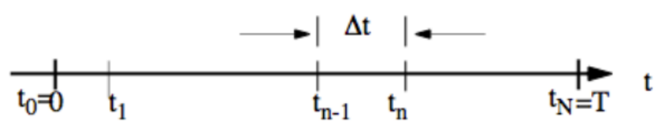
NE 255, Fa16
Equation Discretization
September 22 and 27, 2016

Start from the general time-dependent NTE without delayed neutrons, with 7 independent variables. We need to discretize each variable.

$$\begin{aligned}
&\frac{1}{v}\frac{\partial \psi}{\partial t}(\vec{r}, E, \hat{\Omega}, t) + \hat{\Omega}\cdot\nabla\psi(\vec{r}, E, \hat{\Omega}, t) + \Sigma_t(\vec{r}, E)\psi(\vec{r}, E, \hat{\Omega}, t) \\
&\quad = \int_0^\infty \int_{4\pi} \Sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega})\psi(\vec{r}, E', \hat{\Omega}', t) d\hat{\Omega}' dE' \\
&\qquad + \frac{\chi_p(E)}{4\pi}\int_0^\infty \int_{4\pi} \nu(E')\Sigma_f(\vec{r}, E')\psi(\vec{r}, E', \hat{\Omega}', t) d\hat{\Omega}' dE' \\
&\qquad + S(\vec{r}, E, \hat{\Omega}, t).
\end{aligned} \tag{1}$$

Time

Discretize the time interval $[0, T]$ into N timesteps: Integrate the equation from $t = t_{n-1}$ to $t = t_n$,



where we will use the following definitions:

$$\psi(\vec{r}, E, \hat{\Omega}, t_n) = \psi_n(\vec{r}, E, \hat{\Omega})$$
$$\Delta t = t_n - t_{n-1}$$
$$\bar{\psi}(\vec{r}, E, \hat{\Omega}) = \frac{1}{\Delta t}\int_{t_{n-1}}^{t_n} dt\, \psi(\vec{r}, E, \hat{\Omega}, t)$$

(Note that this integration is functionally ignoring what actually happens in the integration by giving us a time-averaged angular flux; we don't care about more details than that).

To update the equation we simply convert each term to this time-averaged angular flux *except* the term containing a time derivative. We need to handle that specially by using *First Order Backward Difference*:

$$\frac{1}{v}\int_{t_{n-1}}^{t_n} dt\, \frac{\partial \psi}{\partial t}(\vec{r}, E, \hat{\Omega}, t) = \frac{1}{v}\frac{\psi_n(\vec{r}, E, \hat{\Omega}) - \psi_{n-1}(\vec{r}, E, \hat{\Omega})}{\Delta t}$$

Combining all of that we get the following:

$$
\begin{aligned}
&\frac{1}{v}\frac{\psi_n(\vec{r},E,\hat{\Omega})-\psi_{n-1}(\vec{r},E,\hat{\Omega})}{\Delta t}+\hat{\Omega}\cdot\nabla\bar{\psi}(\vec{r},E,\hat{\Omega})+\Sigma_t(\vec{r},E)\bar{\psi}(\vec{r},E,\hat{\Omega})= \\
&\quad\int_0^\infty dE'\int_{4\pi}d\hat{\Omega}'\,\Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\to\hat{\Omega})\bar{\psi}(\vec{r},E',\hat{\Omega}') \\
&\quad+\frac{\chi_p(E)}{4\pi}\int_0^\infty dE'\,\nu(E')\Sigma_f(\vec{r},E')\int_{4\pi}d\hat{\Omega}'\,\bar{\psi}(\vec{r},E',\hat{\Omega}')+\bar{S}(\vec{r},E,\hat{\Omega})
\end{aligned}
$$

Note(!): we now have two unknowns (ψ_n and $\bar{\psi}$). We need to relate them; we choose a linear combination with a weighting parameter, β:

$$\bar{\psi}=\beta\psi_n+(1-\beta)\psi_{n-1}$$

We substitute this in to get

$$
\begin{aligned}
\hat{\Omega}\cdot\nabla\bar{\psi}(\vec{r},E,\hat{\Omega})+\big(\Sigma_t+\frac{1}{v\beta\Delta t}\big)\bar{\psi}(\vec{r},E,\hat{\Omega})&=\frac{1}{v\beta\Delta t}\psi_{n-1}(\vec{r},E,\hat{\Omega}) \\
&+\int_0^\infty dE'\int_{4\pi}d\hat{\Omega}'\,\Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\to\hat{\Omega})\bar{\psi}(\vec{r},E',\hat{\Omega}') \\
&+\frac{\chi_p(E)}{4\pi}\int_0^\infty dE'\,\nu(E')\Sigma_f(\vec{r},E')\int_{4\pi}d\hat{\Omega}'\,\bar{\psi}(\vec{r},E',\hat{\Omega}')+\bar{S}(\vec{r},E,\hat{\Omega})
\end{aligned}
$$

Aside about Finite Difference

Finite difference is a common way to numerically approximate derivatives. **Example** Given f is $C^2\in[a,b]$ and $x_0\in[a,b]$, find an approximation to $f'(x_0)$ and or $f''(x_0)$, etc.

