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ICTP 40th Anniversary

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Workshop on
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Lattice transport theory of WIMS

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Resonance Theory and Transport Theory in WIMSD

J L Hutton

2 March 2004

Outline of Talk

- Resonance Treatment
  - Outline of problem -
    - pin cell geometry
    - U^{238} cross section
  - Simple non-mathematical ideas
  - More rigorous treatment
- Neutron Transport Theory
  - Homogeneous - B1
  - Collision probabilities - PIJ
  - Sn - DSN

DISCRETISATION OF GEOMETRY

Infinite Homogeneous Problem

- No geometry subdivision required.

Heterogeneous Problem

- Minimum subdivision: one calculation "mesh" per material region

- In practice, material regions are normally subdivided into several meshes of about one transport mean free path in size (~ 1 cm in H_2O)

GEOMETRY OPTIONS

HOMOGENEOUS

SLAB

REGULAR PINCELL ARRAY

CLUSTER (PRESSURE TUBE)

MULTICELL

+ choice of boundary conditions

Typical cluster - subdivision into ~ 30 meshes

Computing time and storage vary as :

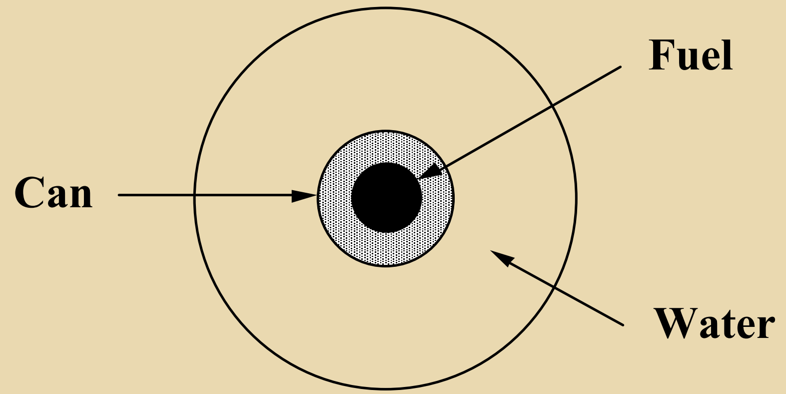
Number of groups x Number of meshes

PIN CELL GEOMETRY

A "Pin Cell" consists essentially of a cylindrical fissile region surrounded by clad and coolant.

Infinite arrays are generated, but leakage can be introduced.

Isolated cylinders can be obtained by adopting a "free” boundary.

