22.211 Lecture 13

Diffusion Theory

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Outline

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Objectives

- Anisotropic scattering
- P_N equations
- Diffusion approximation

Neutron Transport Equation

$$
\begin{aligned}
\hat{\Omega} \cdot \nabla \psi(\mathbf{r}, \boldsymbol{\Omega}, E) + \Sigma_t(\mathbf{r}, E)\psi(\mathbf{r}, \boldsymbol{\Omega}, E) = & \\
& + \int_0^\infty dE' \int_{4\pi} d\Omega' \nu_s \Sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E' \to E)\psi(\mathbf{r}, \boldsymbol{\Omega}', E') \\
& + \frac{\chi(E)}{4\pi} \int_0^\infty dE' \nu \Sigma_f(\mathbf{r}, E')\phi(\mathbf{r}, E') \\
& + s(\mathbf{r}, \boldsymbol{\Omega}, E) \, .
\end{aligned}
$$

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Scattering

In realistic problems, the scattering is usually never isotropic and the effects of the anisotropy can be fairly important.

- Angular variation in the scattering kernel can usually be approximated by

$$\Sigma_s(\Omega' \rightarrow \Omega) = \Sigma_s(\Omega \cdot \Omega') = \Sigma(\mu_0)$$

- Scattering thus depends only on angle between Ω' and Ω
- This is usually a valid assumption, except for moving medium and single crystals
- The scattering kernel can then be expanded using an orthogonal basis set

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Legendre Polynomials

Solutions to Legendre's differential equation, which corresponds to solving Laplace's equation in spherical coordinates. They are only valid between -1 and 1.

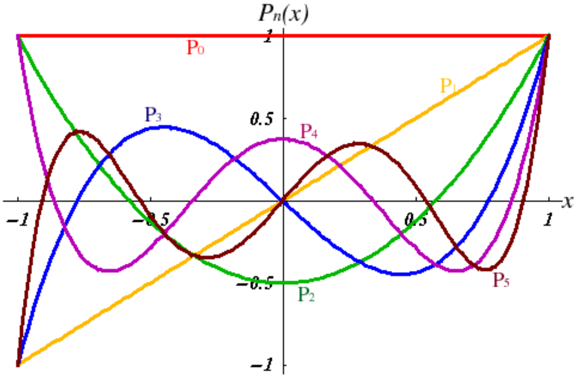
$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{3x^2 - 1}{2}$$

$$P_l(x) = \frac{1}{2^l l!} \frac{dl}{dx^l} (x^2 - 1)^l$$

Legendre Polynomials



Orthogonality

They satisfy the following orthogonality relationship on the -1 to 1 interval

$$\int_{-1}^{1} P_m(x) P_n(x) dx = \frac{2\delta_{mn}}{2n+1}$$

Recurrence Relations

$$xP_l(x) = \frac{1}{2l+1}((l+1)P_{l+1}(x) + lP_{l-1}(x))$$

$$(x^2-1)\frac{d}{dx}P_l(x) = l(xP_l(x) - P_{l-1}(x))$$

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Addition Theorem

$$P_l(\mu_0) = P_l(\mu)P_l(\mu') + 2\sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P_l^m(\mu)P_l^m(\mu') \cos(m(\varphi - \varphi'))$$

Scattering Kernel

$$\Sigma_s(\mu_0) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{sl} P_l(\mu_0)$$

where

$$\Sigma_{sl} = 2\pi \int_{-1}^{1} \Sigma_s(\mu_0) P_l(\mu_0) d\mu_0$$

1D Transport

we get

$$\mu \frac{d\psi(x,\mu)}{dx} + \Sigma_t(x)\psi(x,\mu) = \frac{1}{2}\nu\Sigma_f(x)\phi(x)$$
$$+ \int_{2\pi} d\varphi' \int_{-1}^{1} d\mu' \Sigma_s(x,\mu_0)\psi(x,\mu',\varphi') + S(x,\mu)$$

which becomes

$$\mu \frac{d\psi(x,\mu)}{dx} + \Sigma_t(x)\psi(x,\mu) = \frac{1}{2}\nu\Sigma_f(x)\phi(x)$$
$$\sum_{l=0}^{\infty} \frac{2l+1}{2}\Sigma_{sl}(x)P_l(\mu)\int_{-1}^{1}\psi(x,\mu')P_l(\mu')d\mu' + S(x,\mu)$$

Outline

Angular Flux Expansion

Expand angular flux in terms of Legendre polynomials

$$\psi(x,\mu) = \sum_{m=0}^{\infty} \frac{2m+1}{4\pi} \psi_m(x) P_m(\mu)$$

where

$$\psi_m(x) = 2\pi \int_{-1}^{1} \psi(x,\mu) P_m(\mu) d\mu$$

Instead of solving for the angular flux, we will solve for angular moments of the angular flux. Moments are then used to rebuild the angular flux.

