}}{2} \frac{d^2}{dx^2} [\phi]_i^+ + \frac{[D]_i h_x^i}{2} \frac{d^2}{dx^2} [\phi]_i^- \right)
\end{aligned} \tag{EQ 27}$$

Now let us multiply (23) by $h_x^{i-1}/2$ and (24) by $h_x^i/2$, and adding,

$$\begin{aligned}
& -\frac{h_x^{i-1}}{2} [D]_{i-1} \frac{d^2}{dx^2} [\phi]_i^+ - \frac{h_x^i}{2} [D]_i \frac{d^2}{dx^2} [\phi]_i^- \\
& \quad + (h_x^{i-1} [\Sigma]_{i-1} + h_x^i [\Sigma]_i) [\phi]_i \\
& = \frac{1}{\gamma} h_x^{i-1} [\chi] [\nu \Sigma_f]_{i-1}^T [\phi]_i^+ + \frac{1}{\gamma} h_x^i [\chi] [\nu \Sigma_f]_i^T [\phi]_i^-
\end{aligned}$$

finally we substitute (27) in this last result to get

$$\begin{aligned}
& -\frac{[D]_{i-1}}{h_x^{i-1}} [\phi]_{i-1} + \left(\frac{[D]_{i-1}}{h_x^{i-1}} + \frac{[D]_i}{h_x^i} \right) [\phi]_i - \frac{[D]_i}{h_x^i} [\phi]_{i+1} \\
& \quad + \frac{1}{2} (h_x^{i-1} [\Sigma]_{i-1} + h_x^i [\Sigma]_i) [\phi]_i \\
& = \frac{1}{2} \left(\frac{h_x^{i-1}}{\gamma} [\chi] [\nu \Sigma_f]_{i-1}^T + \frac{h_x^i}{\gamma} [\chi] [\nu \Sigma_f]_i^T \right) [\phi]_i
\end{aligned} \tag{EQ 28}$$

Boundary Conditions

Zero Flux. The simplest boundary conditions are those of zero flux on the external surfaces of the reactor. In this case, we can force the fluxes $[\phi]_1$ or $[\phi]_N$ to zero as needed. Since they are known, they can be

eliminated from the linear system to be solved. For example, the equation for the flux closest to the left boundary of the reactor, $[\phi]_2$, can be written as

$$\begin{aligned} & \left(\frac{[D]_{i-1}}{h_x^{i-1}} + \frac{[D]_i}{h_x^i} \right) [\phi]_i - \frac{[D]_i}{h_x^i} [\phi]_{i+1} \\ & + \frac{1}{2} (h_x^{i-1} [\Sigma]_{i-1} + h_x^i [\Sigma]_i) [\phi]_i \\ & + \frac{1}{2} \left(\frac{h_x^{i-1}}{\gamma} [\chi] [\nu \Sigma_f]_{i-1}^T + \frac{h_x^i}{\gamma} [\chi] [\nu \Sigma_f]_i^T \right) [\phi]_i \end{aligned} \quad (\text{EQ 29})$$

while the flux closest to the right boundary of the reactor will be given by

$$\begin{aligned} & - \frac{[D]_{i-1}}{h_x^{i-1}} [\phi]_{i-1} + \left(\frac{[D]_{i-1}}{h_x^{i-1}} + \frac{[D]_i}{h_x^i} \right) [\phi]_i \\ & + \frac{1}{2} (h_x^{i-1} [\Sigma]_{i-1} + h_x^i [\Sigma]_i) [\phi]_i \\ & + \frac{1}{2} \left(h_x^{i-1} \frac{1}{\gamma} [\chi] [\nu \Sigma_f]_{i-1}^T + h_x^i \frac{1}{\gamma} [\chi] [\nu \Sigma_f]_i^T \right) [\phi]_i \end{aligned} \quad (\text{EQ 30})$$

Other Conditions. The other boundary conditions, such as zero current, zero flux at extrapolated distance, and albedo can all be obtained by going through the derivation process for the coupling coefficient for the boundary in question, and taking into account the proper conditions existing on the boundary.