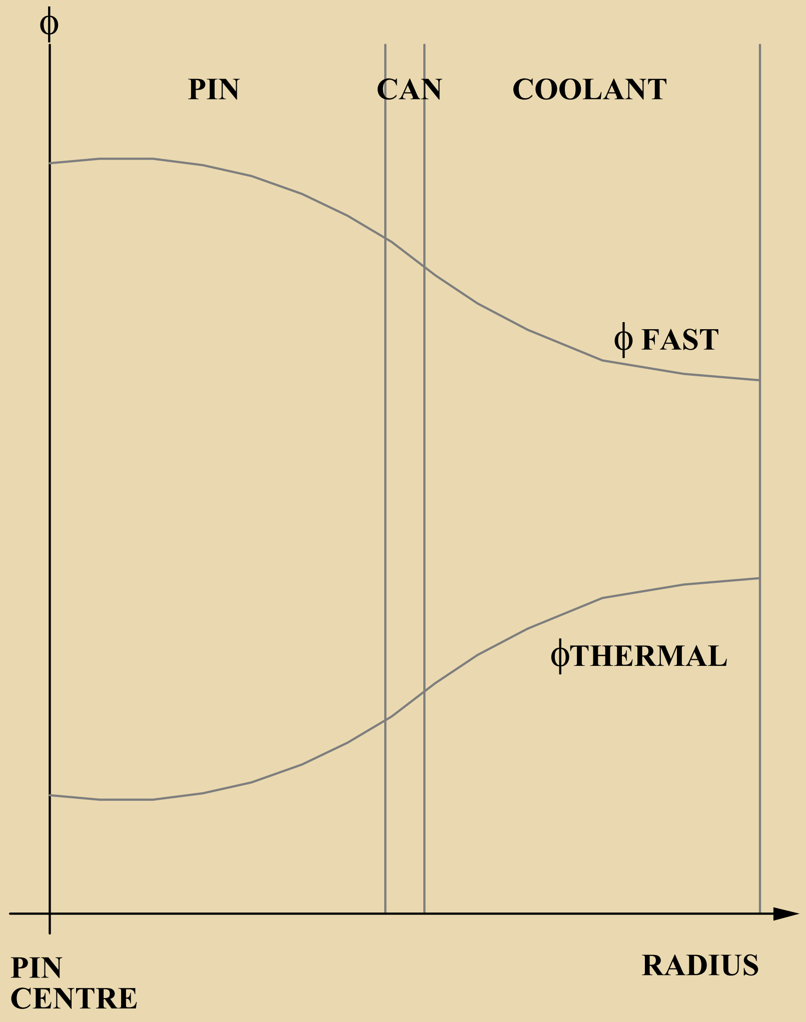


A WIMS Pin Cell

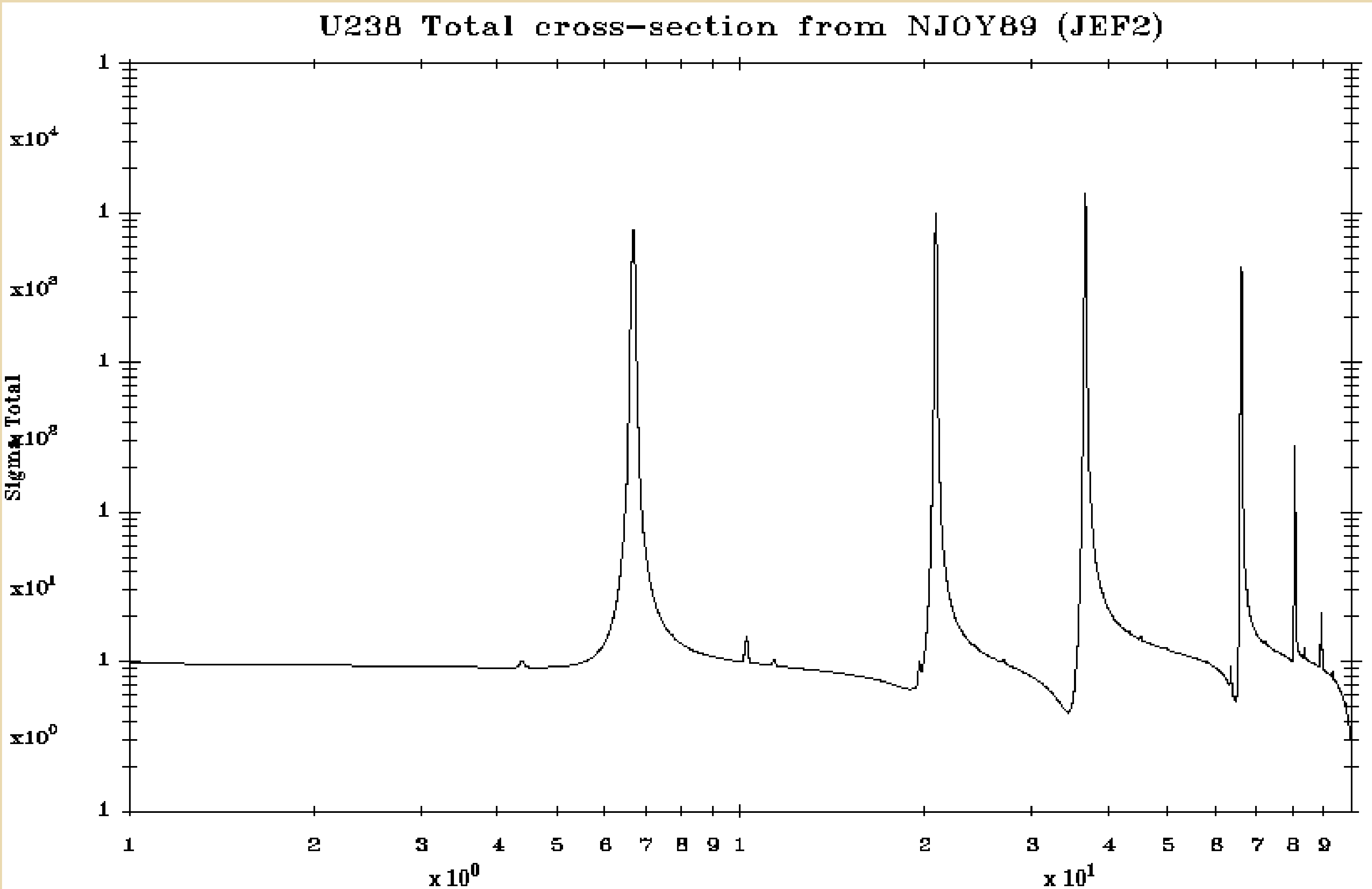
Examples: Regular lattice benchmarking

Safe number of CAGR pins in water

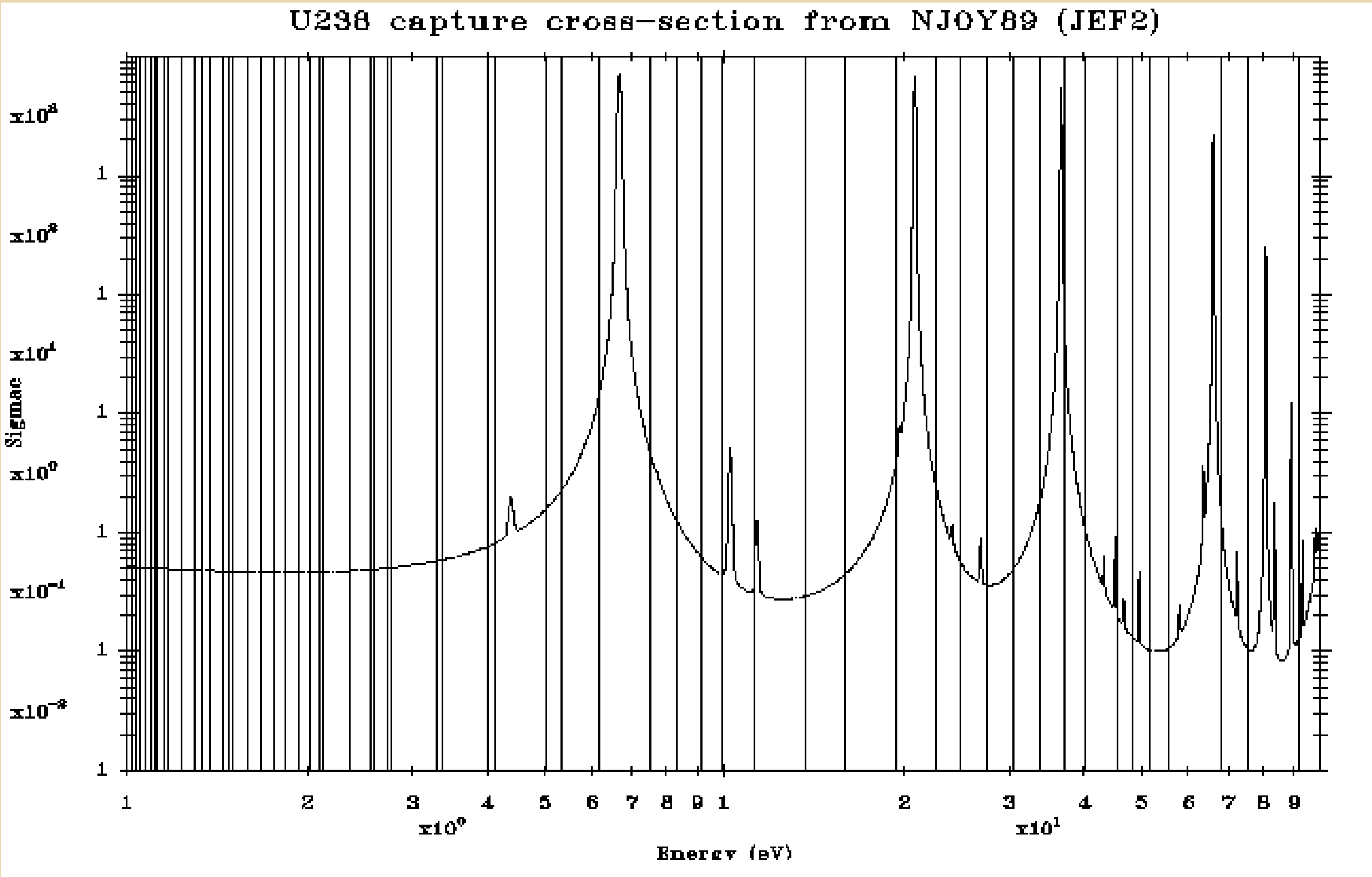
FLUX DISTRIBUTION WITHIN A FLUX CELL



U238 σ_T

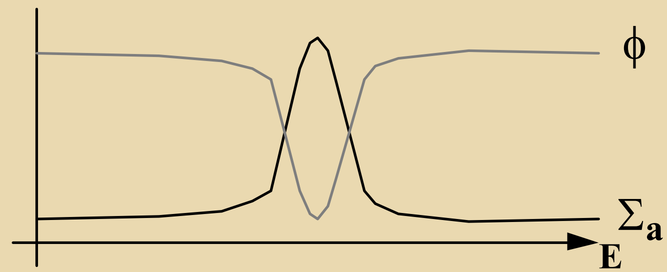

U238 Total cross-section from NJOY89 (JEF2)
Sigma Total
