22.211 Lecture 16

Finite Difference for Diffusion Equation

Benoit Forget

April 5, 2023

Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Objectives

- Develop 2 group 1D finite difference equations
- Power iteration
- Simple nodal model

Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

2 group diffusion

Group 1

$$-\nabla \cdot D_1(\vec{r})\nabla\phi_1(\vec{r}) + \left[\Sigma_{a,1}(\vec{r}) + \Sigma_{s,1\to 2}(\vec{r})\right]\phi_1(\vec{r}) = \nu\Sigma_{f,1}(\vec{r})\phi_1(\vec{r}) + \nu\Sigma_{f,2}(\vec{r})\phi_2(\vec{r}) + S_1(\vec{r})$$

Group 2

$$-\nabla \cdot D_2(\vec{r})\nabla\phi_2(\vec{r}) + \Sigma_{a,2}(\vec{r})\phi_2(\vec{r}) = \Sigma_{s,1\to 2}(\vec{r})\phi_1(\vec{r}) + S_2(\vec{r})$$

Discretize in space (1D)

Massachusetts Institute of Technology

Spatial discretization

Integrate the diffusion equation over each mesh cell, and assume constant material properties in the mesh, for mesh n

$$\int_{x_{n-1}}^{x_n} -\frac{d}{dx} D_1^n \frac{d\phi_1(x)}{dx} dx + \left[\Sigma_{a,1}^n + \Sigma_{s,1\to 2}^n\right] \phi_1^n \Delta^n = \nu\Sigma_{f,1}^n \phi_1^n \Delta^n + \nu\Sigma_{f,2}^n \phi_2^n \Delta^n + S_1^n \Delta^n$$

$$\int_{x_{n-1}}^{x_n} -\frac{d}{dx} D_2^n \frac{d\phi_2(x)}{dx} dx + \Sigma_{a,2}^n \phi_2^n \Delta^n = \Sigma_{s,1\to 2}^n \phi_1^n \Delta^n + S_2^n \Delta^n$$

Divergence theorem

Using divergence theorem, we get

$$D_1^n \frac{d\phi_1(x)}{dx}\bigg|_{x_{n-1}} - D_1^n \frac{d\phi_1(x)}{dx}\bigg|_{x_n} + \left[\Sigma_{a,1}^n + \Sigma_{s,1\to 2}^n\right]\phi_1^n \Delta^n = \nu\Sigma_{f,1}^n \phi_1^n \Delta^n + \nu\Sigma_{f,2}^n \phi_2^n \Delta^n + S_1^n \Delta^n$$

$$D_2^n \frac{d\phi_2(x)}{dx}\bigg|_{x_{n-1}} - D_2^n \frac{d\phi_2(x)}{dx}\bigg|_{x_n} + \Sigma_{a,2}^n \phi_2^n \Delta^n = \Sigma_{s,1\to 2}^n \phi_1^n \Delta^n + S_2^n \Delta^n$$

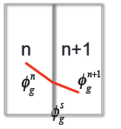
At the interface

$$J_g^{n,R} = -D_g^n \frac{d\phi_g(x)}{dx}\bigg|_{x_n} = -D_g^n \frac{\phi_g^s - \phi_g^n}{\Delta^n/2}$$

$$J_g^{(n+1),L} = -D_g^{n+1} \frac{d\phi_g(x)}{dx}\bigg|_{x_n} = -D_g^{n+1} \frac{\phi_g^{n+1} - \phi_g^s}{\Delta^{n+1}/2}$$

Imposing continuity of the current, and assuming constant mesh spacing

$$D_g^n \frac{\phi_g^s - \phi_g^n}{\Delta/2} = D_g^{n+1} \frac{\phi_g^{n+1} - \phi_g^s}{\Delta/2} \Rightarrow \phi_g^s = \frac{D_g^{n+1}\phi_g^{n+1} + D_g^n \phi_g^n}{D_g^{n+1} + D_g^n}$$



