Nuclear Reactions

Two types

1. Spontaneous *(decay)*

- α: ${}^A_Z X \rightarrow^{A-4}_{Z-2} X +^4_2 \alpha$
- β: ${}^A_Z X \rightarrow^{A}_{Z+1} X + \beta + \bar{\nu}$
- γ: $X^* \rightarrow X + \gamma$

Decay Equations

$t \rightarrow N(t)$
$t + dt \rightarrow N(t + dt)$

$dN(t) = N(t + dt) - N(t)$
$dN(t) = -\lambda N(t)dt$ where λ is the decay constant.

... working through, with B.C. $N(t = 0) = N_0$ ...

$$N(t) = N_0 e^{-\lambda t}$$

Mean Lifetime:

$\frac{dN(t)}{N_0} = \lambda e^{-\lambda t}dt = p_d(t)$ where $p_d(t)dt$ is the probability of decay in time dt

$$\bar{t} = \int_0^\infty tp(t)dt = \frac{1}{\lambda}$$

Half-Life:

$T_{1/2}$is defined as the time s.t. $N(T_{1/2}) = \frac{N_0}{2}$

$$T_{1/2} = \frac{ln2}{\lambda}$$

2. Induced *(projectile/target)*

This will be the emphasis of NE 250

Neutron-Nucleus

- elastic scattering
- inelastic scattering/compound nuclear reaction

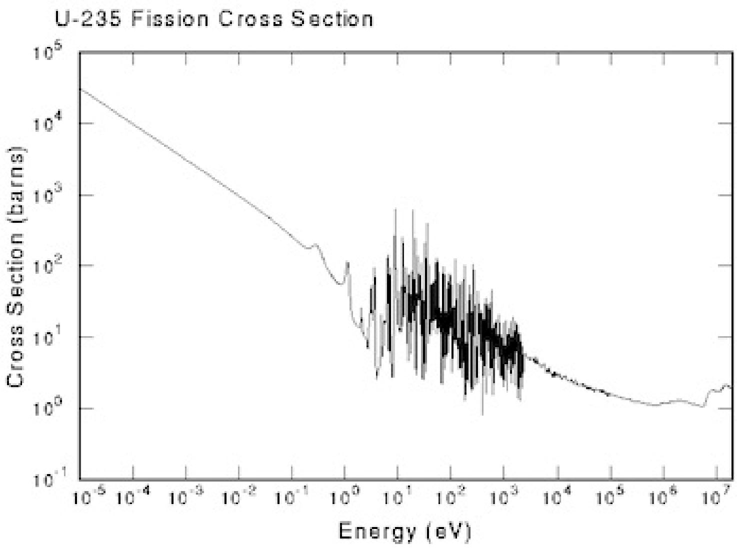
  $$n +^A_Z X \rightarrow^{A+1}_Z X^*$$

  (could result in production of a γ or α, emission of a n, or fission)

  Capture is a subset of absorption!
  Absorption: $(n, \alpha), (n, \gamma), (n, f)$
  Capture: (n, γ)

Cross Sections (σ)
- A property of the isotope and reaction
- A function of the isotope temperature (vibrational motion) and neutron speed (linear motion)
- Tabulated in XSec libraries **(3 common formats)**

- ENDF (USA)
- JEFF (Europe/NEA)
- JENDL (Japan)



- Resonances in X-Sec plots due to excited energy levels that can be reached; nuclei only all excitation to these levels, and so only neutrons with this energy amount will be absorbed
- Cross sections measured at 300K (room temp); calculated using

$$E = k_B T$$

  where k_B is Boltzmann's constant and $T = 300$ K $\Rightarrow E = 0.0253$ eV
- Higher temperatures cause resonant peak widths to broaden (less time spent near center of vibrational trajectory) $\rightarrow$ **Doppler Broadening**

Units

1 barn $= 10^{24}$ cm^2
1 eV $= 1.602 \times 10^{-19}$ J

Fission

Can be spontaneous or induced

$$n +^{235}\text{U} \rightarrow X + Y + \bar{\nu}n + E$$

$\bar{\nu}$ is the average number of neutrons produced in a given fission event.
$E_f \approx 200$ MeV (this is much higher than chemical reactions which are on the order of eV!)

Fissile Isotopes

$E_b > E_{\text{threshold}}$

These neutrons could (almost) be considered as "able to fission from 0 KE neutrons."

Includes ^{235}U, ^{233}U, ^{239}Pu, ^{241}Pu

Fissionable Isotopes

Fission requires collision with high E neutrons.

For ^{235}U this is empirically given by

$$\chi(E) = 0.453e^{-1.036E}\sinh(\sqrt{2.29E})$$

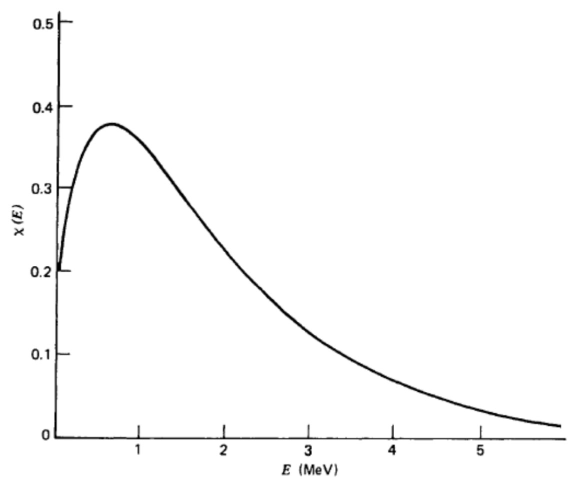


Figure 4: Fission spectrum for thermal neutron induced fission in ^{2}35U

Also, note that $\bar{\nu}$ depends on the isotope. Below is a plot of $\bar{\nu}$ for ^{239}Pu, ^{233}U and ^{235}U:

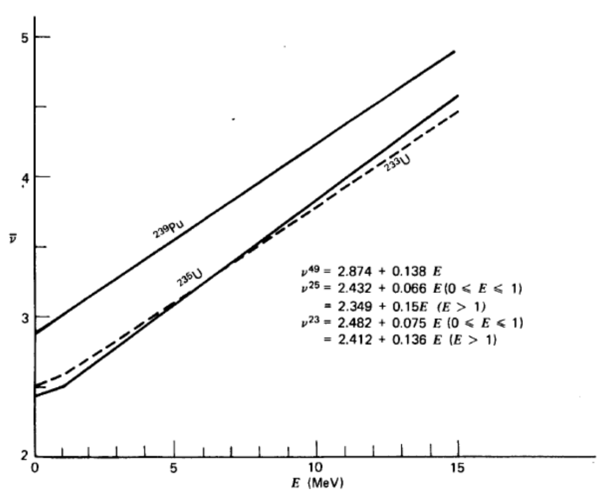


Figure 3: average # of neutrons released per fission as a function of energy

Fertile Isotopes

Isotopes which either undergo neutron capture (and subsequent decay) to become fissile isotopes.

Energy breakdown of fission outputs

- 180 MeV in the KE of fission products
- 5 MeV in the kinetic energy of neutrons
- 7 MeV in prompt γs
- 8 MeV in β^- decay of fission products
- 7 MeV in delayed γs
- 12 MeV in neutrinos

The energy from all outputs can be captured except for neutrinos.

Criticality

Multiplication Factor, k

$$k = \frac{\text{\# neutrons generated}}{\text{\# neutrons lost}}$$

\# neutrons generated = neutrons fission
\# neutrons lost = \# neutrons absorbed + \# neutrons leaked

- $k = 1$: the reaction is critical; the chain reaction is controlled (reactor)
- $k < 1$: the reactor is subcritcal; boring
- $k > 1$: the reaction is supercritical; this is a bomb

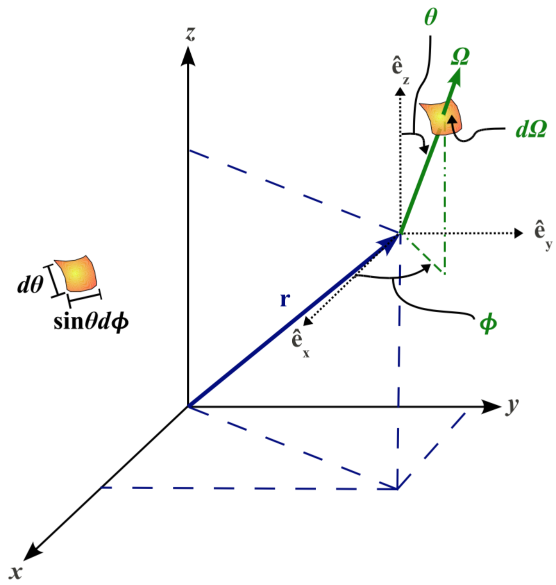
Derivation of the Neutron Transport Equation

Solving for the multiplication factor requires that we know:

1. n: neutron density [n/cm^3]
2. N: atom/nuclide density [nuclei/cm^3]
3. σ: microscopic cross section [cm^2]

Reaction rate: $R = nN\sigma$
Macroscopic cross section [1/**cm**]**:** $\Sigma = N\sigma$
Angular neutron density [$\frac{n}{\mathbf{cm}^3 \cdot \mathbf{sr}}$]**:** $n(\vec{r}, E, \hat{\Omega}, t)$

$\vec{v} = v\,\hat{\Omega}$, $|\hat{\Omega}| = 1$ (describes a sphere, formed by θ and ϕ)
$dr^3 = dx\;dy\;dz$
dE
$d\hat{\Omega} = \sin\theta\;d\theta\;d\phi$; $d\hat{\Omega}$ is a scalar, about the original position defined by vector $\hat{\Omega}$.



Altogether, $n(\vec{r}, E, \hat{\Omega}, t)\ d^3r\ dE\ d\hat{\Omega}$, gives the # of neutrons in the small volume about $\vec{r}$ with energy E, and moving in direction $d\hat{\Omega}$ about $\hat{\Omega}$ at time t.