x10^4
x10^3
x10^2
x10^1
x10^0
1
1 2 3 4 5 6 7 8 9 1 2 3 4 5 6 7 8 9
x 10^0
x 10^1

POSITIONS OF WIMS LIBRARY GROUP BOUNDARIES AND PRINCIPAL RESONANCES



RESONANCE TREATMENT (Non-mathematical)

HOMOGENEOUS MIXTURE OF ABSORBER $\Sigma a(E)$ AND SCATTERER Σs (constant)



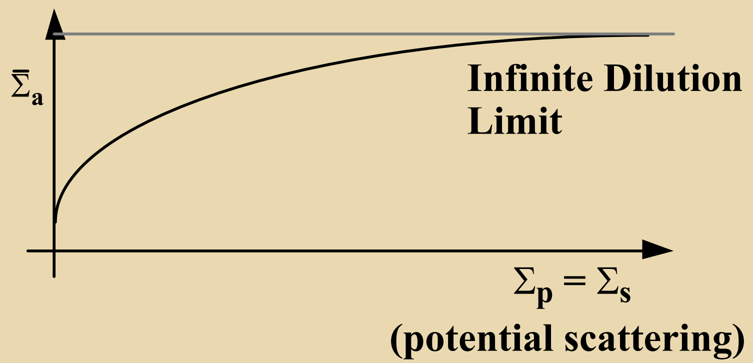
ABSORPTION RATE ~ $\int \Sigma_a \phi$

EFFECTIVE $\bar{\Sigma}_a = \dfrac{\int \Sigma_a \phi}{\int \phi}$

If Σs is very large, flux depression is small and

$$\bar{\Sigma}_a \rightarrow \int \Sigma_a \quad = \text{infinite dilution limit}$$

RESONANCE TREATMENT (Non-mathematical)



ISOLATED PINS

Neutrons pour in from the moderator as well as slowing down within the pin and tend to flatten the flux depression.