We're going to come at this from **Taylor's theorem**, which gives an approximation of a k-times differentiable function around a given point by a k-th order Taylor polynomial.

$$f(x)=\sum_0^k\frac{f^{(n)}(x_0)}{n!}(x-x_0)^n$$

To approximate any type of derivative to a specified order of accuracy, we Taylor expand several points in our collection. Then, we choose how many points to combine and in what ways.

$$\begin{aligned}
f(x_0) &= f(x_0) \\
f(x_0 \pm h) &= f(x_0) \pm hf'(x_0) + h^2\frac{f''(x_0)}{2} \pm h^3\frac{f'''(x_0)}{6} + f^{(4)}(c_1)\frac{h^4}{24} \\
f(x_0 \pm 2h) &= f(x_0) \pm 2hf'(x_0) + 2h^2f''(x_0) \pm \frac{4}{3}h^3f'''(x_0) + \frac{2}{3}h^4f^{(4)}(c_2)
\end{aligned}$$

We combine the expanded expressions, rearrange to group terms, and solve for what we want:

For $O(h)$ Backwards Difference: combine the point and the next point backward:

$$\begin{aligned}
f(x_0) &= f(x_0) \\
f(x_0 - h) &= f(x_0) - hf'(x_0) + h^2\frac{f''(c)}{2} \\
af(x_0) + bf(x_0 - h) &= f'(x_0) \\
af(x_0) + b\big(f(x_0) - hf'(x_0) + h^2\frac{f''(c)}{2}\big) &= f'(x_0) \\
(a+b)f(x_0) - bhf'(x_0) + bh^2\frac{f''(c)}{2} &= f'(x_0)
\end{aligned}$$

Now, we solve for the coefficients to get what we want

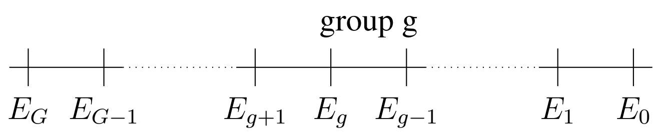
$$\begin{aligned}
a + b = 0 \quad & - bh = 1 \\
b = -\frac{1}{h} \quad & a = \frac{1}{h}
\end{aligned}$$

We now sub in a and b. This gives the first order ($O(h)$) Backwards Difference approximation, which is what we used for the time derivative.

$$\begin{aligned}
\text{error } &= -\frac{1}{h}h^2\frac{f''(c)}{2} \\
f'(x_0) &= \frac{f(x_0) - f(x_0 - h)}{h} + \frac{1}{2}hf''(\mu)
\end{aligned}$$

Energy Discretization

We'd also like to handle the energy dimension by breaking continuous energy into groups:



We will use the following definitions:

$$\psi_g(\vec{r},\hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} dE\, \psi(\vec{r},\hat{\Omega},E) \qquad \phi_g(\vec{r}) \equiv \int_{E_g}^{E_{g-1}} dE\, \phi(\vec{r},E)$$
$$S_g(\vec{r},\hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} dE\, S(\vec{r},\hat{\Omega},E) \qquad \chi_g \equiv \int_{E_g}^{E_{g-1}} dE\, \chi(E)$$

To perform these integrals, we need to introduce approximations. We *assume the each item is separable in energy*. For example:

$$\psi(\vec{r},\hat{\Omega},E) \approx f(E)\psi_g(\vec{r},\hat{\Omega})\;, \quad E_g < E \le E_{g-1}\;,$$

where $f(E)$ is normalized such that $\int_g dE\, f(E) = 1$.

Before we can integrate the whole transport equation over energy, we will need a way to create multigroup cross sections. Options for how to do that in more detail are covered in NE250, so we will do the most common/generic here: weight with the angular flux,

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

similarly for fission

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

If we use all of those definitions and integrate the TE over energy, we get

$$[\hat{\Omega}\cdot\nabla + \Sigma_{tg}(\vec{r})]\psi_g(\vec{r},\hat{\Omega}) = \sum_{g'=1}^{G} \int_{4\pi} d\hat{\Omega}'\, \Sigma_{s,gg'}(\vec{r},\hat{\Omega}'\cdot\hat{\Omega})\psi_{g'}(\vec{r},\hat{\Omega}')$$
$$+ \frac{\chi_g}{4\pi} \sum_{g'=1}^{G} \nu\Sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}) + q_g(\vec{r},\hat{\Omega})$$

This is exact in the magical case where (1) the separability in energy holds and (2) the cross sections are constant within each energy group.

Angular Discretization

And the complicated one: angle. We have two main approaches, **Discrete Ordinates** (S_N) and **Spherical Harmonics** (which we simplify to Legendre polynomials and thus call P_N, not to be confused with the scattering expansion).

Discrete Ordinates

The idea of discrete ordinates approximation is that the TE is only valid along a selected set of angles μ_n, and we apply a compatible quadrature approximation to the integral term.

$$\begin{aligned}
\mu_n \frac{\partial \psi_n}{\partial x} + \Sigma_t(x)\psi_n(x,\mu_n) &= \sum_{l=0}^{L}(2l+1)\Sigma_{s,l}(x)P_l(\mu_n)\phi_l(x) + S(x,\mu_n) \\
\psi_n(x) &= \psi(x,\mu_n) \\
\phi(x) &= \frac{1}{2}\sum_{n=1}^{N} w_n\psi_n(x) \\
\phi_l(x) &= \frac{1}{2}\sum_{n=1}^{N} w_n P_l(\mu_n)\psi_n(x) \\
w_n > 0 \quad & \sum_n w_n = 2
\end{aligned}$$

The collection of μ_n, w_n is known as the angular quadrature set.