In all cases, note that the coupling coefficients are all stopped on one side of the reactor or the other.

Mesh Centered Finite Differences

The mesh centered finite difference method uses as unknowns the average fluxes of each region. It can be shown that in one dimension it corresponds to the flux at the center of the region. This is the usual interpretation, but it has to be used carefully. This interpretation does not hold in two or three dimensions. The correct point of view is that of the region average flux.

Derivation

To obtain mesh centered finite differences, let us mention that the average flux of a region i is given by

$$[\bar{\phi}]_i = \frac{1}{h_x^i} \int_{x_i}^{x_{i+1}} [\phi(x)] dx \quad (\text{EQ 31})$$

The diffusion equation (22) is then integrated over the spatial variable in region i , and divided by h_x^i ,

$$\frac{1}{h_x^i} \int_{x_i}^{x_{i+1}} -\frac{d}{dx}[D] \frac{d}{dx}[\phi(x)] dx + [\Sigma] \frac{1}{h_x^i} \int_{x_i}^{x_{i+1}} [\phi(x)] dx =$$

$$\frac{1}{K_{\text{eff}}} [\chi][\nu \Sigma_f]_i \frac{1}{h_x^i} \int_{x_i}^{x_{i+1}} [\phi(x)] dx$$

By applying the definition of the average flux (31), we find

$$\begin{aligned}
 -[D]_i \frac{d}{dx} [\phi(x_{i+1})] + [D]_i \frac{d}{dx} [\phi(x_i)] + h_x^i [\Sigma]_i [\bar{\phi}]_i = \\
 \frac{1}{K_{\text{eff}}} h_x^i [\chi] [\nu \Sigma_f]_i^T [\bar{\phi}]_i
 \end{aligned}
 \tag{EQ 32}$$

Again, to get rid of the current at the region interfaces, we use Taylor series expansions,

$$\begin{aligned}
 [\bar{\phi}]_i &= [\phi(x_i)] + \frac{h_x^i}{2} [D]_i^{-1} [D]_i \frac{d}{dx} [\phi(x_i)] \\
 [\bar{\phi}]_i &= [\phi(x_{i+1})] - \frac{h_x^i}{2} [D]_i^{-1} [D]_i \frac{d}{dx} [\phi(x_{i+1})]
 \end{aligned}$$

which can also be written

$$[\bar{\phi}]_i = [\phi(x_i)] + \frac{h_x^i}{2} [D]_i^{-1} [J(x_i)]
 \tag{EQ 33}$$

$$[\bar{\phi}]_i = [\phi(x_{i+1})] - \frac{h_x^i}{2} [D]_i^{-1} [J(x_{i+1})]
 \tag{EQ 34}$$

Equation (34) can be written for region $i - 1$,

$$[\bar{\phi}]_{i-1} = [\phi(x_i)] - \frac{h_x^{i-1}}{2} [D]_{i-1}^{-1} [J(x_i)]
 \tag{EQ 35}$$

Subtracting (35) from (33),

$$[\bar{\phi}]_i - [\bar{\phi}]_{i-1} = [\phi(x_i)] - [\phi(x_i)] \\ + \frac{h_x^i}{2} [D]_i^{-1} [J(x_i)] + \frac{h_x^{i-1}}{2} [D]_{i-1}^{-1} [J(x_i)]$$

and we find for the interface current at x_i ,

$$[J(x_i)] = \left(\frac{h_x^i}{2} [D]_i^{-1} + \frac{h_x^{i-1}}{2} [D]_{i-1}^{-1} \right)^{-1} ([\bar{\phi}]_i - [\bar{\phi}]_{i-1}) \quad (\text{EQ 36})$$