As pin radius $\rightarrow \infty$, **this effect** $\rightarrow 0$

$\rightarrow 0$, **source completely swamps the absorptions**

Use $\Sigma_p \sim \Sigma_s + \frac{1}{d}$ **where d is pin diameter.**

RESONANCE TREATMENT
(Non-mathematical)

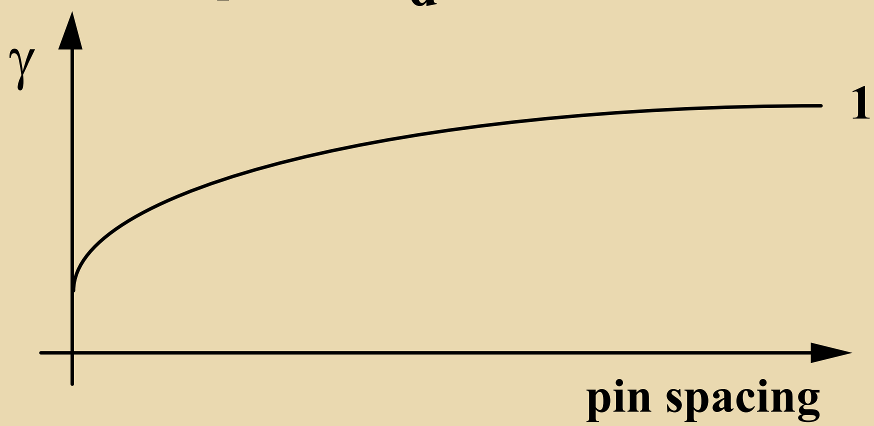
ARRAY OF PINS

The source of neutrons from the moderator at the resonance energy is reduced by absorptions in neighbouring pins.

Multiply 1/d effect by $\rightarrow$ **0 as pins are compacted to solid.**

$\rightarrow$ **1 as pins are widely separated**

Use $\Sigma_p \sim \Sigma_s + \frac{\gamma}{d}$



γ **is known as the** **<u>DANCOFF FACTOR</u>**

RESONANCE TREATMENT

- HOMOGENEOUS

$$\phi\,(\Sigma_p + \Sigma_a) \sim \Sigma_p$$

$$\phi \sim \int \frac{\Sigma_p}{\Sigma_p + \Sigma_a}\, du$$

Resonance Integral I

$$= \int \phi \Sigma_a\, du$$

$$= \int \frac{\Sigma_a \Sigma_p}{\Sigma_p + \Sigma_a}\, du$$

$$\phi = \int \left(\frac{\Sigma_p + \Sigma_a}{\Sigma_p + \Sigma_a} - \frac{\Sigma_a}{\Sigma_p + \Sigma_a} \right) du$$

$$= \Delta u - \frac{I}{\Sigma_p}$$

$$\therefore \quad \bar{\Sigma}_a = \frac{I}{\phi} = \frac{I}{\Delta u - \frac{I}{\Sigma_p}}$$

RESONANCE TREATMENT

HETEROGENEOUS (isolated pin)

2 region model (f=fuel, m=moderator)

$$V_f \Sigma_f \phi_f \sim V_f \Sigma_p P_{ff} + V_m \Sigma_m P_{mf} \qquad (1)$$

but

$$V_m \Sigma_m P_{mf} = V_f \Sigma_f P_{fm} = V_f \Sigma_f (1 - P_{ff}) \qquad (2)$$

$$\therefore \quad \Sigma_f \phi_f \sim \Sigma_p P_{ff} + \Sigma_f (1 - P_{ff}) \qquad (3)$$

RESONANCE TREATMENT

Rational Approximation

$$P_{ff} = \frac{\Sigma_f}{\Sigma_f + \frac{a}{\bar{l}}} \qquad \text{(a=Bell Factor)} \qquad (4)$$

$$I = \int \Sigma_a \phi_f = \int \Sigma_a \left[\frac{\Sigma_p}{\Sigma_f} P_{ff} + (1 - P_{ff}) \right] du$$

$$= \int \left[\frac{\Sigma_a \Sigma_p}{\Sigma_f + \frac{a}{\bar{l}}} + \frac{\Sigma_a \frac{a}{\bar{l}}}{\Sigma_f + \frac{a}{\bar{l}}} \right] du = \int \frac{\Sigma_a \left(\Sigma_p + \frac{a}{\bar{l}} \right)}{\Sigma_a + \left(\Sigma_p + \frac{a}{\bar{l}} \right)} du$$