Angular neutron flux (scalar): $\phi(\vec{r}, E, \hat{\Omega}, t) = v\ n(\vec{r}, E, \hat{\Omega}, t)$
Angular neturon current (vector): $\vec{J}(\vec{r}, E, \hat{\Omega}, t) = \hat{\Omega}\ \phi(\vec{r}, E, \hat{\Omega}, t)$

We can find the number of neutrons in a volume V using

$$\int_V n(\vec{r}, E, \hat{\Omega}, t)\ d^3r$$

Change with time is then

$$\frac{\partial}{\partial t}\left[\int_V n(\vec{r}, E, \hat{\Omega}, t)\ d^3r\right] dE\ d\hat{\Omega} = \text{ \# neutrons gained - \# neutrons lost}$$

neutrons gained: source (fission), in-scattering $(E', \hat{\Omega}' \to E, \hat{\Omega})$
neutrons lost: absorption, scattering $(E, \hat{\Omega} \to E', \hat{\Omega}')$

We also add a streaming term, to quantify neutrons leaking out (and in) to the system.

The chance of a collision in the system is given by

$$\left[\int_V \Sigma_{\text{tot}}(\vec{r}, E) v n(\vec{r}, E, \hat{\Omega}, t)\ d^3r\right] dE\ d\hat{\Omega}$$

The chance of fission in system...

(See paper notes...)

The Transport Equation

$$\frac{1}{v}\frac{\partial\psi}{\partial t} + \hat{\Omega}\cdot\nabla\psi + \Sigma_t\psi = \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\Sigma_s(E',\hat{\Omega}' \to E,\hat{\Omega})\psi(E',\hat{\Omega}') + \frac{\chi(E)}{4\pi}\int_0^\infty dE'\nu(E')\Sigma_f(E')\int_{4\pi} d\hat{\Omega}'\phi(\vec{r},E',\hat{\Omega}',t) + s(\vec{r},E,\hat{\Omega},t)$$

Initial condition: $\psi(\vec{r},E,\hat{\Omega},0) = \psi_0(\vec{r},E,\hat{\Omega})$

Interface condition: angular flux must be continuous at all points

Other conditions

Fixed condition: incoming flux is specified $\psi(\vec{r}_s,E,\hat{\Omega},t) = \psi_{\text{in}}(\vec{r},E,\hat{\Omega},t)$
(Vacuum or black if $\psi_{\text{in}}(\vec{r},E,\hat{\Omega},t) = 0$)
Reflective conditions: mirror symmetry at some surface, $\psi(\hat{\Omega}_{\text{in}},t) = \psi(\hat{\Omega}_{\text{out}},t)$
Periodic conditions: $\psi(\vec{r}_s) = \psi(\vec{r}_s + \vec{p})$
Finiteness conditions: (can't have infinite flux) $0 \leq \psi(\vec{r},E,\hat{\Omega},t) < \infty$
Source condition: localized (pt.) sources introduce mathemetaical singularities
$S(\vec{r},E,\hat{\Omega},t) = \lim_{\vec{r}\to\vec{r_0}} \int dS\ \hat{e}\cdot\hat{\Omega}$

Approximations to the Transport Equation

One-speed Transport Equation

Assume all particles are the same speed: $\vec{v} = v_0 \cdot \hat{\Omega}$

The equation becomes

$$\frac{1}{v}\frac{\partial\psi(\vec{r},\hat{\Omega},t)}{\partial t} + \hat{\Omega}\nabla\psi(\vec{r},\hat{\Omega},t) + \Sigma_t\psi(\vec{r},\hat{\Omega},t) = \int_{4\pi} d\hat{\Omega}'\Sigma_s(\hat{\Omega}'\to\hat{\Omega})\psi(\vec{r},\hat{\Omega}',t) + \frac{\nu\Sigma_f}{4\pi}\int_{4\pi} d\hat{\Omega}'\psi(\vec{r},\hat{\Omega}',t) + S(\vec{r},\hat{\Omega},t)$$

One-dimensional

$\vec{r} = (x,y,z)$
$d\hat{\Omega} = sin\theta\ d\theta\ d\varphi = d\mu\ d\varphi$, where $\mu = cos\theta$

$$\frac{1}{v}\frac{\partial\psi(x,\hat{\Omega},t)}{\partial t} + \Omega_x\frac{\partial}{\partial x}\psi(x,\hat{\Omega},t) + \Sigma_t(x)\psi(x,\hat{\Omega},t) = \int_{4\pi} d\hat{\Omega}'\Sigma_s(\hat{\Omega}'\to\hat{\Omega})\psi(x,\hat{\Omega}',t) + \frac{v\Sigma_f}{4\pi}\int_{4\pi} d\hat{\Omega}'\psi(x,\hat{\Omega}',t) + S(x,\hat{\Omega},t)$$

The Diffusion Equation

Usually the scalar flux is all that is needed to get a fairly accurate picture of our system. Reaction rates usually only depend on the neutron flux, not the direction of neutron motion.

Assume that the angular flux depends only weakly on direction.

Recall:

$\phi(\vec{r},t) = \int_{4\pi} d\hat{\Omega}\psi(\vec{r},\hat{\Omega},t)$
$\vec{J}(\vec{r},t) = \int_{4\pi} d\hat{\Omega}\ \hat{\Omega}\ \psi(\vec{r},\hat{\Omega},t)$

The Neutron Continuity Equation

"The Zeroth Moment of the Transport Equation":
Integrate transport equation over all angles

$$\int_{4\pi} d\hat{\Omega} \left[\underbrace{\frac{1}{v}\frac{\partial \psi(\vec{r},\hat{\Omega},t)}{\partial t}}_{1} + \underbrace{\hat{\Omega}\cdot\nabla\psi(\vec{r},\hat{\Omega},t)}_{6} + \underbrace{\Sigma_t\psi(\vec{r},\hat{\Omega},t)}_{2} \right] = \int_{4\pi} d\hat{\Omega} \left[\underbrace{\int_{4\pi} d\hat{\Omega}'\, \Sigma_s(\hat{\Omega}'\to\hat{\Omega})\psi(\vec{r},\hat{\Omega},t)}_{5} \right.$$
$$\left. + \underbrace{\frac{\nu\Sigma_f}{4\pi}\int_{4\pi} d\hat{\Omega}'\, \psi(\vec{r},\hat{\Omega}',t)}_{3} + \underbrace{s(\vec{r},\hat{\Omega},t)}_{4} \right]$$

1. **Time:** No approximations in time
$$\frac{1}{v}\frac{\partial}{\partial t}\int_{4\pi} d\hat{\Omega}\ \psi(\vec{r},\hat{\Omega},t) = \frac{1}{v}\frac{\partial}{\partial t}\phi(\vec{r},t)$$
2. **Absorption:** No approximations in absorption
$$\Sigma_t \int_{4\pi} d\hat{\Omega}\ \psi(\vec{r},\hat{\Omega},t) = \Sigma_t\ \phi(\vec{r},t)$$
3. **Fission:** No approximations in fission
$$\int_{4\pi} d\hat{\Omega} = \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\varphi = 4\pi$$
$$\int_{4\pi} d\hat{\Omega}\frac{\nu\Sigma_f}{4\pi}\int_{4\pi} d\hat{\Omega}'\psi(\vec{r},\hat{\Omega}',t) = \nu\Sigma_f\phi(\vec{r},t)$$
4. **Source:** No approximations in source
$$\int_{4\pi} d\hat{\Omega}\ s(\vec{r},\hat{\Omega},t) \equiv S(\vec{r},t)$$
5. **Scattering:** For scattering, interchange the order of integration
$$\int_{4\pi} d\hat{\Omega}\int_{4\pi} d\hat{\Omega}'\ \Sigma_s(\hat{\Omega}'\to\hat{\Omega})\ \psi(\vec{r},\hat{\Omega}',t) = \int_{4\pi} d\hat{\Omega}'\int_{4\pi} d\hat{\Omega}\ \Sigma_s(\hat{\Omega}'\to\hat{\Omega})\ \psi(\vec{r},\hat{\Omega}',t)$$
   Now we assume that scattering is azimuthally symmetric (scattering depends only on cosine). The particle is as likely to scatter at angle θ in any direction off $\hat{\Omega}$.
$$\int_{4\pi} d\hat{\Omega}\ \Sigma_s(\hat{\Omega}'\cdot\hat{\Omega}) = 2\pi\int_{-1}^{1} d\mu\ \Sigma_s(\mu) = \Sigma_s$$
   Then, if we substitute this in above
$$\Sigma_s\int_{4\pi} d\hat{\Omega}'\ \psi(\vec{r},\hat{\Omega}',t) = \Sigma_s\phi(\vec{r},t)$$
6. **Streaming:** To adjust streaming, we first manipulate the order
$$\int_{4\pi} d\hat{\Omega}\ \hat{\Omega}\cdot\nabla\ \psi(\vec{r},\hat{\Omega},t) = \nabla\cdot\int_{4\pi} d\hat{\Omega}\ \hat{\Omega}\ \psi(\vec{r},\hat{\Omega},t) = \nabla\cdot\vec{J}(\vec{r},t)$$

Put all the above integrations together to get the **neutron continuity equation (NCE)**. Notice that we have three equations (each $\vec{r}$ has x, y, z components) and 4 unknown quantities.

$$\frac{1}{v}\frac{\partial\phi(\vec{r},t)}{\partial t} + \nabla\cdot\vec{J}(\vec{r},t) + \Sigma_t\phi(\vec{r},t) = \Sigma_s\phi(\vec{r},t) + \nu\Sigma_f\phi(\vec{r},t) + S(\vec{r},t)$$

First angular moment

Multiply the TE by $\hat{\Omega}$ and integrate. We will drop the fission term (technically we will assume it is part of the source), though the procedure is nearly the same when it is included.