In the same way, the interface current at x_{i+1} is

$$[J(x_{i+1})] = \left(\frac{h_x^i}{2} [D]_i^{-1} + \frac{h_x^{i+1}}{2} [D]_{i+1}^{-1} \right)^{-1} ([\bar{\phi}]_{i+1} - [\bar{\phi}]_i) \quad (\text{EQ 37})$$

Let us substitute (36) and (37) into (32),

$$-\left(\frac{h_x^i}{2} [D]_i^{-1} + \frac{h_x^{i+1}}{2} [D]_{i+1}^{-1} \right)^{-1} [\bar{\phi}]_{i+1} - \left(\frac{h_x^i}{2} [D]_i^{-1} + \frac{h_x^{i-1}}{2} [D]_{i-1}^{-1} \right)^{-1} [\bar{\phi}]_{i-1} \\ + \left[\left(\frac{h_x^i}{2} [D]_i^{-1} + \frac{h_x^{i+1}}{2} [D]_{i+1}^{-1} \right)^{-1} + \left(\frac{h_x^i}{2} [D]_i^{-1} + \frac{h_x^{i-1}}{2} [D]_{i-1}^{-1} \right)^{-1} \right] [\bar{\phi}]_i \quad (\text{EQ 38}) \\ + h_x^i [\Sigma]_i [\bar{\phi}]_i = \frac{1}{K_{\text{eff}}} h_x^i [\chi] [\nu \Sigma_f]_i^T [\bar{\phi}]_i$$

which constitutes the expression for the coupling coefficients of the mesh centered finite difference method.

Boundary Conditions

Zero Flux. At the left side of the reactor, (33) will be

$$[\bar{\phi}]_1 = [\phi(x_1)] + \frac{h_x^1}{2} [D]_1^{-1} [J(x_1)]$$

$$[\bar{\phi}]_1 = \frac{h_x^1}{2} [D]_1^{-1} [J(x_1)]$$

from which we get a relationship between the interface current and the average flux of the region,

$$[J(x_1)] = \left(\frac{h_x^1}{2} [D]_1^{-1} \right)^{-1} [\bar{\phi}]_1 \quad (\text{EQ 39})$$

The equation for the fluxes of the left region of the reactor becomes

$$-\left(\frac{h_x^1}{2} [D]_1^{-1} + \frac{h_x^2}{2} [D]_2^{-1} \right)^{-1} [\bar{\phi}]_2$$

$$+ \left[\left(\frac{h_x^1}{2} [D]_1^{-1} + \frac{h_x^2}{2} [D]_2^{-1} \right)^{-1} + \left(\frac{h_x^1}{2} [D]_1^{-1} \right)^{-1} \right] [\bar{\phi}]_1 \quad (\text{EQ 40})$$

$$+ h_x^1 [\Sigma]_1 [\bar{\phi}]_1 = \frac{1}{K_{\text{eff}}} h_x^1 [\chi] [v \Sigma_f]_1^T [\bar{\phi}]_1$$

In the rightmost region of the reactor, we find, starting from (34),

$$[J(x_{N+1})] = - \left(\frac{h_x^N}{2} [D]_N^{-1} \right)^{-1} [\bar{\phi}]_N \quad (\text{EQ 41})$$

and we have for the flux,

$$\begin{aligned}
& - \left(\frac{h_x^i}{2} [D]_i^{-1} + \frac{h_x^{i-1}}{2} [D]_{i-1}^{-1} \right)^{-1} [\bar{\phi}]_{N-1} \\
& + \left[\left(\frac{h_x^N}{2} [D]_N^{-1} \right)^{-1} + \left(\frac{h_x^N}{2} [D]_N^{-1} + \frac{h_x^{N-1}}{2} [D]_{N-1}^{-1} \right)^{-1} \right] [\bar{\phi}]_N \quad (\text{EQ 42}) \\
& + h_x^N [\Sigma]_N [\bar{\phi}]_N = \frac{1}{K_{\text{eff}}} h_x^N [\chi] [\nu \Sigma_f]_N^T [\bar{\phi}]_N
\end{aligned}$$

Here again, we note that the coupling is cut-off on the regions bounding the core, because of the boundary conditions.