Net currents

We can then replace the surface flux to express the net currents in terms of mesh fluxes

$$J_g^{n,R} = \frac{-2D_g^n}{\Delta}\left(\frac{D_g^{n+1}\phi_g^{n+1} + D_g^n\phi_g^n}{D_g^{n+1} + D_g^n} - \phi_g^n\right)$$

$$J_g^{n,R} = \frac{2D_g^n D_g^{n+1}}{\Delta(D_g^n + D_g^{n+1})}\phi_g^n - \frac{2D_g^n D_g^{n+1}}{\Delta(D_g^n + D_g^{n+1})}\phi_g^{n+1}$$

where we can define

$$\tilde{D}_g^{n,n+1} = \frac{2D_g^n D_g^{n+1}}{\Delta(D_g^n + D_g^{n+1})}$$

Massachusetts Institute of Technology

Replacing in diffusion equation

Assuming equal mesh spacing

$$\begin{aligned}\tilde{D}_1^{n-1,n}\left(\phi_1^n-\phi_1^{n-1}\right)-\tilde{D}_1^{n,n+1}\left(\phi_1^{n+1}-\phi_1^n\right)+\Sigma_{r,1}^n\phi_1^n\Delta \\ =\nu\Sigma_{f,1}^n\phi_1^n\Delta+\nu\Sigma_{f,2}^n\phi_2^n\Delta+S_1^n\Delta\end{aligned}$$

$$\tilde{D}_2^{n-1,n}\left(\phi_2^n-\phi_2^{n-1}\right)-\tilde{D}_2^{n,n+1}\left(\phi_2^{n+1}-\phi_2^n\right)+\Sigma_{a,2}^n\phi_2^n\Delta=\Sigma_{s,1\to2}^n\phi_1^n\Delta+S_2^n\Delta$$

Re-arranging

$$\begin{aligned}-\tilde{D}_1^{n-1,n}\phi_1^{n-1}-\tilde{D}_1^{n,n+1}\phi_1^{n+1}+\left[\Sigma_{r,1}^n\Delta+\tilde{D}_1^{n-1,n}+\tilde{D}_1^{n,n+1}\right]\phi_1^n \\ =\nu\Sigma_{f,1}^n\phi_1^n\Delta+\nu\Sigma_{f,2}^n\phi_2^n\Delta+S_1^n\Delta\end{aligned}$$

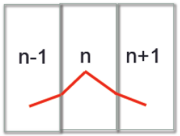
$$\begin{aligned}-\tilde{D}_2^{n-1,n}\phi_2^{n-1}-\tilde{D}_2^{n,n+1}\phi_2^{n+1}+\left[\Sigma_{a,2}^n\Delta+\tilde{D}_2^{n-1,n}+\tilde{D}_2^{n,n+1}\right]\phi_2^n \\ =\Sigma_{s,1\to2}^n\phi_1^n\Delta+S_2^n\Delta\end{aligned}$$

Massachusetts Institute of Technology

Final form

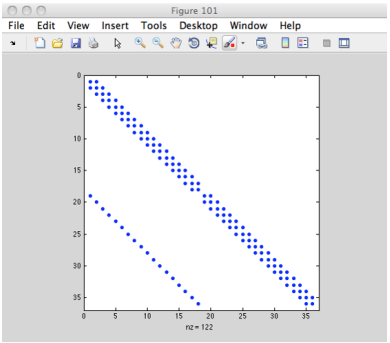
$$-\tilde{D}_1^{n-1,n}\phi_1^{n-1} - \tilde{D}_1^{n,n+1}\phi_1^{n+1} + \left[\Sigma_{r,1}^n\Delta + \tilde{D}_1^{n-1,n} + \tilde{D}_1^{n,n+1}\right]\phi_1^n = \nu\Sigma_{f,1}^n\phi_1^n\Delta + \nu\Sigma_{f,2}^n\phi_2^n\Delta + S_1^n\Delta$$