Note:

$\int_{4\pi} d\hat{\Omega}\, \hat{\Omega} = 0$

$\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\hat{\Omega} = \frac{4\pi}{3}\bar{\bar{I}},$ $\qquad \bar{\bar{I}}$ is the identity tensor:

$$\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}_i\hat{\Omega}_j = \begin{cases} 0, & i \neq j \\ \frac{4\pi}{3}, & i = j \end{cases}$$

$\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\hat{\Omega}\hat{\Omega} = 0$

When multiplied out, we have

$$\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}[\text{TE}]$$

$$\underbrace{\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\frac{1}{v}\frac{\partial\psi(\vec{r},\hat{\Omega},t)}{\partial t}}_{1} + \underbrace{\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\hat{\Omega}\nabla\psi(\vec{r},\hat{\Omega},t)}_{5} + \underbrace{\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\Sigma_t\psi(\vec{r},\hat{\Omega},t)}_{2}$$
$$= \underbrace{\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\int_{4\pi} d\hat{\Omega}' Xs_s(\hat{\Omega}' \to \hat{\Omega})\psi(\vec{r},\hat{\Omega}',t)}_{4} + \underbrace{\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\frac{\nu\Sigma_f}{4\pi}\int_{4\pi} d\hat{\Omega}'\psi(\vec{r},\hat{\Omega}',t) + \int_{4\pi} d\hat{\Omega}\, \hat{\Omega}S(\vec{r},\hat{\Omega},t)}_{3}$$

Like we did to derive the continuity equation, we can break down each term.

1. **Time:**
$$\frac{1}{v}\frac{\partial}{\partial t}\int_{4\pi} d\hat{\Omega}'\, \hat{\Omega}\psi(\vec{r},\hat{\Omega},t) = \frac{1}{v}\frac{\partial\vec{J}}{\partial t}$$

2. **Absorption:**
$$\Sigma_t\int_{4\pi} d\hat{\Omega}\hat{\Omega}\psi(\vec{r},\hat{\Omega},t) = \Sigma_t\vec{J}(\vec{r},t)$$

3. **Source (fission now absent):**
$$\int_{4\pi} d\hat{\Omega}\, \hat{\Omega}S(\vec{r},\hat{\Omega},t) \equiv S(\vec{r},t)$$

4. **Scattering:** Expand scattering cross section in Legendre Polynomials (a sequence of orthogonal polynomials)
$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[(x^2-1)^n\right]$$

   Expand $\Sigma_s(\hat{\Omega}' \cdot \hat{\Omega})$ in Legendre polynomials
$$\Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) = \sum_0^{\infty}\frac{2\ell+1}{4\pi}\Sigma_{s\ell}P_\ell(\hat{\Omega}')P_\ell(\hat{\Omega})$$

   - $\ell = 0$ is isotropic
     $P_0(\hat{\Omega}) = 1 \quad \Rightarrow \quad \Sigma_s(\hat{\Omega}',\hat{\Omega}) \approx \frac{1}{4\pi}\Sigma_{s0}$
   - $\ell = 1$ is linearly anisotropic
     $P_1(\hat{\Omega}) = \hat{\Omega} \quad \Rightarrow \quad \Sigma_s(\hat{\Omega}',\hat{\Omega}) \approx \frac{1}{4\pi}(\Sigma_{s0} + 3\hat{\Omega}' \cdot \hat{\Omega}\Sigma_{s1})$

     Assume scattering is at most linearly anisotropic (if its not, there's some "weird" stuff going on")

Substitute the linearly anistropic approximation into the expression for streaming. We note the prevously defined identities and defintion of neutron current:

$$\frac{1}{4\pi}\int_{4\pi} d\hat{\Omega}\hat{\Omega}\int_{4\pi} d\hat{\Omega}(\Sigma_{s0}+3\hat{\Omega}'\cdot\hat{\Omega}\Sigma_{s1})\,\psi(\vec{r},\hat{\Omega},t) = \frac{1}{4\pi}\underbrace{\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}}_{0}\int_{4\pi}\hat{\Omega}'\Sigma_s\,\psi(\vec{r},\hat{\Omega}',t) + \frac{1}{4\pi}\underbrace{\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}}_{4\pi/3\bar{\bar{I}}}\underbrace{\int_{4\pi} d\hat{\Omega}'\,\hat{\Omega}'3\Sigma_{s1}\,\psi(\vec{r},\hat{\Omega}',t)}_{3\Sigma_{s1}\vec{J}(\vec{r},t)}$$

Substituting those identities and simplifying, we get

$$\left(\frac{1}{4\pi}\right)\left(\frac{4\pi}{3\bar{\bar{I}}}\right)\left(3\Sigma_{s1}\vec{J}(\vec{r},t)\right) = \Sigma_{s1}\,J(\vec{r},t)$$

5. **Streaming:**

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\hat{\Omega}\cdot\nabla\psi(\vec{r},\hat{\Omega},t) = \nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\,\hat{\Omega}\,\psi(\vec{r},\hat{\Omega},t)$$

Putting each of these 5 components back together the **current continuity equation (CCE)** is

$$\frac{1}{v}\frac{\partial\vec{J}}{\partial t} + \nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\,\psi(\vec{r},\hat{\Omega},t) + \Sigma_t\vec{J}(\vec{r},t) = \Sigma_{s1}\vec{J}(\vec{r},t) + S_1(\vec{r},t)$$

Now we have 2 moment equations (zeroth and first) so a total of 4 equations (neutron continuity and 3 tensor equations). There are now 10 unknowns: ϕ (1), $\vec{J}$ (3), and the new tensor term (6). There is little point to continuing with this technique any longer.

Angular Flux Approximation

Assume now that the flux is at most linearly anisotropic (for the current continuity equation we assumed that *scattering* was linearly anisotropic).

$$\psi(\hat{\Omega}) \approx \frac{1}{4\pi}\left(\psi_0 + 3\hat{\Omega}\cdot\vec{\psi}_1\right)$$

Substitute expansion into the streaming term of the current continuity equation.

$$\nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\,\psi(\vec{r},\hat{\Omega},t) = \nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\,\frac{1}{4\pi}\left(\psi_0 + 3\hat{\Omega}\cdot\vec{\psi}_1\right)$$

$$\nabla\cdot\frac{1}{4\pi}\int d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\left(\psi_0 + 3\hat{\Omega}\vec{\psi}_1\right) = \nabla\cdot\frac{1}{4\pi}\left[\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\,\psi_0 + 3\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\hat{\Omega}\,\vec{\psi}_1\right]$$

Using the same identities as before, we have

$$\nabla\cdot\frac{1}{4\pi}\int d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\left(\psi_0 + 3\hat{\Omega}\vec{\psi}_1\right) = \nabla\cdot\frac{1}{4\pi}\frac{4\pi}{3}\bar{\bar{I}}\,\phi(\vec{r},t)$$

(Note, that this assumes $\psi_0 = \phi \leftarrow$ figure out where this comes from) and

$$\nabla\cdot\frac{1}{4\pi}\int d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\left(\psi_0 + 3\hat{\Omega}\vec{\psi}_1\right) = \frac{1}{3}\nabla\phi(\vec{r},t)$$

Now the current continuity equation is

$$\frac{1}{v}\frac{\partial\vec{J}}{\partial t} + \frac{1}{3}\nabla\phi(\vec{r},t) + \Sigma_t\vec{J}(\vec{r},t) = \Sigma_{s1}\vec{J}(\vec{r},t) + S_1(\vec{r},t)$$

Define absorption and transport cross sections:
$\Sigma_a \equiv \Sigma_t - \Sigma_{s0}$
$\Sigma_{tr} \equiv \Sigma_t - \Sigma_{s1}$

Using these cross sections we can reform both the neutron and current continuity equations.

NCE:

$$\frac{1}{v}\frac{\partial \phi(\vec{r},t)}{\partial t} + \nabla \cdot \vec{J}(\vec{r},t) + \Sigma_a \phi(\vec{r},t) = S(\vec{r},t)$$

CCE:

$$\frac{1}{v}\frac{\partial \vec{J}}{\partial t} + \frac{1}{3}\nabla \phi(\vec{r},t) + \Sigma_{tr}\vec{J}(\vec{r},t) = S_1(\vec{r},t)$$

Fick's Law

With the following conditions

- Steady state ($\frac{\partial}{\partial t}(X) = 0$)
- Isotropic source ($S_1 = 0$)

The current continuity equation becomes

$$\frac{1}{3}\nabla \phi(\vec{r}) + \Sigma_{tr}\vec{J}(\vec{r}) = 0$$

which we can solve for $\vec{J}$:

$$\vec{J}(\vec{r}) = -\frac{1}{3\Sigma_{tr}}\nabla \phi(\vec{r}).$$

If we let $D = \frac{1}{3\Sigma_{tr}} = \frac{1}{3(\Sigma_t - \Sigma_{s1})}$ be the diffusion coefficient, then this simplifies further to

$$\vec{J}(\vec{r}) = -D\nabla \phi(\vec{r})$$

Recall:
$\Sigma_{s1} = \int d\hat{\Omega}\, \hat{\Omega}\Sigma_s$
Include azimuthally symmetric assumptions and $\Sigma_{s1} = \bar{\mu}_0 \Sigma_s$, where $\bar{\mu}_0$ = average scattering cosine = $\frac{2}{3A}$, where A is the atomic mass number.

Then $\Sigma_{tr} = \Sigma_t - \bar{\mu}_0 \Sigma_s$.

