The finite difference methods

Alain Hébert

alain.hebert@polymtl.ca

Institut de génie nucléaire

École Polytechnique de Montréal

Content (week 4)

- Discretization of the neutron diffusion equation
- Mesh-corner finite differences
- Mesh-centered finite differences

Discretization of the diffusion equation 1

- discretization is the technique we use to transform an algebraic operator into a matrix operator.
- A discretization of the neutron diffusion equation allows its transformation into a matrix system that can be solved by standard numerical analysis techniques.
  - A discretization technique is said to be consistent if the discretization of a Laplace operator $\nabla^2\phi(\boldsymbol{r})$ produces a symmetric, positive-definite and diagonally dominant matrix.
  - Consistent discretization techniques are generally based on polynomial approximation of the neutron flux in each region. Each homogeneous region of the reactor can be sub-divided into sub-regions in order to increase the number of piecewise polynomials. This operation is called sub-meshing.
  - A numerical solution of a consistent discretization technique must tend to the exact solution of the differential problem
    - as the number of sub-regions increases to infinity, for a given order of the polynomial basis,
    - as the polynomial order of the polynomial basis increases to infinity, for a given number of sub-regions.

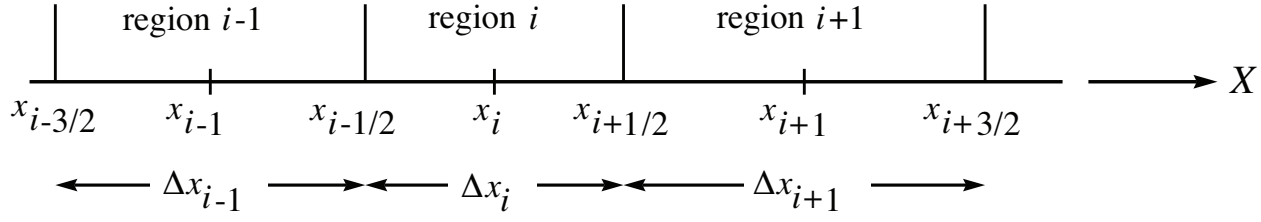
Discretization of the diffusion equation 2

- The symmetry of the matrix operator is important to ensure that the discretization of an adjoint differential equation leads to the transposed matrix operator obtained from the discretization of the direct differential equation.
- The positive-definite and diagonally dominant criteria ensure the success of the standard numerical analysis techniques used to solve the matrix system.
- Discretization techniques can be derived from the differential formulation of the neutron diffusion equation by replacing the dependent variable with Taylor's expansions or by using a weighted residual approach.
- They can also be obtained from a variational formulation by finding a stationary point of an ad-hoc functional (aka Rayleigh-Ritz method). The choice of the functional is arbitrary, the only condition being that the Euler equations of the functional must be identical to the neutron diffusion equation with its continuity and boundary conditions.
- A discretization technique can be primal if it belongs to the family of mesh-corner finite difference, or dual if it belongs to the family of mesh-centered finite difference methods. A discretization technique can be simultaneously primal and dual (primal-dual agreement), a characteristic of superconvergent approximations.

Both mesh-corner and mesh-centered techniques are consistent discretization approaches that can be obtained from the differential formulation of the neutron diffusion equation.

Mesh-corner finite differences 1

The 1D Cartesian mesh-corner finite difference formulation can be derived from the differential formulation of the neutron diffusion equation, by replacing the flux derivative terms in the diffusion equation by finite-difference relations written in terms of the neutron flux values at specific abscissa points.



In its mesh-corner formulation, the abscissa points where the neutron flux is explicitly calculated are chosen on the boundary between sub-regions and are numbered as depicted in the figure. We will use Taylor expansions to represent the flux at points $x_{i-3/2}$ and $x_{i+1/2}$ in terms of the flux at point $x_{i-1/2}$, so that

(1) $$\phi(x_{i-3/2}) = \phi(x_{i-1/2}) - \Delta x_{i-1}\,\phi'(x^-_{i-1/2}) + \frac{1}{2}\Delta x^2_{i-1}\,\phi''(x^-_{i-1/2})$$

and

(2) $$\phi(x_{i+1/2}) = \phi(x_{i-1/2}) + \Delta x_i\,\phi'(x^+_{i-1/2}) + \frac{1}{2}\Delta x^2_i\,\phi''(x^+_{i-1/2})$$

where the energy group index was omitted, in order to simplify the notation.