Source Expansion

Expand source in terms of Legendre polynomials

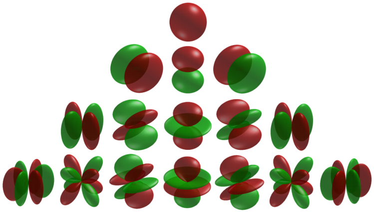
$$S(x, \mu) = \sum_{m=0}^{\infty} \frac{2m+1}{4\pi} S_m(x) P_m(\mu)$$

where

$$S_m(x) = 2\pi \int_{-1}^{1} S(x, \mu) P_m(\mu) d\mu$$

In 3D ...

We use spherical harmonics



$$Y_l^m(\theta,\varphi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(cos\theta)e^{im\varphi}$$

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Replace in TE

$$\sum_{m=0}^{\infty} \frac{2m+1}{4\pi} \left(\mu \frac{d\psi_m(x)}{dx} + \Sigma_t(x)\psi_m(x) \right) P_m(\mu) =$$

$$\sum_{m=0}^{\infty} \frac{2m+1}{4\pi} S_m(x) P_m(\mu) + \frac{1}{4\pi} \nu\Sigma_f(x)\psi_0(x) +$$

$$\sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{sl}(x) P_l(\mu)\psi_l(x)$$

Recurrence relation

$$\mu P_m(\mu) = \frac{m+1}{2m+1} P_{m+1}(\mu) + \frac{m}{2m+1} P_{m-1}(\mu)$$

we get

$$\sum_{m=0}^{\infty} \Big((m+1) P_{m+1}(\mu) + m P_{m-1}(\mu) \Big) \frac{d\psi_m(x)}{dx} +$$

$$\sum_{m=0}^{\infty} (2m+1) \Sigma_t(x) \psi_m(x) P_m(\mu) =$$

$$\sum_{m=0}^{\infty} (2m+1) S_m(x) P_m(\mu) + \nu \Sigma_f(x) \psi_0(x) +$$

$$\sum_{l=0}^{\infty} (2l+1) \Sigma_{sl}(x) P_l(\mu) \psi_l(x)$$

Orthogonality

Multiply by $P_n(\mu)$, integrate over all μ, use orthogonality relation, express in terms of n

$$\frac{n+1}{2n+1}\frac{d\psi_{n+1}(x)}{dx} + \frac{n}{2n+1}\frac{d\psi_{n-1}(x)}{dx} + \Sigma_t(x)\psi_n(x) = S_n(x) + \nu\Sigma_f(x)\psi_0(x) + \Sigma_{sn}(x)\psi_n(x)$$

Truncated expansion

$$
\begin{aligned}
n = 0 \qquad & \frac{d\psi_1(x)}{dx} + (\Sigma_t - \Sigma_{s0})\psi_0(x) = \nu\Sigma_f\psi_0(x) + S_0(x) \\
n = 1 \qquad & \frac{2}{3}\frac{d\psi_2(x)}{dx} + \frac{1}{3}\frac{d\psi_0(x)}{dx} + (\Sigma_t - \Sigma_{s1})\psi_1(x) = S_1(x) \\
n = 2 \qquad & \frac{3}{5}\frac{d\psi_3(x)}{dx} + \frac{2}{5}\frac{d\psi_1(x)}{dx} + (\Sigma_t - \Sigma_{s2})\psi_2(x) = S_2(x) \\
n = N \qquad & \frac{N}{2N+1}\frac{d\psi_{N-1}(x)}{dx} + (\Sigma_t - \Sigma_{sN})\psi_N(x) = S_N(x)
\end{aligned}
$$