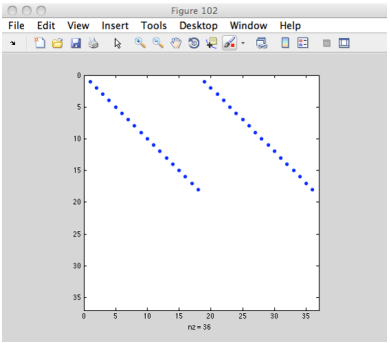
$$-\tilde{D}_2^{n-1,n}\phi_2^{n-1} - \tilde{D}_2^{n,n+1}\phi_2^{n+1} + \left[\Sigma_{a,2}^n\Delta + \tilde{D}_2^{n-1,n} + \tilde{D}_2^{n,n+1}\right]\phi_2^n = \Sigma_{s,1\to 2}^n\phi_1^n\Delta + S_2^n\Delta$$



Massachusetts Institute of Technology

Matrix form





$$H\phi = F\phi + S$$

Looking at the figures, how was the flux vector ordered (space first or energy first)?

Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Boundary conditions - Vacuum

$$J_g^+(0) = 0 = \frac{\phi_g(0)}{4} - \frac{D_g^1}{2}\frac{d\phi_g(x)}{dx}\bigg|_{x=0} = \frac{\phi_g(0)}{4} + \frac{J_g(0)}{2}$$

thus

$$J_g(0) = -\frac{\phi_g(0)}{2} \Rightarrow \phi_g(0) = -2J_g(0)$$

the net current can also be defined from

$$J_g(0) = \frac{-D_g^1(\phi_g^1 - \phi_g(0))}{\Delta/2} = \frac{-D_g^1(\phi_g^1 + 2J_g(0))}{\Delta/2}$$

Massachusetts Institute of Technology

Boundary conditions - Vacuum

Express $J_g(0)$ as a function of ϕ_g^1

$$J_g(0) = -\frac{2D_g^1}{\Delta}\left[\frac{1}{1+4D_g/\Delta}\right]\phi_g^1 = -\tilde{D}_g^1\phi_g^1$$

Thus for mesh 1 in 2 groups

$$-\tilde{D}_1^{1,2}\phi_1^2 + \left[\Sigma_{r,1}^1\Delta + \tilde{D}_1^1 + \tilde{D}_1^{1,2}\right]\phi_1^1 = \nu\Sigma_{f,1}^1\phi_1^1\Delta + \nu\Sigma_{f,2}^1\phi_2^1\Delta + S_1^1\Delta$$

$$-\tilde{D}_2^{1,2}\phi_2^2 + \left[\Sigma_{a,2}^1\Delta + \tilde{D}_2^1 + \tilde{D}_2^{1,2}\right]\phi_2^1 = \Sigma_{s,1\to 2}^1\phi_1^1\Delta + S_2^1\Delta$$

A similar expression can be derived for the right surface with $J_g^-(L) = 0$.

Massachusetts Institute of Technology

Boundary conditions - Reflective

$$J^+(0) = J^-(0)$$

This implies that the net current ($J(0)$) is equal to 0. Thus for mesh 1 in 2 groups

$$-\tilde{D}_1^{1,2}\phi_1^2 + \left[\Sigma_{r,1}^1\Delta + \tilde{D}_1^{1,2}\right]\phi_1^1 = \nu\Sigma_{f,1}^1\phi_1^1\Delta + \nu\Sigma_{f,2}^1\phi_2^1\Delta + S_1^1\Delta$$

$$-\tilde{D}_2^{1,2}\phi_2^2 + \left[\Sigma_{a,2}^1\Delta + \tilde{D}_2^{1,2}\right]\phi_2^1 = \Sigma_{s,1\to 2}^1\phi_1^1\Delta + S_2^1\Delta$$

One thing to keep in mind

The expression for partial currents

$$J^{\pm}(x) = \frac{\phi(x)}{4} \mp \frac{D(x)}{2} \frac{d\phi(x)}{dx}\bigg|_x$$

is for a surface normal aligned with the x axis. This means that an incoming current on the left boundary is for J^+ and an incoming current on the right boundary is for J^-.

Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Power iteration

In reactor analysis we mainly care about the dominant eigenvalue (which yields a positive flux). The simplest way to obtain the dominant eigenvalue is the power iteration, on system $Ax = \lambda x$. Suppose A is diagonalizable with ordered eigenvalues:

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$$

then we have $A = V\Lambda V^{-1}$ where Λ is a diagonal matrix of eigenvalues. Note that

$$A^k = (V\Lambda V^{-1})^k = V\Lambda^k V^{-1} \Rightarrow A^k V = V\Lambda^k$$

For a random initial guess of x, that can be expressed as $x = V\tilde{x}$, we can show

$$A^{(k)}x = A^k V\tilde{x} = \sum_{j=1}^{n} v_j \lambda_j^k \tilde{x}_j$$

Massachusetts Institute of Technology

Power iteration

We can also pull out the dominant eigenvalue λ_1

$$A^k x = \lambda_1^k \left(\sum_{j=1}^{n} v_j \left(\frac{\lambda_j}{\lambda_1} \right)^k \tilde{x}_j \right)$$

Thus, as we increase the value of k (iterations), all higher modes will go to zero except for the dominant eigenvalue. In reactor physics, we actually use a slight variant called the inverse power iteration, because of the way we setup our problem. The ratio of λ_2/λ_1 is the slowest mode to go to zero, and is referred to as the dominance ratio.

Massachusetts Institute of Technology

Krylov methods

The power iteration method created a series of vectors that form a Krylov subspace

$$\kappa = span\left\{x^0, Ax^0, A^2x^0, ...A^kx^0\right\}$$

Krylov solvers will store multiple vectors in such a subspace (orthogonalized subspace) and project the matrix to a subspace on which accurate approximations of eigenvalues and eigenvectors can be obtained (Arnoldi's method).

Massachusetts Institute of Technology

How to solve - power iteration

1. Guess an initial normalized flux vector $\phi^{(0)}$ and eigenvalue $k^{(0)}$
2. Compute source $b^{(0)} = \frac{1}{k^{(0)}} F\phi^{(0)}$
3. Perform linear solve for $H\phi^{(1)} = b^{(0)}$
4. Compute $k^{(1)} = \frac{\langle F\phi^{(1)} \rangle}{\langle F\phi^{(0)} \rangle} k^{(0)}$
5. Normalize flux
6. Iterate until convergence (k, flux, fission source, ...)

Massachusetts Institute of Technology

Normalization

A normalized vector is a vector in the same direction but with a known length.

$$\hat{x} = \frac{x}{||x||}$$

where $||x||$ can take many forms

$$L_\infty \Rightarrow ||x||_\infty = max|x_j|$$

$$L_m \Rightarrow ||x||_m = \sqrt{\sum_{j=1}^{N} |x_j|^m}$$

Massachusetts Institute of Technology

Convergence

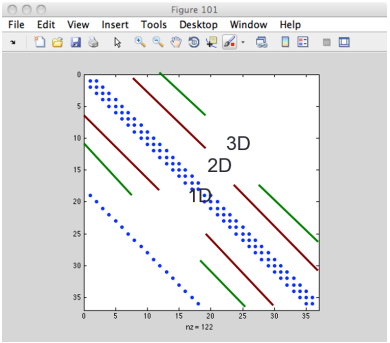
Convergence is obtained by comparing the change between successive iterations and comparing to a given threshold ϵ