From this implementation of Fick's law, we can write the diffusion equation as only a function of ϕ:

$$\frac{1}{v}\frac{\partial}{\partial t}\phi(\vec{r},t) - \nabla \cdot D\nabla \phi(\vec{r},t) + \Sigma_a \phi(\vec{r},t) = \nu\Sigma_f \phi(\vec{r},t) + S(\vec{r},t)$$

Due to our assumptions, however, the diffusion equation is not valid at

1. Boundaries/interfaces
2. Sources
3. Strong absorbers
4. Voids

The angular flux expansion can then be written as

$$\psi(\vec{r},\hat{\Omega},t) \approx \frac{1}{4\pi}\left(\phi(\vec{r},t) - \frac{1}{\Sigma_{tr}}\nabla \phi(\vec{r},t)\right)$$

At equilibrium, $\vec{J} = 0$ (net migration is opposed to gradient, hence negative into Fick's Law)

Mean Free Path: the median distance from the last collision
$\lambda_t = \frac{1}{\Sigma_t}$ or $\lambda_{tr} = \frac{1}{\Sigma_{tr}}$

If scattering is

- isotropic $\rightarrow \bar{\mu}_0 = 0, \lambda_t = \lambda_{tr}$
- forward peaked $\rightarrow \bar{\mu}_0 > 0, \lambda_t > \lambda_{tr}$

Initial Conditions:

$\phi(\vec{r}, 0) = \phi(\vec{r})\ \forall \vec{r} \in V$

Basic requirements:
- real and nongegative ($\phi \geq 0$)
- bounded ($\phi > \infty$)

Interface conditions:

-Zeroth and first moments must be continuous
$\phi_1(\vec{r}, t) = \phi_2(\vec{r}, t)$
$\vec{J}_1(\vec{r}, t) = \vec{J}_2(\vec{r}, t)$

Vacuum BCs:

In the DE use partial current
$J_-(\vec{r}, t) = \int_{2\pi^-} d\hat{\Omega}\hat{\Omega} \cdot \hat{e}_s \psi(\vec{r}, \hat{\Omega}, t) = 0$
$J_+(\vec{r}, t) = \int_{2\pi^+} d\hat{\Omega}\hat{\Omega} \cdot \hat{e}_s \psi(\vec{r}, \hat{\Omega}, t) = 0$

$J_\mp = \int_{2\pi^-} d\hat{\Omega}\hat{\Omega}\hat{e}_s \left(\frac{1}{4\pi}\left(\phi \pm \frac{1}{\Sigma_{tr}}\nabla\phi\right)\right) \approx \frac{1}{4}\phi \pm \frac{D}{2}\hat{e}_s \cdot \nabla\phi = 0$

In 1D problems $J_-(\vec{r}_s, t) = J_-(x_s, t) = \frac{1}{4}\phi(x_s, t) + \frac{D}{2}\frac{d\phi}{dx}|_{x_s} = 0$

The extrapolation distance, where $\phi = 0$ is

$$\tilde{x}_s = x_s + 2D = x_s + \frac{2}{3}\lambda_{tr}$$

and so replace $J_-(x_s) = 0$ with $\phi(\tilde{x}_s) = 0$.

Helmholtz Form of the Diffusion Equation

$$\nabla^2\phi - \frac{1}{L^2}\phi = \frac{-Q}{D}$$

where $L \equiv \sqrt{\frac{D}{\Sigma_a}}$

The solution to this equation is $\phi = \phi_H(\vec{r}) + \phi_P(\vec{r})$, where the homogeneous solution is $\phi_H = Ae^{\frac{-|\vec{r}|}{L}} + Be^{\frac{|\vec{r}|}{L}}$

Criticality

For the equation

$$\nabla \cdot D\nabla\phi + \Sigma_a\phi = \nu\Sigma_f\phi, \quad \phi(\pm\tilde{x}_s) = 0.$$

There is no general solution unless we get it exactly right.

Introduce k. For any k, there is always a solution. We use an iterative porcess to find k. You might consider k as tuning the neutrons produced per fission.

$$\nabla \cdot D\nabla\phi + \Sigma_a\phi = \frac{1}{k}\nu\Sigma_f\phi$$

This causes our problem to become an eigenvalue problem. At long times, the non-negative largest, real eigenvalue is the dominant mode (eigenvalue k; eigenvector ϕ).

Prompt and Delayed Neutrons

Fission produces

- Prompt n's (within 10^{-10} s of fission)
- Fission Products (FPs)

Delayed neutrons come from the decay of FPs. For example ^{87}Br has a half-life of 55.9 s.

Use $T_{1/2}$ to bin delayed neutrons into either 6 or 8 groups (generally). Define the group index as j.

Decay constant of group j: λ_j^d
Delayed neutron fraction: β_j
Reactivity: $\rho = \frac{k-1}{k}$
$0 < \rho < \beta$: delayed supercritcal
$\rho = 0$: critical
$\rho > \beta$: prompt supercritical
$\rho = \beta$: 1$

The total delayed neutron faction (β) from thermal fission in ^{235}U is 0.0065, and the average neutron lifetime is 0.1 s.

Critical: Prompt + Delayed holds criticality
Prompt Critical: Critcal only on prompt n's
Prompt Supercritical: $k > 1$ from only prompt n's

Thought experiment:

$\ell =$ mean n generation time
$n(t+\ell) = n(t) + \ell\frac{dn}{dt} = kn(t)$

We can solve for the rate of neutron change

$$\frac{dn}{dt} = \left(\frac{k-1}{\ell}\right) n(t),$$

and then solve the differential equation

$$n(t) = n_0 e^{\frac{(k-1)t}{\ell}}$$

The reactor period is given by $T \equiv \frac{\ell}{k-1}$.

If a reactor has $k = 1.005$, at $t = 1$ s, what is the ration of $n(t)$ to n_0 for
a.) $\ell = 0.1s$
$n(1s)/n_0 = e^{(1.0005-1)(1s)/0.1s}$
$\boxed{n(1s)/n_0 = 1.005}$
b.) $\ell = 1 \times 10^{-4}$s
$n(1s)/n_0 = e^{(1.0005-1)(1\text{ s})/(1\times 10^{-4})\text{ s}}$
$\boxed{n(1s)/n_0 = 148.4}$

Diffusion Equation and the P_N equations

We assumed that the angular flux is linearly anisotropic (P_1 expansion), and it is valid away from boundaries, sources, sinks, and voids. Other assumptions included

- one speed
- isotropic source
- azimuthally symmetric, linearly anisotropic scattering
- n current changes slowly compared to the mean coillision time ($\frac{1}{|\vec{J}(\vec{r},t)|}\frac{\partial \vec{J}}{\partial t} \ll v\Sigma_t$)

Fick's Law and the 1-speed Diffusion Equation gave us

$$\frac{1}{v}\frac{\partial \phi}{\partial t} = S(\vec{r},t) - \Sigma_a(\vec{r})\phi(\vec{r},t) + \nabla \cdot D(\vec{r})\nabla\phi(\vec{r},t)$$

Start by looking at the energy dependent P_1 equations (NCE,CCE but with energy dependence)

$$\frac{1}{v}\frac{\partial \phi}{\partial t} = S(\vec{r},E,t) + \int_0^\infty dE'\Sigma_s(\vec{r},E' \to E)\phi(\vec{r},E',t) - \Sigma_t(\vec{r},E)\phi(\vec{r},E,t) - \nabla \cdot \vec{J}(\vec{r},E,t)$$

and

$$\frac{1}{v}\frac{\partial \vec{J}}{\partial t} = S_1(\vec{r},E,t) + \int_0^\infty dE'\bar{\mu}_0\Sigma_{s1}(\vec{r},E' \to E)\vec{J}(\vec{r},E',t) - \Sigma_t(\vec{r},E)\vec{J}(\vec{r},E,t) - \frac{1}{3}\nabla \cdot \phi(\vec{r},E,t)$$

We apply asusmptions

1. Slow current change $\left(\frac{1}{|\vec{J}(\vec{r},t)|}\frac{\partial \vec{J}(\vec{r},t)}{\partial t} \ll v\Sigma_t \;\therefore\; \frac{1}{v}\frac{\partial \vec{J}(\vec{r},t)}{\partial t} = 0\right)$
2. Isotropic source, $S_1(\vec{r},E,t) = 0$
3. Isotropic scattering, $\Sigma_{s1}(E' \to E) = 0$

Condition #3 is usually too strong, so we introduce a different diffusion coefficient.

$$D(\vec{r},E) = \frac{1}{3}\left[\Sigma_t(\vec{r},E) - \frac{\int_0^\infty \Sigma_{s1}(\vec{r},E' \to E)J_i}{J_i(\vec{r},E,t)}\right]^{-1}$$

where J_i denotes the current in $i = x, y, z$. This gives

...

This isn't great, so we neglect anisotropic contribution to energy transfer in scattering.
..

$$\int_0^\infty dE'\Sigma_{s1}(\vec{r},E)\delta(E' \to E)J_i(\vec{r},E,t) = \bar{\mu_0}\Sigma_s(\vec{r},E)J_i(\vec{r},E,t)$$

..

which, when plugged into the neutron continuity equation gives

$$\frac{1}{v}\frac{\partial \phi}{\partial t} = S(\vec{r},E,t) + \int_0^\infty dE'\Sigma_s(\vec{r},E' \to E)\phi(\vec{r},E,t) - \Sigma_t(\vec{r},E)\phi(\vec{r},E,t) + \nabla \cdot D(\vec{r},E)\nabla\phi(\vec{r},E,t)$$

↑ check that

Before, we had just 1 speed. Now we have 1 group (a set of different speeds in 1 bin). To get get the group, we integrate the equation over energy, and we weight based on the flux.

*Note this requires we solve for the flux, based on the flux. We often make estimations of the flux shape.

The group constants:
The effective group cross section, $\Sigma_{t,1}(\vec{r}) = \frac{\int_0^\infty dE\Sigma_t(\vec{r},E)\phi(\vec{r},E,t)}{\int_0^\infty dE\phi(\vec{r},E,t)}$ $\phi_1(\vec{r},t) = \int_0^\infty dE\phi(\vec{r},E,t)$
...

Integrate the source: $\int_0^\infty dES(\vec{r},E,t) = S(\vec{r},t)$

$\int_0^\infty dE \int_0^\infty dE'\Sigma_s(\vec{r},E' \to E)\phi(\vec{r},E',t) = \int_0^\infty dE'\Sigma()\phi(\vec{r},E',t) = \Sigma_{s,1}\phi_1$

...