Boundary Conditions

- $N+1$ equations require $N+1$ BC's, in 1D, we need $\frac{N+1}{2}$ on each side
- We will look at the left hand side only

$$\psi(x_s,\mu) = \Gamma(\mu) \qquad \mu \geq 0$$

- There are two main types of approximation for the P_N methods: Marshak and Mark

Marshak

Express BC in integral sense such that

$$\int_0^1 f_n(\mu)\psi(x_s,\mu)d\mu = \int_0^1 f_n(\mu)\Gamma(\mu)d\mu$$

- Replace f_n by the odd Legendre moments
- Even moments are symetric about 0, only odd moments quantify neutron flow

$$\int_0^1 P_{2n-1}(\mu)\psi(x_s,\mu)d\mu = \int_0^1 P_{2n-1}(\mu)\Gamma(\mu)d\mu$$

Expand angular flux

$$\psi(x_s,\mu) = \sum_{m=0}^{M} \frac{2m+1}{4\pi}\psi_m(x_s)P_m(\mu)$$

Marshak

$$\sum_{m=0}^{M} \frac{2m+1}{4\pi} \psi_m(x_s) \int_0^1 P_{2n-1}(\mu) P_m(\mu) d\mu = \frac{\Gamma_n}{2\pi}$$

For $n = 1$ case, using orthogonality relation

$$\int_0^1 P_1(\mu)\psi(x_s,\mu)d\mu = \int_0^1 P_1(\mu)\Gamma(\mu)$$

$$2\pi \int_0^1 \mu\psi(x_s,\mu)d\mu = J^+(x_s) = \Gamma_1$$

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Mark

Use fixed angles μ_n

$$\psi(x_s, \mu_n) = \Gamma(\mu_n)$$

$$\sum_{m=0}^{N} \frac{2m+1}{4\pi} \psi_m(x_s) P_m(\mu_n) = \Gamma(\mu_n)$$

Choose μ_n such that we can integrate polynomials of order $N+1$ exactly, which is equivalent to finding μ_n such that

$$P_{N+1}(\mu_n) = 0 \qquad \mu > 0$$

P_N Notes

- Marshak BC are generally more accurate
- Even N in the P_N approximation leads to inconsistent BC
- Interface conditions are also inconsistent when N is even
- Other orthogonal functions can also be used, i.e. Chebyshev polynomials

Flux angular moments

$$\psi_m(x) = 2\pi \int_{-1}^{1} \psi(x,\mu) P_m(\mu) d\mu$$

For n=0, we have the scalar flux

$$\psi_0(x) = 2\pi \int_{-1}^{1} \psi(x,\mu) P_0(\mu) d\mu = \phi(x)$$

For n=1, we have the scalar current

$$\psi_1(x) = 2\pi \int_{-1}^{1} \psi(x,\mu) P_1(\mu) d\mu = J(x)$$

One group P_1 Approximation

Let $\psi_0 = \phi$ and $\psi_1 = J$, assume isotropic source

$$\frac{dJ(x)}{dx} + (\Sigma_t - \Sigma_{s0})\phi(x) = \nu\Sigma_f\phi(x) + S_0(x)$$

$$\frac{1}{3}\frac{d\phi(x)}{dx} + (\Sigma_t - \Sigma_{s1})J(x) = 0$$

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P_1 Approximation with Energy

Let $\psi_0 = \phi$ and $\psi_1 = J$, assume isotropic source

$$\frac{dJ(x,E)}{dx} + \Sigma_t(x,E)\phi(x,E) - \int_0^\infty \Sigma_{s0}(x,E' \rightarrow E)\phi(x,E')dE' =$$
$$\chi(E)\int_0^\infty \nu\Sigma_f(x,E')\phi(x,E')dE' + S_0(x,E)$$

$$\frac{1}{3}\frac{d\phi(x,E)}{dx} + \Sigma_t(x,E)J(x,E) - \int_0^\infty \Sigma_{s1}(x,E' \rightarrow E)J(x,E')dE' = 0$$

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Fick's Law

Using

$$J(x,E) = -D(x,E)\nabla\phi(x,E)$$

where

$$D(x,E) = \frac{1}{3\left(\Sigma_t(x,E) - \frac{\int_0^\infty \Sigma_{s1}(x,E'\to E)J(x,E')dE'}{J(x,E)}\right)} = \frac{1}{3\Sigma_{tr}(x,E)}$$

Out-Scatter Approximation

In a weakly absorbing media, the in-scatter rate will approximately balance the out-scatter rate.

$$\int_0^\infty \Sigma_{s1}(x, E' \to E) J(x, E') dE' \approx \int_0^\infty \Sigma_{s1}(x, E \to E') J(x, E) dE'$$

which allows us to write

$$\int_0^\infty \Sigma_{s1}(x, E \to E') J(x, E) dE' = \mu_0 \Sigma_s(x, E) J(x, E)$$

DO NOT USE FOR HYDROGEN-BASED SYSTEMS!