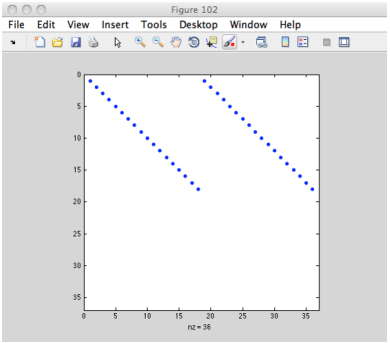
$$\left|\left|\frac{x^i - x^{i-1}}{x^i}\right|\right| < \epsilon$$

Converging the eigenvalue is not sufficient, you must also verify convergence of the eigenvector. Common practice is to check convergence of fission source since it weighs the flux by the important regions of the problem.

Massachusetts Institute of Technology

Multi-dimensional



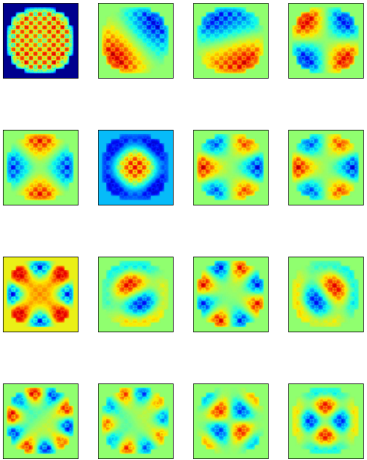


Exact position of the diagonals will depend on node ordering.

Oscillation sensitivities

- Core size
- Decoupling of radial zones
  - Control rod insertion
  - Asymmetric core loadings
  - Xenon distributions
- Axial zones
  - Partially inserted rods
  - Axial enrichment zoning
  - Axial burnable absorber loading

The eigenmodes of the system play an important role in design and operation of nuclear reactors.



Massachusetts Institute of Technology

Outline

Massachusetts Institute of Technology

Diffusion equation

$$\frac{\partial}{\partial x} J^k_{g,x}(x,y,z) + \frac{\partial}{\partial y} J^k_{g,y}(x,y,z) + \frac{\partial}{\partial z} J^k_{g,z}(x,y,z) + \Sigma^k_{r,g} \phi^k_g(x,y,z) = Q^k_g(x,y,z)$$

with

$$J^k_{g,x}(x,y,z) = -D^k_g \frac{\partial}{\partial x} \phi^k_g(x,y,z)$$

Massachusetts Institute of Technology

Balance on a node

$$\frac{1}{\Delta x}\left[J^k_{g,x^+} - J^k_{g,x^-}\right] + \frac{1}{\Delta y}\left[J^k_{g,y^+} - J^k_{g,y^-}\right] + \frac{1}{\Delta z}\left[J^k_{g,z^+} - J^k_{g,z^-}\right] + \Sigma^k_{r,g}\bar{\phi}^k_g = \bar{Q}^k_g$$

where the node average flux is defined as

$$\bar{\phi}^k_g = \frac{1}{V}\int_{-\Delta x/2}^{\Delta x/2} dx \int_{-\Delta y/2}^{\Delta y/2} dy \int_{-\Delta z/2}^{\Delta z/2} dz \phi^k_g(x,y,z)$$

and the surface average current as

$$J^k_{g,x^+} = \frac{1}{\Delta y \Delta z}\int_{-\Delta y/2}^{\Delta y/2} dy \int_{-\Delta z/2}^{\Delta z/2} dz - D^k_g \frac{\partial}{\partial x}\phi^k_g(x,y,z)\Big|_{x=\Delta x/2}$$

Massachusetts Institute of Technology

Expressing the current

The goal of any discretization scheme is to find a form that allows us to express the net current.

- Finite Difference

$$J^k_{g,x^+} = -D^k_g \frac{\phi^k_g - \phi^k_{g,x+}}{\Delta/2}$$

The mesh required in finite difference is too small, thus nodal methods introduce a higher order approximation of the flux shape within an homogeneous node.