The one group diffusion equation is then

$$\frac{1}{v}\frac{\partial\phi_1}{\partial t} = S_1(\vec{r},t) - \Sigma_a(\vec{r})\phi_1(\vec{r},t) + \nabla \cdot D_1(\vec{r})\nabla\phi_1(\vec{r},t)$$

P_n equations

Discrete Ordinates

Generally, $\hat{\Omega}$ is continuous in 4π. Since computation requires discrete values, we can treat the continous distribution as $\{\hat{\Omega}_1, \hat{\Omega}_2, .., \hat{\Omega}_n\}$. This leads to ray effects, however.

Legendre Polynomials:

$$P$$

...

When S_0 is at x,

$$-D\frac{d\phi}{dx}\bigg|_{+\epsilon} + D\frac{d\phi}{dx}\bigg|_{-\epsilon} = J_x(0^+) - J_x(0^-) = S_0$$

Now we look at boundary conditions:

(1) $x < 0$, the left half
$\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi(X) = 0$
$\lim_{x\to 0^+} \vec{J}(x) = \frac{S_0}{2}$

$\lim_{x\to 0^-\infty} |\phi(x)| < \infty$
$\phi(x) \geq 0$

(2) $x > 0$, the right half
$\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi(X) = 0$
$\lim_{x\to 0^-} \vec{J}(x) = -\frac{S_0}{2}$

$\lim_{x\to 0^+\infty} |\phi(x)| < \infty$
$\phi(x) \geq 0$

The generic solution is

$$\phi(x) = C_1 e^{-x/L} + C_2 e^{x/L}$$

Due to the finiteness condition, $C = 0$.
Then ...

Plane source in a vacuum

We have an infinite plane source in a slab of thickness a, surrounded by vacuum.

(1) $x > 0$

$\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi(X) = 0$
$\lim_{x\to 0^+} \vec{J}(x) = \frac{S_0}{2}$
$\phi(\frac{\tilde{a}}{2}) = 0$

(2) $x < 0$

$\frac{d^2\phi}{dx^2} - \frac{1}{L^2}\phi(X) = 0$
$\lim_{x\to 0^-} \vec{J}(x) = -\frac{S_0}{2}$
$\phi(-\frac{\tilde{a}}{2}) = 0$

Again, $\phi(X) = C_1 e^{-|x|/L} + C_2 e^{|x|/L}$.

If instead we had a uniformly distributed source, the diffusion equation would be

$$\frac{d^2\phi(x)}{dx^2} - \frac{1}{L^2}\phi(x) = \frac{S_0}{D}$$

Our boundary conditions would then be...

Now consider the uniform source in a reflector. For that reflector, assume $Xs_s \approx \Sigma_t$ and $\Sigma_s > \Sigma_a$.

The diffusion equation then can be written as

$$\frac{d^2\phi(x)_f}{dx^2} - \frac{1}{L_f^2}\phi(x) = \frac{S_0}{D_f}$$

Boundary conditions are:

$\phi_f(-\frac{a}{2}) = \phi_r(-\frac{a}{2})$, or
$\phi_f(\frac{a}{2}) = \phi_r(\frac{a}{2})$

$\vec{J}_f(-\frac{a}{2}) = \vec{J}_r(-\frac{a}{2}), or$
$\vec{J}_f(\frac{a}{2}) = \vec{J}_r(\frac{a}{2})$

... (finiteness)...

$$\frac{d^2\phi(x)_r}{dx^2} - \frac{1}{L_r^2}\phi(x) = 0$$

For more complicated functions,

$$D\nabla^2\phi(\vec{r}) - \Sigma_a\phi(\vec{r}) = -S(\vec{r}).$$

Reexpress this as

$$M\phi(\vec{r}) = f(\vec{r}),$$

where M is a differential operator of order n, and

$$M = a_0\phi^{(n)} + a_1\phi^{(n-1)} + ... + a_n\phi = f(\vec{r})$$

We've been using $M = \frac{d^2}{dx^2} - \frac{1}{L_r^2}$, where $a_0 = 1$, $a_1 = 0$, and $a_2 = \frac{-1}{L}$.

If we use variation of parameters,
$M\phi_{\text{homogeneous}} = 0$
$M\phi_{\text{particular}} = f(\vec{r})$
$\phi = \phi_{\text{homogeneous}} + \phi_{\text{particular}}$

Reactor Overview

BWRs

-cans surround assemblies; prevent boiling water from evacuating central channels
-control rods inserted from bottom; more water $\Rightarrow$ better moderation $\Rightarrow$ more neutronic control

TRISO Fuel

-directly placed in reactor (like gumball machine... pebbles move up or down depending on moderator/coolant)
-can also be embedded in graphite compacts, assembled into core configuration

Diffusion Equation Solution Methods

Green's Functions

Say we have a unit source at $\vec{r}'$.

$$\nabla \cdot D\nabla\phi(\vec{r}) + \Sigma_a\phi(\vec{r}) = -S(\vec{r})\forall\vec{r} \in V$$

...

$$\nabla \cdot D\nabla G(\vec{r}, \vec{r}') + \Sigma_a G(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}')\forall\vec{r} \in V$$

... Let $HG = \delta$ and $H\phi = S$ ...

$$= \int_V dV\,(S(\vec{r}')G(\vec{r}, \vec{r}') - \delta(\vec{r} - \vec{r}')\phi(\vec{r}))$$

and using the divergence theorem and our boundary conditions

$$\int_{\mathcal{S}} d\mathcal{S}\hat{e}_s \cdot D\left[\nabla\phi G(\vec{r}, \vec{r}') - ...\right] = 0$$

$$\begin{aligned}\int_V dV S(\vec{r})G(\vec{r}, \vec{r}') &= \int_V dV \delta(\vec{r} - \vec{r}')\phi \\ &= \phi(\vec{r}')\end{aligned}$$

or

$$\phi(\vec{r}) = \int_V dV S(\vec{r}')G(\vec{r}, \vec{r}')$$

Note: $G(\vec{r}, \vec{r}')$ is a **kernel**.

Example: Plane source in an infinite medium

...

$$\frac{d^2G(x,x')}{dx^2} - \frac{1}{L^2}G(x,x') = -S(x)\delta(x), \text{ and } \lim_{x\to\pm\infty} G(x,x') = 0$$

Variation of constants: $G(x,x') = \frac{L}{2D}H(x-x')e^{-|x-x'|/L} + \frac{L}{2D}H(x-x')e^{|x-x'|/L}$, where $H(x-x')$ is the heaviside function.

Then

$$\phi = \int dx' G(x,x')\delta(x')S$$

$$\phi(x) = \frac{SL}{2D}e^{-|x|/L}$$

Eigenfunction expansion method

We use this method to get the DE solution as a functional expansion of eigenvectors.

Eigenvalues

A special set of scalars associated with a linear system of equations. They are also known as characteristic roots. Each eigenvalue has a corresponding eigenvector.

$\mathbf{A} \in \mathbb{C}^n \times \mathbb{C}^n$, then $\mathbf{A}$ can be composed into eigenvectors and eigenvalues as long as $\mathbf{A}$ is square.

Let $\mathbf{A} \in \mathbb{R}^{n\times n}$. If there is a $\vec{x} \in \mathbb{R}^n$ s.t. $\mathbf{A}\vec{x} = \lambda\vec{x}$.

...

Solve for λs and $\vec{x}$s that go w/ them. There are nontrivial solutions iff $\det(\mathbf{A} - \lambda\mathbb{1}) = 0$. $\mathbf{A}_{n\ timesn}$ is guaranteed to have n eigenvalues, some of which ay be repeated. This spectrum of $\mathbf{A}$ is

$$\sigma(A) \equiv [\lambda \in \mathbb{C} : \det(\mathbf{A} - \lambda\mathbb{1}) = 0], \, \lambda \in \sigma(\mathbf{A})$$

...

$$\nabla^2\phi(\vec{r}) - \Sigma_a\phi(\vec{r}) = \frac{-S(\vec{r})}{D}, \, \forall\, \vec{r} \in V$$

where our boundary conditions

$$\phi(\vec{r}) = 0, \, \forall\, \vec{r} \in \mathcal{S}$$

Now, let ψ be an eigenvector, and n be the n^{th} mode.

...

where $\nabla^2 = \mathbf{A}$ and $-B_n^2 = \lambda$.

$$... - \frac{1}{L^2}\sum_{n=1}^{N} c_n\psi_n = \frac{-1}{D}\sum_{n=1}^{N} S_n\psi_n$$

$$\sum_{n=1}^{N} c_n\left(B + \frac{1}{L^2}\right)\psi_n = \frac{1}{D}\sum_{n=1}^{N} S_n\psi_n.$$

Now we use the orthonormality of eigenvectors,

$$\int_V dV \psi_n \psi_m = \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases}$$

to find c_n.

$$\int_V dV \sum_{n=1}^{N} c_n \left(B_n^2 + \frac{1}{L^2} \right) = \frac{1}{D} S_n$$

$$c_n \left(B_n^2 + \frac{1}{L^2} \right) = \frac{1}{D} S_n$$

$$c_n = \frac{S_n}{D} \left(B_n^2 + \frac{1}{L^2} \right)^{-1}$$

$$S_n = \int_V dV S(\vec{r}) \psi_n$$

$$\phi(\vec{r}) = \int_V dV \sum_{n=1}^{N} \frac{S(\vec{r})}{D} \left(B_n^2 + \frac{1}{L^2} \right) \psi_n \psi_n$$

1D Slab with a source

... with boundary conditions $\phi(\pm\frac{\tilde{a}}{2}) = 0$.

$$\frac{d^2\psi}{dx^2} - B^2\psi = 0, \; -\frac{a}{2} \leq x \leq \frac{a}{2}$$

... and $\psi(\pm\frac{\tilde{a}}{2}) = A_1 \cos(\frac{B\tilde{a}}{2}) + A_2 \sin(...) = 0$. ...

...

$$\psi_n = \begin{cases} A_n \cos(\frac{n\pi}{\tilde{a}} x), & n \text{ is odd} \\ A_n \sin(\frac{n\pi}{\tilde{a}} x), & n \text{ is even} \end{cases}$$

The eigenvalue is $B_n = \frac{n\pi}{\tilde{a}}$ and the eigenvectors (or normal/harmonic modes are $\psi_n = \frac{n\pi}{\tilde{a}}$.