Mesh-corner finite differences 2

The neutron current continuity condition at $x_{i-1/2}$ causes a discontinuity in the first derivative of the neutron flux at this point:

(3) $$D_{i-1}\,\phi'(x^-_{i-1/2}) = D_i\,\phi'(x^+_{i-1/2}) \quad .$$

We multiply Eqs. (1) and (2) by $D_{i-1}/\Delta x_{i-1}$ and $D_i/\Delta x_i$, respectively, add the resulting relations and introduce Eq. (3):

(4) $$\begin{aligned}&\frac{1}{2}\left[\Delta x_{i-1} D_{i-1}\,\phi''(x^-_{i-1/2}) + \Delta x_i D_i\,\phi''(x^+_{i-1/2})\right]\\ &\quad = \frac{D_i}{\Delta x_i}\left[\phi(x_{i+1/2}) - \phi(x_{i-1/2})\right] - \frac{D_{i-1}}{\Delta x_{i-1}}\left[\phi(x_{i-1/2}) - \phi(x_{i-3/2})\right] \quad .\end{aligned}$$

Equation (4) is used as a finite difference relation valid for the internal points. We also need relations valid on boundary points where an albedo boundary condition is imposed:

(5) $$\phi(x_{3/2}) = \phi(x_{1/2}) + \Delta x_1\,\phi'(x_{1/2}) + \frac{1}{2}\Delta x_1^2\,\phi''(x_{1/2}) \quad \text{(left boundary)}$$

(6) $$\phi(x_{I-1/2}) = \phi(x_{I+1/2}) - \Delta x_I\,\phi'(x_{I+1/2}) + \frac{1}{2}\Delta x_I^2\,\phi''(x_{I+1/2}) \quad \text{(right boundary)}$$

Mesh-corner finite differences 3

We recall the mathematical expression of an albedo condition, written as

$$\mp D_g(x)\,\frac{d\phi_g}{dx} + \frac{1}{2}\frac{1-\beta(x)}{1+\beta(x)}\,\phi_g(x) = 0 \tag{7}$$

We multiply these two relations by $D_1/\Delta x_1$ and $D_I/\Delta x_I$, respectively, and introduce Eq. (7). We obtain

$$\frac{1}{2}\Delta x_1 D_1\ \phi''(x_{1/2}) = \frac{D_1}{\Delta x_1}\left[\phi(x_{3/2}) - \phi(x_{1/2})\right] - \frac{1}{2}\frac{1-\beta_-}{1+\beta_-}\,\phi(x_{1/2}) \tag{8}$$

and

$$\frac{1}{2}\Delta x_I D_I\ \phi''(x_{I+1/2}) = \frac{D_I}{\Delta x_I}\left[\phi(x_{I-1/2}) - \phi(x_{I+1/2})\right] - \frac{1}{2}\frac{1-\beta_+}{1+\beta_+}\,\phi(x_{I+1/2}) \tag{9}$$

where β_- and β_+ are the left– and right–domain albedos, respectively.

Our Taylor expansions are truncated after the term in Δx_i^2. Consequently, the difference relations (4), (8) and (9) are accurate only to the second order in Δx_i^2. This order is the smallest one that leads to a consistent discretization of the diffusion equation.

Mesh-corner finite differences 4

Substitute the finite difference relations into the neutron diffusion equation. On both sides of point $x_{i-1/2}$, the nuclear properties are uniform, so that the diffusion equation reduces to

$$
\begin{aligned}
-D_{i-1}\,\phi''(x^{-}_{i-1/2}) + \Sigma_{\mathrm{r},i-1}\,\phi(x_{i-1/2}) &= Q^{\diamond}_{i-1} \\
\text{and}\quad -D_{i}\,\phi''(x^{+}_{i-1/2}) + \Sigma_{\mathrm{r},i}\,\phi(x_{i-1/2}) &= Q^{\diamond}_{i}
\end{aligned}
\tag{10}
$$

where the flat-source approximation leading to constant terms $Q^{\diamond}_{i-1}$ and $Q^{\diamond}_{i}$ is compatible with the truncation order of the Taylor series. A higher truncation order would have required spatially dependent neutron sources in the right term.