Massachusetts Institute of Technology

Second order nodal methods

- First, let's assume that each mesh is normalized by its width, such that each mesh varies between $x = -1/2$ and $x = 1/2$.
- Define the flux shape as second order using polynomials that integrate to zero on the interval as to preserve the average flux.

$$\phi(x) = \bar{\phi} + a_1 x + a_2(3x^2 - 1/4)$$

Massachusetts Institute of Technology

Expressing net current at an interface

Our goal is to replace the net current in the balance equation by an expression that depends only on the cell average fluxes. For 2 neighboring node sharing an interface (in 1 group), we have 2 nodal balance equations, continuity of the current and continuity of the flux. These 4 conditions will allow us to determine the 4 coefficients and express the current as a function of cell average fluxes.

$$\frac{d\phi}{dx} = a_1 + 6a_2x$$

$$\frac{d^2\phi}{dx^2} = 6a_2$$

Massachusetts Institute of Technology

2 node system

We have 4 equations and 4 unknowns.

$$-D^k(6a_2) + \Sigma_a^k \bar{\phi}^k = \frac{1}{k}\nu\Sigma_f^k \bar{\phi}^k \Rightarrow -D^k(6a_2) = \bar{S}^k \bar{\phi}^k$$

$$-D^{k+1}(6b_2) + \Sigma_a^{k+1} \bar{\phi}^{k+1} = \frac{1}{k}\nu\Sigma_f^{k+1} \bar{\phi}^{k+1} \Rightarrow -D^{k+1}(6b_2) = \bar{S}^{k+1} \bar{\phi}^{k+1}$$

$$J^k(1/2) = J^{k+1}(-1/2) \Rightarrow D^k(a_1 + 3a_2) = D^{k+1}(b_1 - 3b_2)$$

$$\phi^k(1/2) = \phi^{k+1}(-1/2) \Rightarrow \bar{\phi}^k + \frac{1}{2}(a_1 + a_2) = \bar{\phi}^{k+1} - \frac{1}{2}(-b_1 + b_2)$$

Massachusetts Institute of Technology

Solving for the coefficients

$$a_2 = \frac{-\bar{S}^k \bar{\phi}^k}{6D^k}$$

$$b_2 = \frac{-\bar{S}^{k+1} \bar{\phi}^{k+1}}{6D^{k+1}}$$

with

$$D^k(a_1 + 3a_2) = D^{k+1}(b_1 - 3b_2)$$

Massachusetts Institute of Technology

from flux continuity

$$b_1 = 2\bar{\phi}^{k+1} - 2\bar{\phi}^{k} - a_1 - a_2 + b_2$$

replace in the previous equation

$$D^k \left(a_1 + 3a_2\right) = D^{k+1} \left(2\bar{\phi}^{k+1} - 2\bar{\phi}^{k} - a_1 - a_2 + b_2 - 3b_2\right)$$

thus

$$a_1 = \frac{\frac{D^{k+1}}{D^k}\left(2\bar{\phi}^{k+1} - 2\bar{\phi}^{k} - a_2 - 2b_2\right) - 3a_2}{1 + \frac{D^{k+1}}{D^k}}$$

Massachusetts Institute of Technology

Expression for the current

$$J^k(1/2) = -D^k(a_1 + 3a_2)$$

with

$$a_1 = \frac{\frac{D^{k+1}}{D^k}\left(2\bar{\phi}^{k+1} - 2\bar{\phi}^k - a_2 - 2b_2\right) - 3a_2}{1 + \frac{D^{k+1}}{D^k}}$$

and

$$a_2 = \frac{-\bar{S}^k\bar{\phi}^k}{6D^k} \qquad b_2 = \frac{-\bar{S}^{k+1}\bar{\phi}^{k+1}}{6D^{k+1}}$$

Very similar to the finite difference equations, just different coefficients in front of the cell average fluxes. You can thus use the same solver and just replace how you calculate the tri-diagonal terms.

Massachusetts Institute of Technology