If normalize the power ($A_n = 1$),

$$\phi(x) = \sum_{n=1}^{N} c_n \psi_n$$

$$S(x) = \sum_{n=1}^{N} \psi_n S_n$$

$$S_n = ...$$

Altogether,

$$\frac{d^2}{dx^2} \sum_{n=1}^{N} c_n \psi_n - ... = -\frac{1}{D} \sum_{n=1}^{N} \psi_n S_n$$

$$...$$

$$c_n = \frac{S_n}{D} \left(\frac{1}{L^2} + B_n^2 \right)^{-1}$$

$$\phi(x) = \frac{1}{D} \sum_{n=1}^{N} S_n \left(\frac{1}{L^2} + B_n^2 \right)^{-1} \psi_n$$

Now substitute the source into the flux expression we just found.

$$\phi(x) = \int_{-\frac{\tilde{a}}{2}}^{\frac{\tilde{a}}{2}} dx \left[\frac{2}{\tilde{a}D} \sum_{n=1}^{N} \frac{\psi_n(x)\psi_n(x')}{\frac{1}{L^2} + B_n^2} \right] S(x')$$

Recall Green's function,

$$\phi(x) = \int_{-\frac{\tilde{a}}{2}}^{\frac{\tilde{a}}{2}} dx\, G(x, x') S(x')$$

and we see that

$$G(x, x') = \frac{2}{\tilde{a}D} \sum_{n=1}^{N} \frac{\psi_n(x)\psi_n(x')}{\frac{1}{L^2} + B_n^2}$$

Separation of Variables: Time Dependence in a Uniform Slab

$$\frac{1}{v}\frac{\partial \phi(x,t)}{\partial t} - D\frac{\partial^2 \phi(x,t)}{\partial x^2} + \Sigma_a \phi(x,t) = \nu\Sigma_f(x,t)$$

Our boundary conditions are

$$\phi(\pm\frac{\tilde{a}}{2}, t) = 0 \text{ (vacuum)}$$

$$\phi(x, 0) = \phi_0(x) = \phi_0(-x) \text{ (symmetric)}$$

...

Now we have 2 ODEs

$$\frac{dT}{dt} = -\lambda T(t)$$

$$D\frac{d^2\psi}{dx^2} = ...$$

...

Use the eigenvalue approach, solve

$$\frac{d^2\psi_n}{dx^2} + B_n^2 \psi_n(x) = 0$$

$$\psi_n(\pm\frac{\tilde{a}}{2}) = 0$$

Now, due to symmetry, $\psi_n = \cos(B_n x)$ are the eigenvectors (no odd sine functions).

$$B_n^2 = \left(\frac{n\pi}{\tilde{a}}\right)^2, \text{ where } n = \text{odd (the “space eigenvalue”}$$

$$\lambda = v\Sigma_a + vDB_n^2 - v\nu\Sigma_f \equiv \lambda_n$$

We can solve for λ, where λ_n is the time eigenvalue of the equation.

$$\phi(x,t) = \sum_{\text{n=odd}} A_n e^{-\lambda_n t} \cos\left(\frac{n\pi x}{\tilde{a}}\right)$$

...

...

$$\phi(x,t) = \sum_{n=\text{odd}} [...]\, e^{-\lambda n t} \cos(B_n x)$$

At long times:
$\lambda_1 > \lambda_2 > \lambda_3 ...$
$B_1 > B_2 > B_3 ...$
... this is the geometric buckling (a measure of the curvature of the shape of the dominant mode).

$$B_1^2 = -\frac{1}{\psi_1} d^2\psi_1 ...$$

Criticality

Geometric Buckling:

$$B_g^2 \equiv \left(\frac{\pi}{\tilde{a}}\right)^2$$

...

$$\phi(x,t) = \sum_{n=\text{odd}} A_n e^{\lambda_n t} \cos\left(\frac{n\pi x}{\tilde{a}}\right)$$

$$\phi(x,t) = ...$$

Material Buckling

$$B_m^2 \equiv \frac{\nu\Sigma_f - \Sigma_a}{D}$$

When a reactor is critical, the geometric buckling and material buckling must match.

$$\begin{aligned} B_m^2 = B_g \Rightarrow \lambda_1 = 0 \quad &\text{(critical)} \\ B_m^2 > B_g \Rightarrow \lambda_1 < 0 \quad &\text{(supercritical)} \\ B_m^2 < B_g \Rightarrow \lambda_1 > 0 \quad &\text{(subcritical)} \end{aligned}$$

This relates to the multiplication factor, k. Recall

$$k = \frac{\int_V dV \nu\Sigma_f \phi}{...} = 1 \qquad k_\infty \equiv \frac{\nu\Sigma_f}{\Sigma_a} \qquad L^2 = \frac{D}{\Sigma_a}$$

...

and so we have criticality when

$$B^2 = \frac{k_\infty - 1}{L^2} = B_m^2$$

Integral Form of the Transport Equation

We are going to use the Method of Characteristics (MOC) formalism to derive an integral equation (as opposed to the previous integro-differential equation).

Note: We cannot have a purely differential equation. This arises from the fact that while space and time are continuous, energy and direction can be discontinuous in time.

The transport eqaution is: linear, 1$^{\text{st}}$ order, partial differential, integral

Steady State Transport Equation:

$$\hat{\Omega} \cdot \nabla\psi(\vec{r}, E, \hat{\Omega}) + \Sigma_t \psi(\vec{r}, E, \hat{\Omega}) = q(\vec{r}, E, \hat{\Omega})$$

When ...

$$\hat{\Omega} \cdot \nabla \psi = \mu \frac{\partial \psi}{\partial x} + \eta \frac{\partial \psi}{\partial y} + \xi \frac{\partial \psi}{\partial z}$$

$$\mu^2 + \eta^2 + \xi^2 = 1$$

where $\mu = \cos(x)$, $\eta = \cos(y)$, and $\xi = \cos(z)$.

(figure)

This can be treated like n moving along "characteristic" line along $\hat{\Omega}$

$$\vec{r} = \vec{r}_0 + s(\mu\hat{x} + \eta\hat{y} + \xi\hat{z})$$

$$x = x_0 + \mu s$$
$$y = y_0 + \mu s$$
$$z = z_0 + \mu s$$

Use this to get the Cartesian streaming

$$\frac{\partial \psi}{\partial s} = \frac{\partial \psi}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial \psi}{\partial y}\frac{\partial y}{\partial s} + \frac{\partial \psi}{\partial z}\frac{\partial z}{\partial s}$$

and so indeed,

$$\frac{\partial \psi}{\partial s} = \hat{\Omega} \cdot \nabla \psi$$

Look at the Transport

$$\frac{\partial}{\partial s}\psi(\vec{r}_0 + \hat{\Omega}_s, \hat{\Omega}, E) + \Sigma_t \psi(\vec{r}_0 + \hat{\Omega}_s, \hat{\Omega}, E) = q(\vec{r}_0 + \hat{\Omega}_s, \hat{\Omega}, E)$$

This is a derivative along a characteristic curve. It's linear, 1$^{\text{st}}$ order and an ODE (we can integrate it). Use an integrating factor.

$$\text{\# of MFP from } \vec{r} \text{ at distance } s \text{ away} = \exp\left[\int_S ds'' \Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right]$$

Note:

$$\frac{d}{ds}\exp\left[\int_S ds''\Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right] = \Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\,\frac{d}{ds}\exp\left[\int_S ds''\Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right]$$

$$\frac{d}{ds}\left[\exp\left[\int_S ds''\Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right]\psi((\vec{r}_0 + \hat{\Omega}s'', E)\right] = \exp\left[\int_S ds''\Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right]\frac{d\psi}{ds} + \psi\Sigma_t \exp\left[\int_S ds''\Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right]$$

$$\frac{d}{ds}\left[\left[\int_S ds''\Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right]\psi\right] = (L$$

$$= (R$$

LHS:

$$\int_{-\infty}^{s} ds' \frac{d}{ds'}\left[\exp\left[\int^{s'} ds''\Sigma_t(\vec{r} + ...)\right]\right]\psi(\vec{r} + \hat{\Omega}s', \hat{\Omega}, E)$$

... (Repeat this with $\left[\int_S ds''\Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right] = \mathcal{I}$)...

And so we finally have:

$$\psi(\vec{r}_0 + \hat{\Omega}s, \hat{\Omega}, E) = \int_{-\infty}^{s} ds' \exp\left[-\int_{s'}^{s} ds'' \Sigma_t(\vec{r}_0 + \hat{\Omega}s'', E)\right] q(\vec{r}_0 + \hat{\Omega}s', \hat{\Omega}, E)$$

The integro-differential form expresses a local balance with local coupling.
In the integral form, we are tracking particles from birth to observation; an accumulation process, so the coupling is global.

Let $\rho' \equiv s - s', d\rho' = -ds'$ and $\rho'' = s - s'', d\rho'' = -ds''$. Then

$$\phi(\vec{r}, E, \hat{\Omega}) = -\int_{\infty}^{0} d\rho' \exp\left[\Sigma_t(\vec{r}_0 + \hat{\Omega}s - \hat{\Omega}s + \hat{\Omega}s'', E)\right] q(\vec{r}_0 + \hat{\Omega}s - \hat{\Omega}s - \hat{\Omega}s', E, \hat{\Omega})$$

$$... = \int_0^{\infty} ...$$

$$\psi(\vec{r}, E, \hat{\Omega}) = \int_0^{\infty} d\rho' \exp\left[-\int_0^{\rho'} d\rho'' \Sigma_t(\vec{r} - \rho''\hat{\Omega}, \hat{\Omega}, E)\right] q(\vec{r} - \rho''\hat{\Omega}, \hat{\Omega}, E)$$

Let Q' by the integrated fixed source, and k is the integral operator.

$$k\psi = \text{n production from scattering and fission}$$

$$\psi_t = k\psi_{t-1} + Q'$$

The total flux is

$$\psi = \sum_{j=0}^{n} \psi_j$$

where the "uncollided flux" is $\psi_0 = Q'$, the "once collided flux" is $\psi_1 = k\psi_0$, and the "twice collided flux" is $\psi_2 = k\psi_1$.