We multiply each of Eqs. (10) with Δx_{i-1} and Δx_i, respectively, and we add the resulting relations. Introducing the finite difference relations (4), (8) and (9), we obtain

- in mesh points internal to the domain:

$$
\begin{aligned}
&\frac{D_i}{\Delta x_i}\left[\phi_{i+1/2}-\phi_{i-1/2}\right] - \frac{D_{i-1}}{\Delta x_{i-1}}\left[\phi_{i-1/2}-\phi_{i-3/2}\right] \\
&\quad = \frac{1}{2}\,\phi_{i-1/2}\left[\Delta x_i \Sigma_{\mathrm{r},i} + \Delta x_{i-1}\Sigma_{\mathrm{r},i-1}\right] - \frac{1}{2}\left[\Delta x_i Q^{\diamond}_{i} + \Delta x_{i-1} Q^{\diamond}_{i-1}\right]
\end{aligned}
\tag{11}
$$

  where we used the notation $\phi_{i-1/2} = \phi(x_{i-1/2})$;

Mesh-corner finite differences 5

- on zero-flux boundary points:

(12) $$\phi_{1/2} = 0 \quad \text{or} \quad \phi_{I+1/2} = 0$$

- on the left boundary point, assuming an albedo boundary condition:

(13) $$\frac{D_1}{\Delta x_1}\left[\phi_{3/2} - \phi_{1/2}\right] - \frac{1}{2}\frac{1-\beta_-}{1+\beta_-}\,\phi_{1/2} = \frac{1}{2}\Delta x_1 \Sigma_{\mathrm{r},1}\,\phi_{1/2} - \frac{1}{2}\Delta x_1\, Q_1^{\diamond}$$

- on the right boundary point, assuming an albedo boundary condition:

$$\frac{D_I}{\Delta x_I}\left[\phi_{I-1/2} - \phi_{I+1/2}\right] - \frac{1}{2}\frac{1-\beta_+}{1+\beta_+}\,\phi_{I+1/2} = \frac{1}{2}\Delta x_I \Sigma_{\mathrm{r},I}\,\phi_{I+1/2} - \frac{1}{2}\Delta x_I\, Q_I^{\diamond} \quad .$$

(14)

Mesh-corner finite differences 6

The discretization process involves the transformation of Eq. (36) with its continuity and boundary conditions into a matrix system whose unknown vector, denoted $\boldsymbol{\Phi}$, is a set of neutron flux values selected at specific abscissa:

(15)
$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_{1/2} \\ \phi_{3/2} \\ \vdots \\ \phi_{I+1/2} \end{pmatrix} .$$

The matrix system is written

(16)
$$\mathbb{A}\,\boldsymbol{\Phi} = \boldsymbol{Q}$$

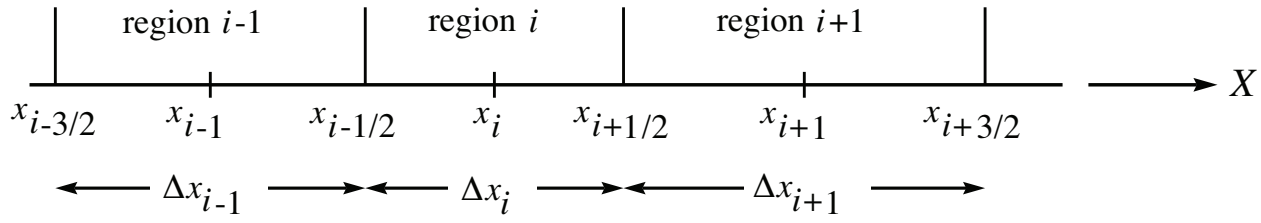
where coefficient matrix $\mathbb{A}$ and source vector $\boldsymbol{Q}$ components correspond to the various terms of Eqs. (11) to (14). Matrix $\mathbb{A}$ is symmetric, positive definite and diagonally dominant.

The numerical solution of Eq. (16) is greatly simplified by the particular structure of matrix $\mathbb{A}$. All its components are located in a tri-diagonal structure, each component $\phi_{i-1/2}$ being related only to its two closest neighbors, $\phi_{i-3/2}$ and $\phi_{i+1/2}$. The wide acceptance of the mesh-corner finite difference method is due to the observation that similar tri-diagonal layouts are observed with two- and three-dimensional domains.