Other Conditions. The boundary conditions of zero current or of albedo can be derived starting from equations (33) and (34) with the particular relationships applied to the fluxes and currents. In all these cases, coupling coefficients will result that will reflect these particular conditions. The coupling coefficients will also be cut-off in the corresponding regions.

Matrix Structure

Whether using classical or mesh centered finite differences, we find difference equations whose coefficients are slightly different, given either by (28) or by (38).

Let us consider for example the case of mesh centered finite differences. There will be N flux $[\phi]_i$ to determine. But the discretisation technique gives rise to exactly N equations relating these $[\phi]_i$ between each other. In other words, the fluxes are the unknowns in the problem. We can regroup them in a vector. Let us define a vector $[\psi]$

whose elements are the N fast fluxes numbered in the same way as the regions, followed by the N fluxes of lower energies, and so on until the lowest energy group. In other words the flux $[\psi]$ is a column vector of $N \times G$ entries,

$$[\psi] = \begin{bmatrix} \left[\begin{array}{c} \phi_1 \\ \cdot \\ \phi_N \end{array} \right]_{g=1} \\ \cdot \\ \left[\begin{array}{c} \phi_1 \\ \cdot \\ \phi_N \end{array} \right]_{g=G} \end{bmatrix} \quad (\text{EQ 43})$$

Define a matrix $[B]$ which will contain the fission production terms,

$$[B] = \begin{bmatrix} \left[h_x^i[\chi_1][\nu\Sigma_f]_i^T \right] & \cdots & \left[h_x^i[\chi_1][\nu\Sigma_f]_i^T \right] \\ \cdot & \cdots & \cdot \\ \left[h_x^i[\chi_G][\nu\Sigma_f]_i^T \right] & \cdots & \left[h_x^i[\chi_G][\nu\Sigma_f]_i^T \right] \end{bmatrix} \quad (\text{EQ 44})$$

Note that in the two energy group case,

$$[B] = \begin{bmatrix} [B]_{11} & [B]_{12} \\ [0] & [0] \end{bmatrix}$$

since the fission spectrum is zero for thermal neutrons.

The coupling coefficients relate only fluxes of adjoining regions together. This is known as nearest neighbor coupling, and is a property most sought after because of the large body of knowledge concerning iterative methods for the type of matrix that it gives rise to. The $[\Sigma]$ matrix takes into account slowing down, and acceleration, in energy of the neutrons. In this way, we can define the $[A]$ matrix which will have the following structure,

$$[A] = \begin{bmatrix} \begin{bmatrix} X & X \\ X & X & X \\ X & X & X \\ \dots & \dots & \dots \\ X & X & X \\ X & X \end{bmatrix} & \begin{bmatrix} X \\ X \\ X \\ \dots \\ X \\ X \end{bmatrix} \\ \dots & \dots \\ \begin{bmatrix} X \\ X \\ X \\ \dots \\ X \\ X \end{bmatrix} & \begin{bmatrix} X & X \\ X & X & X \\ X & X & X \\ \dots & \dots & \dots \\ X & X & X \\ X & X \end{bmatrix} \end{bmatrix} \quad (EQ 45)$$

The matrix $[A]$ thus contains $G \times G$ large blocks of $N \times N$ and is thus of dimensions $(N \times G) \times (N \times G)$. The blocks containing the coupling coefficients contributions by leakage all have a tri-diagonal

structure, because of the nearest neighbor coupling. The discretized equations thus take the form

$$[A][\psi] = \frac{1}{K_{\text{eff}}}[B][\psi] \quad (\text{EQ 46})$$

The structures of the [A] and [B] matrices are identical for the mesh centered finite differences or for classical finite differences. This comes from the coupling coefficients. The individual matrix elements of course will be different for the two methods, which would give rise to a slightly different solution.