Isotropic Scattering

When we have isotropic scattering and sources, we can remove angular dependence.
- Fission: $\frac{\chi(E)}{4\pi} \int_0^{\infty} dE' \nu\Sigma_f(\vec{r}, E') \int_{4\pi} d\hat{\Omega}' \psi(\vec{r}, E', \hat{\Omega}')$
- Fixed Source: $S(\vec{r}, E, \hat{\Omega}) = \frac{S(\vec{r}, E)}{4\pi}$
- Scattering: $\int_0^{\infty} dE' \int_{4\pi} d\hat{\Omega} \frac{\Sigma_s}{...}$

The integrating factor over angle:
<image>

Note: $d\hat{\Omega} = \frac{dA}{\rho''}$ and $d\rho' dA = dV$

...

Remember, $\rho' = |\vec{r} - \vec{r}'|$, and $dv = d^3r'$

If we say τ is the optical path length,

$$\int_0^{\rho'} d\rho'' \Sigma_t(\vec{r} - \rho''\hat{\Omega}, E) \equiv \tau(\vec{r} - \rho'\hat{\Omega} \to \vec{r}, E).$$

Our scalar flux is

$$\phi(\vec{r},E) = \int_V d^3r \left[\frac{\exp\left[\tau(E,\vec{r}' \to \vec{r})\right]}{4\pi|\vec{r}-\vec{r}'|^2}\left(S(\vec{r}',E) + \chi(E)\int_0^\infty dE'\nu\Sigma_f(E')\phi(\vec{r}',E') + \int_0^\infty dE'\Sigma_s(\vec{r}',E' \to E)\phi(\vec{r}',E')\right)\right]$$

The source term is the rate at which neutrons of energy E appear at location $\vec{r}$. Integrating over all $\vec{r}\,'$ gives the total number of neutrons.

This is a Green's function for isotropic source at $\vec{r}\,'$ in an absorbing medium.

Anisotropic Scattering

Use a producition kernel:

$$\Pi() \equiv \Sigma_s() + \frac{\chi(E)}{4\pi}\nu\Sigma_f(\vec{r},E')$$

The collision source of neutorns is

$$k\psi \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\Pi()\psi()$$

The Multigroup Transport Equation

Energy grid (actually choosing this is difficult)

E_G is the lowest energy edge
E_0 is the highest energy edge

An energy group g is between E_g and E_{g-1}.

$$\psi_g(\vec{r},\hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} dE\psi(\vec{r},E,\hat{\Omega})$$

Integrate the transport equation over energy so we can solve for ψ_g.

Assume that the flux is separable in space & energy

$$\psi(\vec{r},E,\hat{\Omega}) \approx f(E)\psi_g(\vec{r},\hat{\Omega}), \qquad E_g \leq$$

Normalize: $\int_g dEf(E) = 1$
*substitute in approximation and integrate

Streaming:

$$\begin{aligned}\int_{E_g}^{E_{g-1}} dE\hat{\Omega}\cdot\nabla\psi(\vec{r},E,\hat{\Omega}) &= \int_{E_g}^{E_{g-1}} \hat{\Omega}\cdot\nabla f(E)\psi_g(\vec{r},\hat{\Omega}) \\ &= \hat{\Omega}\cdot\nabla\psi_g(\vec{r},\hat{\Omega})\end{aligned}$$

External Source:

$$q_g(\vec{r},\hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} dEq(\vec{r},E,\hat{\Omega})$$

Fission:

$$\int_{E_g}^{E_{g-1}} dE \frac{\chi(E)}{4\pi} \int_0^\infty dE' \nu \Sigma_f(E') \int_{4\pi} d\hat{\Omega}' \psi(\vec{r}, E', \hat{\Omega}')$$

where

$$\chi_g \equiv \int_{E_g}^{E_{g-1}} dE\, \chi(E)$$

$$\int_{4\pi} d\hat{\Omega}' \psi_g(\vec{r}', \hat{\Omega}') = \phi_g(\vec{r})$$

Then

$$\int_0^\infty dE' \nu \Sigma_f(E') = \sum_{g'=1}^{G} \int_{E_g}^{E_{g-1}} dE' \nu \Sigma_f(e)$$

$$\nu \Sigma_{f,g'} \equiv \int_{E_g}^{E_{g-1}} dE\, \nu \Sigma_f(E') f(E')$$

$$q_{f,g} = \frac{\chi_g}{4\pi} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \phi_{g'}(\vec{r})$$

Scattering:
(from group g' into group g)

$$q_{s,g,g'}(\hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} dE \int_{E_g'}^{E_{g'-1}} dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(E' \to E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}')$$

where (general scattering cross section)

$$\Sigma_{s,gg'}(\hat{\Omega}' \cdot \hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} dE \int_{E_g'}^{E_{g'-1}} dE' \Sigma_s(E' \to E, \hat{\Omega}' \cdot \hat{\Omega}) f(E')$$

Then

$$q_{s,g}(\hat{\Omega}) = \sum_{g'=1}^{G} \int_{4\pi} d\hat{\Omega}' \Sigma_{s,gg'}(\hat{\Omega}' \cdot \hat{\Omega}) \psi_{g'}(\vec{r}, \hat{\Omega}')$$

Total Interaction:

$$\Sigma_{t,g}(\vec{r}) \equiv \int_{E_g}^{E_{g-1}} dE \Sigma_t(E, \vec{r}) f(E)$$

$$\text{term} = \Sigma_{t,g} ...$$

Combine to yield the full **multigroup transport equation**

$$\left[\hat{\Omega} \cdot \nabla + \Sigma_{t,g}(\vec{r})\right] \psi_g(\vec{r}, \hat{\Omega}) = q_g(\vec{r}, \hat{\Omega}) + \sum_{g'=1}^{G} \int_{4\pi} d\hat{\Omega}' \Sigma_{s,gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi_{g'}(\vec{r}, \hat{\Omega}') + \frac{\chi_g}{4\pi} \sum_{g'=1}^{G} \nu \Sigma_{f,g'}(\vec{r}) \vec{r}_{g'}(\vec{r})$$

and there are $g = 1, ..., G$ of these *coupled* equations.

Typically people use 2 groups, though tens of groups are becoming more common. Hundreds of groups get used in most advanced calculations on cutting-edge architectures.

Group Constants

For these equations to be accurate, we need:

- detailed E-dependence of the cross sections
- details of weighting function, $f(E)$
  - $f(E)$ is easy for smoothly varying cross sections
  - resonance regions are tougher (many energy bins, resonance self-shielding)

In general

1. start w/ ENDF data (1000s of E-groups), an infinite medium, and do a 1-D transport calculation $\rightarrow$ collapse the data to 100s of groups
2. perform another tranpsort calculation at the assembly level, or unit cell $\rightarrow$ collapse in E to a few or 10s of groups (also, we usually homogenize in space)
3. perform a core-level calculation with diffusion theory

Use fine energy index j, coarse energy index h; to collapse fine $\rightarrow$ coarse

$$\Sigma_{x,h} \equiv \frac{\sum_{j\in h} \Sigma_{x,j}\phi_j(\vec{r})}{\sum_{j\in h}\phi_j(\vec{r})}$$

Homogenize in space

$$\Sigma_{x,j}^{\text{homog}} \equiv \frac{\int_v dV \Sigma_{x,j}(\vec{r})\phi_j(\vec{r})}{\int_v dV \phi_j(\vec{r})}$$

Legendre Expansion Techniques

Legendre Addition Theorem:

$$P_\ell(\hat{\Omega}'\cdot\hat{\Omega}) = \frac{1}{2\ell+1}\sum_{m=-\ell}^{\ell}...$$

Flux moments (not scalar flux): $\phi_\ell^m(\vec{r},E') = \int_{4\pi} d\hat{\Omega}'\, Y_{\ell m}(\hat{\Omega}')\,\psi(\vec{r},\hat{\Omega}',E')$

$$\psi(\vec{r},E',\hat{\Omega}') = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{\Omega})\phi_\ell^m(\vec{r},E')$$

Now, we use this information in the scattering term of the transport equation.

$$\begin{aligned}\left[\hat{\Omega}\cdot\nabla + \Sigma_t(\vec{r})\right]\psi(\vec{r},E,\hat{\Omega}) = q(\vec{r},E,\hat{\Omega}) + \frac{\chi(E)}{4\pi}\int_0^\infty dE'\,\nu\Sigma_f(E')\int_{4\pi} d\hat{\Omega}'\psi(\vec{r},E',\hat{\Omega}')\\ + \sum_{\ell=0}^{m}\sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{\Omega}')\int_0^\infty dE'\Sigma_{s,\ell}(E'\\ \rightarrow E)\phi_\ell^m(\vec{r},E')\end{aligned}$$

Next, integrate over energy,

$$q_{s,gg'} = \sum_{\ell=0}^{m}\sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\hat{\Omega}')\int_{E_g}^{E_{g-1}} dE\int_{E_g'}^{E_{g'-1}} dE'\Sigma_{s,\ell}(E'\rightarrow E)\phi_\ell^m(\vec{r},E')$$

Define the group scattering cross section moment

$$\Sigma_{s,\ell,gg'} \approx \frac{\int_{E_g}^{E_{g-1}} dE\int_{E_g'}^{E_{g'-1}} dE'\Sigma_{s,\ell}(E'\rightarrow E)\phi_\ell^m(\vec{r},E')}{\phi_{\ell,g'}^m(\vec{r})}$$

Total Interaction:
Returning to the total interaction term, let's consider the cross section as before

$$\Sigma_{t,g} = \frac{\int_{E_g}^{E_{g-1}} dE \Sigma_t(\vec{r}, E)\psi(\vec{r}, E, \hat{\Omega})}{\psi_g(\vec{r}, \hat{\Omega})}.$$