Mesh-centered finite differences 1

- The mesh-centered finite difference method is an alternative to the mesh-corner finite difference method frequently implemented in production codes for solving the neutron diffusion equation.
- It offers the same accuracy and the same advantages as the mesh-corner finite difference method.
- The discretization errors originating from these two types of finite difference methods are often of opposite sign: an over-estimation of a power peak with one method is often associated with an under-estimation with the other method.
- A careful mathematical study of this phenomenon reveals that the mesh-corner and mesh-centered finite difference methods are the Euler equations of primal and dual variational formulations, respectively.
- The mesh-centered finite difference relations can be obtained by assuming that the average neutron flux in a sub-region is equal to the neutron flux at the center of this sub-region.

Mesh-centered finite differences 2



We consider the sub-region surrounding the abscissa point x_i and write the neutron flux at this point, using the figure to define the other abscissa values. We obtain

(17) $$\phi_i = \phi(x_i) = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} dx\, \phi(x) \quad .$$

The next step consists in integrating the one-speed diffusion equation over each sub-region, so that

(18) $$-D_i \int_{x_{i-1/2}}^{x_{i+1/2}} dx\, \frac{d^2\phi}{dx^2} + \Sigma_{\mathrm{r},i} \int_{x_{i-1/2}}^{x_{i+1/2}} dx\, \phi(x) = \Delta x_i Q_i^{\diamond}$$

where we assumed that neutron sources $Q^{\diamond}(x)$ are uniform and equal to $Q_i^{\diamond}$ over sub-region i.

Mesh-centered finite differences 3

The first term on the left can be integrated analytically. Introducing Eq. (17), we get

(19) $$-D_i\left[\phi'(x^-_{i+1/2})-\phi'(x^+_{i-1/2})\right]+\Delta x_i\Sigma_{\mathrm{r},i}\,\phi(x_i)=\Delta x_i Q^\diamond_i \quad .$$

The differential terms of Eq. (19) are replaced with finite-difference relations. These relations can be obtained from the following two Taylor expansions:

(20) $$\phi(x_{i-1})=\phi(x_{i-1/2})-\frac{\Delta x_{i-1}}{2}\,\phi'(x^-_{i-1/2})$$

and

(21) $$\phi(x_i)=\phi(x_{i-1/2})+\frac{\Delta x_i}{2}\,\phi'(x^+_{i-1/2}) \quad .$$

We also remember the neutron current continuity condition at point $x_{i-1/2}$. This condition is written

(22) $$D_{i-1}\,\phi'(x^-_{i-1/2})=D_i\,\phi'(x^+_{i-1/2}) \quad .$$

Mesh-centered finite differences 4

We multiply Eqs. (20) and (21) by $D_{i-1}/\Delta x_{i-1}$ and $D_i/\Delta x_i$, respectively, and add these relations in such a way as to eliminate the derivatives of the flux with the help of Eq. (22). We obtain

(23) $$\phi(x_{i-1/2}) = \frac{\Delta x_i D_{i-1}\,\phi(x_{i-1}) + \Delta x_{i-1} D_i\,\phi(x_i)}{\Delta x_i D_{i-1} + \Delta x_{i-1} D_i} \quad .$$

After substitution of Eq. (23) into Eq. (21), we obtain our first mesh-centered finite-difference relation as

(24) $$\phi'(x^+_{i-1/2}) = 2D_{i-1}\frac{\phi(x_i) - \phi(x_{i-1})}{\Delta x_i D_{i-1} + \Delta x_{i-1} D_i} \quad .$$

Using a similar approach, we obtain a second mesh-centered finite-difference relation as

(25) $$\phi'(x^-_{i+1/2}) = 2D_{i+1}\frac{\phi(x_{i+1}) - \phi(x_i)}{\Delta x_{i+1} D_i + \Delta x_i D_{i+1}} \quad .$$

Mesh-centered finite differences 5

Let us now consider the case where the left–most surface is characterized by a zero-flux boundary condition. Setting $\phi(x_{1/2}) = 0$ in Eq. (21) leads to the corresponding finite-difference relation. It is written