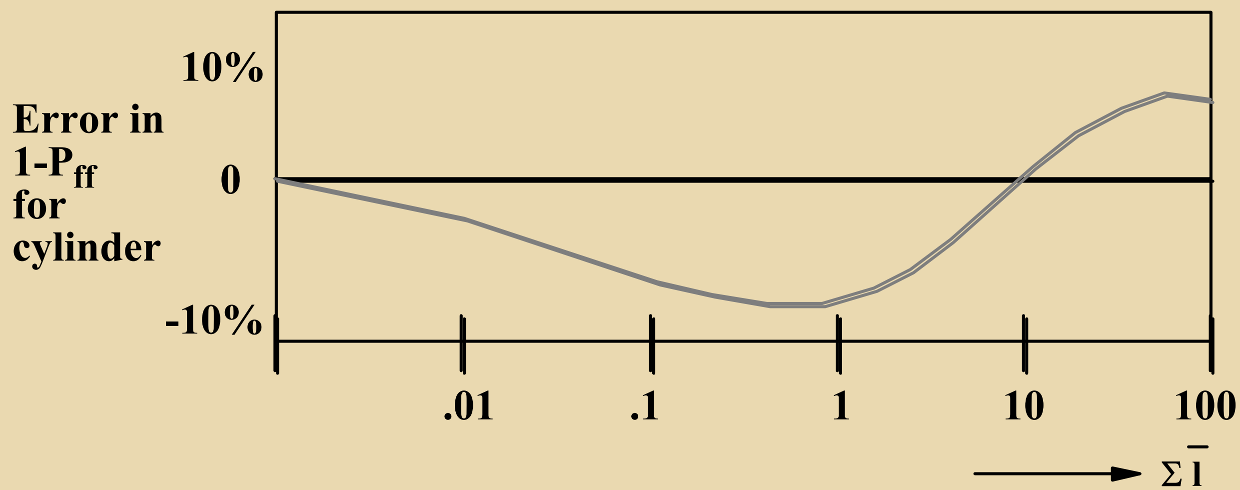
$\equiv$ Homog I with $\sigma p \rightarrow \sigma e = \sigma p + \frac{a}{N\bar{l}}$

RESONANCE TREATMENT

BELL FACTOR

$$P_{ff} = \frac{\Sigma}{\Sigma + \frac{a}{\bar{l}}}$$

where a~1.16



RESONANCE TREATMENT

DANCOFF FACTOR

$$\sigma_e = \sigma_p + \frac{a}{N\bar{l}}$$ for isolated rod

□p (homogeneous value) for ∞packed array

$\therefore$ Require factor on $\frac{a}{N\bar{l}}$ to allow for geometry varying from 1 forisolated rod to 0 for ∞ packing

Dancoff Factor ~ probability of collision in moderator before next fuel collision for neutrons leaving the fuel

$$\Rightarrow \sigma_e = \sigma_p + \frac{\gamma}{\gamma + a(1-\gamma)} \frac{a}{N\bar{l}}$$