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Using

$$J(x,E) = -D(x,E)\nabla\phi(x,E)$$

where

$$D(x,E) = \frac{1}{3(\Sigma_t(x,E) - \mu_0\Sigma_s(x,E))} = \frac{1}{3\Sigma_{tr}(x,E)}$$

DO NOT USE FOR HYDROGEN-BASED SYSTEMS!

Outline

Diffusion Equation

$$
\begin{aligned}
-\nabla D(x,E)\nabla\phi(x,E) + \Sigma_t(x,E)\phi(x,E) = \\
\int_0^\infty \Sigma_{s0}(x,E' \to E)\phi(x,E')dE' + \\
\chi(E)\int_0^\infty \nu\Sigma_f(x,E')\phi(x,E') + S(x,E)
\end{aligned}
$$

Notes on Diffusion Equation

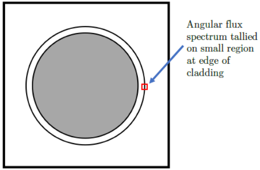
Main assumptions:

- Angular flux only has a linear angular component
- Neutron sources are isotropic (external sources and fission sources)
- Most events happen in a weakly absorbing media (balance of in-scatter and out-scatter rates)

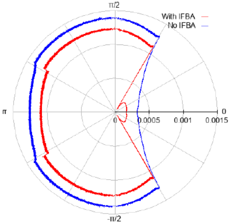
It breaks down:

- Near external boundaries of the system (vacuum BC)
- Abrupt changes in material properties
- Close to localized sources
- Close to strongly absorbing media (e.g. control rods)

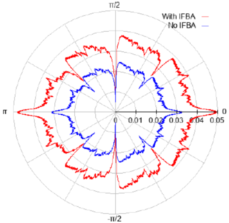
Angular Flux



(a) The sample location for generation.



(b) Thermal neutron energy group angular flux [cm^{-2}] spectrum (thermal group boundaries: 0 eV - 0.005 eV)



(c) Fast neutron energy group angular flux [cm^{-2}] spectrum (fast group boundaries: 6.0655 MeV - 10.0 MeV)

In Multigroup form

$$-\nabla D_g(x)\nabla\phi_g(x) + \Sigma_{t,g}(x)\phi_g(x) =$$

$$\sum_{g'=1}^{G} \Sigma_{s0,g'\to g}(x)\phi_{g'}(x)+$$

$$\chi_g \sum_{g'=1}^{G} \nu\Sigma_{f,g'}(x)\phi_{g'}(x) + S_g(x)$$

Group condensation

Group condensation is performed to preserve reaction rates

$$\Sigma_{t,g} = \frac{\int_0^\infty \Sigma_t(E)\phi(E)dE}{\int_0^\infty \phi(E)dE}$$

... but it cannot directly preserve leakage. Corrections are introduced to preserve both: SPH factors or discontinuity factors.

Things to note

- $\chi(E)$ is isotope dependent
- $\chi(E)$ is also incoming energy dependent, i.e. $\chi(E' \rightarrow E)$
- In the steady-state form, $\chi(E)$ must include both prompt and delayed components.
- Out-scatter approximation is not valid for reactors with lots of hydrogen.
- Diffusion coefficient should be theoretically collapsed with the current, but often approximated by a flux collapse.

Recap

- Scattering kernel can be represented by an orthogonal polynomial expansion
- Scattering kernels are commonly stored in terms of Legendre polynomials
- Angular flux and source can also be expressed in terms of Legendre polynomials
- This expresses all angular dependence from the set of equations as flux moments
- The linear approximation is also known as the Diffusion equation

References

- Duderstadt and Martin, Transport Theory
- Bell and Glasstone. Nuclear Reactor Theory
- Handbook of Nuclear Engineering - Chapter 5 (sections 2, 4 and 8)

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