(26) $$\phi'(x^+_{1/2}) = \frac{2}{\Delta x_1}\phi(x_1) \quad .$$

We recall the mathematical expression of an albedo condition, written as

(27) $$\mp D_g(x)\,\frac{d\phi_g}{dx} + \frac{1}{2}\frac{1-\beta(x)}{1+\beta(x)}\,\phi_g(x) = 0$$

If the left–most surface is characterized by an albedo boundary condition, we combine Eqs. (27) and (20) to obtain

(28) $$\phi'(x^+_{1/2}) = \frac{2(1-\beta_-)}{4D_1(1+\beta_-) + \Delta x_1(1-\beta_-)}\,\phi(x_1) \quad .$$

Mesh-centered finite differences 6

The substitution of finite-difference Eqs. (24) to (28) into Eq. (19) leads to the complete set of mesh-centered finite difference relations:

- the sub-region i is internal to the domain:

$$2\left[D_i D_{i+1}\frac{\phi_{i+1}-\phi_i}{\Delta x_{i+1}D_i+\Delta x_i D_{i+1}}-D_i D_{i-1}\frac{\phi_i-\phi_{i-1}}{\Delta x_i D_{i-1}+\Delta x_{i-1}D_i}\right] = \Delta x_i \Sigma_{\mathrm{r},i}\,\phi_i - \Delta x_i Q_i^{\diamond} \tag{29}$$

- the left–surface of sub-region $i=1$ is characterized by a zero-flux boundary condition:

$$2\left[D_1 D_2\frac{\phi_2-\phi_1}{\Delta x_2 D_1+\Delta x_1 D_2}-\frac{D_1}{\Delta x_1}\phi_1\right] = \Delta x_1 \Sigma_{\mathrm{r},1}\,\phi_1 - \Delta x_1 Q_1^{\diamond} \tag{30}$$

- the left–surface of sub-region $i=1$ is characterized by an albedo boundary condition:

$$2\left[D_1 D_2\frac{\phi_2-\phi_1}{\Delta x_2 D_1+\Delta x_1 D_2}-\frac{D_1(1-\beta_-)}{4D_1(1+\beta_-)+\Delta x_1(1-\beta_-)}\phi_1\right] = \Delta x_1 \Sigma_{\mathrm{r},1}\,\phi_1 - \Delta x_1 Q_1^{\diamond} \tag{31}$$

Mesh-centered finite differences 7

- the right–surface of sub-region $i = I$ is characterized by a zero-flux boundary condition:

$$2\left[-\frac{D_I}{\Delta x_I}\,\phi_I - D_I D_{I-1}\frac{\phi_I - \phi_{I-1}}{\Delta x_I D_{I-1} + \Delta x_{I-1} D_I}\right] = \Delta x_I \Sigma_{\mathrm{r},I}\,\phi_I - \Delta x_I Q_I^{\diamond} \tag{32}$$

- the right–surface of sub-region $i = I$ is characterized by an albedo boundary condition:

$$2\left[-\frac{D_I(1-\beta_+)}{4D_I(1+\beta_+) + \Delta x_I(1-\beta_+)}\,\phi_I - D_I D_{I-1}\frac{\phi_I - \phi_{I-1}}{\Delta x_I D_{I-1} + \Delta x_{I-1} D_I}\right]$$

$$= \Delta x_I \Sigma_{\mathrm{r},I}\,\phi_I - \Delta x_I Q_I^{\diamond}\ . \tag{33}$$

Mesh-centered finite differences 8

The matrix system produced by the mesh-centered finite difference method is similar and has the same numerical properties as the matrix system produced by the mesh-corner finite difference method. The principal distinction comes from the fact that the unknown vector is the set of all mesh-centered neutron flux values. It is written

(34)
$$\mathbf{\Phi} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_I \end{pmatrix} .$$

As before, the matrix system is written

(35)
$$\mathbb{A}\,\mathbf{\Phi} = \boldsymbol{Q}$$

where coefficient matrix $\mathbb{A}$ and source vector $\boldsymbol{Q}$ components correspond to the various terms of Eqs. (29) to (33). Matrix $\mathbb{A}$ is symmetric, positive definite and diagonally dominant.

The spatial discretization order of the mesh-centered finite difference method can be increased beyond the linear order presented in this text, leading to the nodal collocation method.