RESONANCE TREATMENT

CORRECTIONS

MULTIPLE ABSORBERS

$$\bar{\Sigma}_a \rightarrow \frac{I}{\Delta u - \frac{I'}{\Sigma_p}}$$

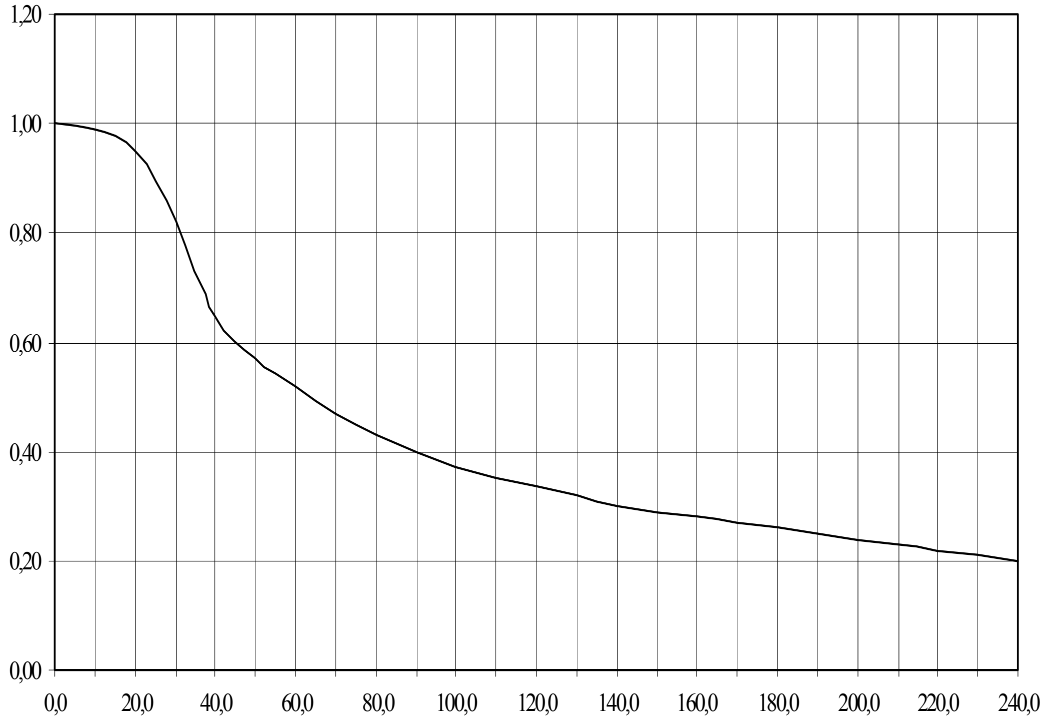
LAMBDA VALUES (Finite Resonance Width)

$\lambda\sigma_p$ used instead of σ_p

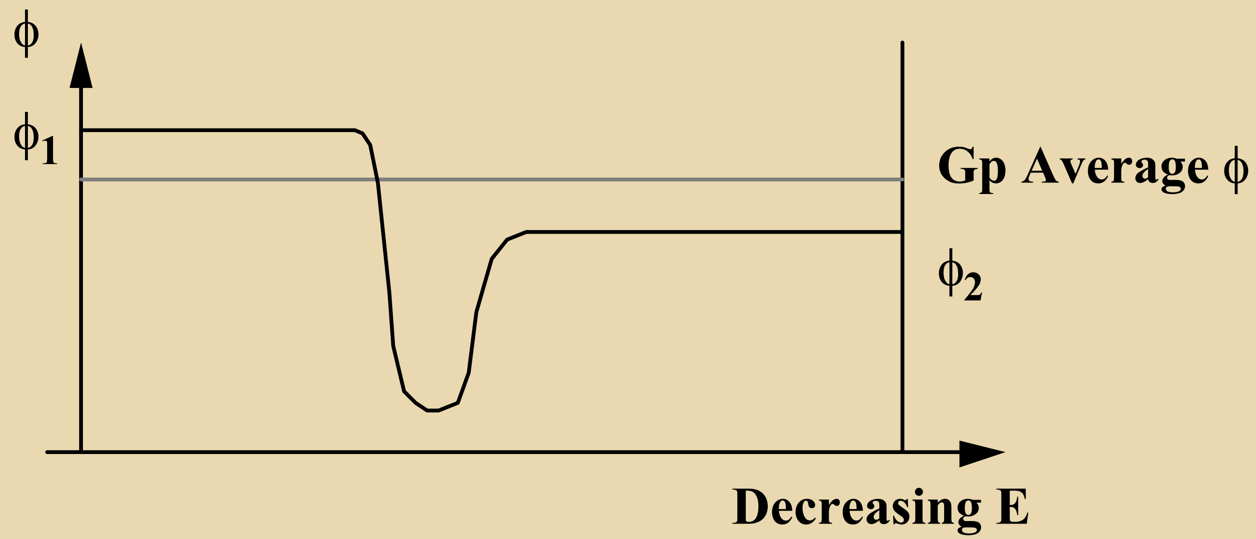
where λ is the effectiveness of a scatterer relative to Hydrogen