But, this is nondesirable because Σ_{tg} is a function of angle $\hat{\Omega}$. Instead, use the Legendre expansion and define Σ_t moments.

$$\int_{E_g}^{E_{g-1}} dE\, \Sigma_t(\vec{r}, E) \sum_{\ell=0}^{m} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\hat{\Omega}')\phi^m_\ell(\vec{r}, E) = \sum_{\ell=0}^{m} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\hat{\Omega}') \int_{E_g}^{E_{g-1}} dE \Sigma_t(\vec{r}, E)\phi^m_\ell(\vec{r}, E)$$

where

$$\Sigma_{t,\ell,g}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} dE \Sigma_t(\vec{r}, E)\phi^m_\ell(\vec{r}, E)}{\phi^m_{\ell,g}(\vec{r})}$$

$$\text{term} = \sum_{\ell=0}^{m} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\hat{\Omega}')\Sigma_{t,\ell,g}(\vec{r})\phi^m_{\ell,g'}(\vec{r})$$

Fission:

$$\nu\Sigma_{f,g'} = \frac{\int_{E'_g}^{E_{g'-1}} dE' \nu\, \Sigma_f(\vec{r}, E')\, \phi(\vec{r}, E')}{\phi_{g'}(\vec{r})}$$

Using all of this in the transport equation: (add $\Sigma_{t,g}\psi_g$ to both sides and move expanded total term to the right-hand side of the equation)

$$\begin{aligned}\left[\hat{\Omega} \cdot \nabla + \Sigma_{t,g}(\vec{r})\right] \psi_g(\vec{r}, \hat{\Omega}) = {} & \frac{\chi_g}{4\pi} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}(\vec{r})\, \phi_{g'}(\vec{r}) + q_g(\vec{r}, \hat{\Omega}) \\ & + \sum_{\ell=0}^{m} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\hat{\Omega}') \sum_{g=1}^{G} \left(\Sigma_{\ell,gg'} + \left(\Sigma_{t,g}(\vec{r}) - \Sigma_{t,\ell,g}(\vec{r})\right) \delta_{gg'}\right) \phi^m_{\ell,g'}(\vec{r})\end{aligned}$$

This looks like the first version we found, except for the scattering term. If we weight the total interaction term with the scalar flux (P_0),

$$\Sigma_{t,g}(\vec{r}) = \Sigma_{tg,0}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} dE\, \Sigma_t(\vec{r}, E)\, \phi(\vec{r}, E)}{\phi_g(\vec{r})}$$

then this is consistent with the P_N approximation (and this is the P_0 approximation in it).

Instead, we could also use the observation that we truncate expansions ($\ell = L$). We choose $\Sigma_{t,g}(\vec{r})$ to make the $\ell = L + 1$ component small.

$$\sum_{m=-(L+1)}^{L+1} Y^*_{(L+1)m}(\hat{\Omega}) \sum_{g'=1}^{G} \left[\Sigma_{s,(L+1),gg'} + \left(\Sigma_t g(\vec{r}) - \Sigma_{t,(L+1),g}(\vec{r})\right) \delta_{gg'}\right) \phi^m_{(L+1),g'}(\vec{r}) \approx 0$$

For reactors, and for most groups, in-scattering $\approx$ out-scattering. In this case,

$$\sum_{g=1}^{G} \Sigma_{s,(L+1),gg'}\ldots \approx \sum_{g'=1}^{G} \Sigma_{s,(L+1),gg'}\ldots$$

$$\Sigma_1(\vec{r}) = \ldots$$

This is the extended transport approximation.

Monte Carlo

Sampling

Use uniformly distributed random variables (ξ between 0 and 1) to choose a value for a variable according to its PDF.

$$F(x) = \xi \rightarrow x = F^{-1}(\xi)$$

Basic

- direct discrete sampling (which reaction)
- direct continuous sampling (# of MFPs)
- rejection sampling (Klein-Nishina formula)

Advanced

- histogram
- piecewise linear
- alias sampling
- advanced continuous PDFs

Example: Distance to a collision

Solve using direct inversion.

$$\Sigma_t = \sum_{j=1}^{J} N_j \sigma_t^j$$

Here the PDF is the

(probability of interaction per unit distance) $\times$ (probability of traveling distance $s$without interacting)

or

$$f(s) = \Sigma_t e^{-\Sigma_t s}$$

To find the CDF we integrate from 0 to s:

$$F(s) = \int_0^s f(s')\, ds'$$

In our case, the CDF is

$$F(s) = \int_0^s \Sigma_t e^{-\Sigma_t s'}\, ds'$$

$$F(s) = -\left[e^{-\Sigma_t s'}\right]_0^s$$

$$F(s) = 1 - e^{-\Sigma_t s}$$

To *sample* we do direct inversion. If $F(s) = \xi$, then $\xi = 1 - e^{-\Sigma_t s}$. Solving for s,

$$e^{-\Sigma_t s} = 1 - \xi$$

$$-\Sigma_t s = \ln(1 - \xi)$$

$$s = \frac{-\ln(1-\xi)}{\Sigma_t}$$

After determining which reaction occurs, we determine which isotope and which collision type were involved. Then

$$\sigma_t = \sigma_{el} + \sigma_{inel} + \sigma_{capture} + \sigma_f + ...$$

The probability of a reaction i is

$$\rho_i = \frac{\sigma_i}{\sigma_t}$$

At this point, we have a set of discrete probabilities. We can sample these probabilities

- **Directly:**
  - get ξ
  - find k s.t. $F_{k-1} \leq \xi F_k$
  - return $i = ik$
- (speed this up with an *alias table*)

Scoring

Each history, i, is a series of interaction sites.

- Estimators convert histories into scores. Histories have different scores (in general).
- Tallies accumulate sets of scores $\{x_i\}$ to form a PDF

We want to find the expected value of underlying PDFs, and we normalize the tallies to the number of source particles, N.

$$E(x) = \frac{1}{N}\sum_{i=1}^{N} x_i$$

Types of Estimators

1. **Point Estimator:** surface crossings, collisions (current tally, surface flux tally)
2. **Track Length Estimator:** track length through a cell (volume flux tally)
3. **Energy Balance Estimator:** energy loss in a cell (pulse height tally)

Example: Surface/Current tally

We have our estimator,

$$x_i = \sum_j w_{ij}$$

The current is

$$\int_A dA \int_{\hat{\Omega}} d\hat{\Omega} \int_E dE \hat{n} \cdot \vec{J}(\vec{r}, E, \hat{\Omega}) \approx \frac{1}{N}\sum_{i=1}^{N} x_i = \frac{1}{N}\sum_{i=1}^{N}\sum_j w_{ij}$$

The surface energy current is

$$\int_A dA \int_{\hat{\Omega}} d\hat{\Omega} \int_E dE \, \hat{n} \cdot E \, \vec{J}(\vec{r}, E, \hat{\Omega}) \approx \sum_{i=1}^{N}\sum_j E_{ij} w_{ij}$$

The flux/fluence is

$$\bar{\phi}_V = \frac{1}{V}\int_V dV \int_E dE \int_t dt\phi(\vec{r}, E, t)$$

where $\phi \equiv vN$ and $vdt = ds$. Then

$$\bar{\phi}_V = \frac{1}{V}\int_s ds \int_E dE\phi(\vec{r}, E, t)$$

Collision; score at collision

$$\phi_V \approx \frac{1}{VN}\sum_{i=1}^{N} x_i = \frac{1}{VN}\sum_{i=1}^{N} w_i$$

Track length (T_ℓ = track length in volume)

$$\phi_V \approx= \frac{1}{VN}\sum_{i=1}^{N} w_i T_{\ell,ij}$$

The surface flux is ...

Statistics

The true mean μ of any PDF is the expected value, $E(x)$, where

$$\mu = E(x) = \int x\, f(x)\, dx$$

Since we often can't find/don't know this value, we estimate the true mean from the sample mean, $\bar{x}$, where

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

and

$$\lim_{n\to\infty} \bar{x} = \mu.$$

The variance of a PDF is a measure of the spread in that PDF. The true variance is

$$\begin{aligned} \sigma^2 = E[(x-\mu)^2] &= \int (x-\mu)^2 f(x) dx \\ &= \int x^2 f(x) dx - 2\mu \int x\, f(x)\, dx + \mu^2 \int f(x)\, dx \end{aligned}$$

and the sample variance is

$$\begin{aligned} S_x^2 &= \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2 \\ &= \frac{1}{N-1}\left[\sum_{i=1}^{N} x_i^2 - 2\bar{x})^2 \sum_{i=1}^{N} x_i + \bar{x})^2 \sum_{i=1}^{N} 1\right] \\ &\approx \overline{x^2} - \bar{x}^2 \end{aligned}$$

The Central Limit Theorem

For N independent random variables, x_i, sampled from identical distributions, their mean allows a normal distribution (IID). From this, we can define confidence intervals.

First, we note $S_{\bar{x}} = \sqrt{\frac{S_x^2}{N}}$.

Our confidence intervals are

$$\bar{x} - S_{\bar{x}} < E(x) < \bar{x} + S_{\bar{x}}(68\%)$$
$$\bar{x} - 2S_{\bar{x}} < E(x) < \bar{x} + 2S_{\bar{x}}(95\%)$$

The standard deviation is a measure of the error in the result.

$$\begin{aligned}
S_{\bar{x}}^2 &= E[(\bar{x} - \mu)^2] \\
&= E[(\frac{1}{N^2}\sum_{i=1}^{N} x_i - \mu)] \\
&= \frac{1}{N^2} E\left[\sum_{i=1}^{N}\sum_{j=1}^{N}(x_i - \mu)(x_j - \mu)\right] \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N} E\left[(x_i - \mu)(x_j - \mu)\right] \\
&= \frac{1}{N^2}\sum_{i=1}^{N} S_x^2 \\
&= \frac{N S_x^2}{N^2} \\
&= \frac{S_x^2}{N} \\
&= S_{\bar{x}}^2
\end{aligned}$$