(λ depends on α, energy loss/collision and resonance width)

GRAPH OF λ(1-GROUP) AGAINST ATOMIC WEIGHT



f(p) CORRECTION TO GROUP REMOVAL



Downscatter from the group = f (p) $\Sigma_r \phi$

For heavy nuclides that remove neutrons only from the bottom of the group,

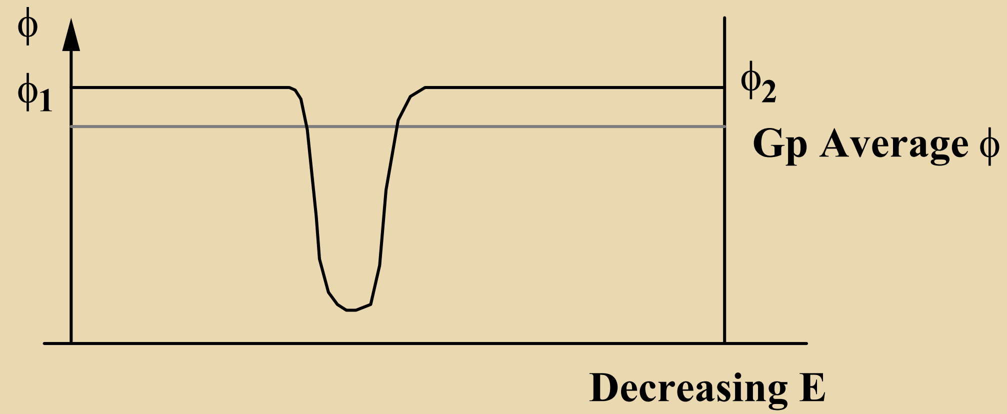
Removals = $\Sigma_r \phi_2$

and f(p)= ϕ_2 / ϕ_{ave}

For Hydrogen f(p)~1.0

f(p) CORRECTION TO GROUP REMOVAL

In a well moderated system:



$\phi_{ave} < \phi_2$ and $f(p) > 1$

NEUTRON TRANSPORT THEORY

METHODS:

Homogeneous	- Leakage Effects (B1)
Differential Transport	- DSN
Integral Transport (Collision Probabilities)	- PERSEUS, PIJ, PRIZE.

Analytic Solutions

- Homogeneous - 1D - equation is

$$\mu\frac{\partial\phi}{\partial z}+\Sigma_t\phi=\iint\Sigma_s\left(E'\rightarrow E\right)\phi dE'd\mu$$
$$+\lambda\chi\left(E\right)\int\upsilon\Sigma_f\left(E'\right)\phi dE'd\mu$$

- Separation of variables

$$\frac{\partial\phi}{\partial z}=F\left(E,\mu\right)\phi=\omega\phi$$

Analytic Solution

- Solution has the form

$$\phi = e^{\omega z}\varphi\left(E,\mu,\omega\right)$$

- Spectrum independent of position
- Spatial variation independent of energy

Bn Solutions

- General solution of **Homogeneous** transport equation - Used in WIMS in CRITIC module
- Solutions of form

$$\phi = e^{iBz}\varphi\left(E, \mu, B\right)$$

Bn Solution

- Using Spherical Harmonics for flux gives following solution of transport equation

$$\Sigma_g \varphi_g^l = \sum_k A_{lk}^g \sum_{g'} \Sigma_{g'g}^k \varphi_{g'}^k + \lambda A_{l0}^g \chi_g \sum_{g'} \upsilon \Sigma_{fg'} \varphi_{g'}^0$$

Bn Solution

Where

$$\varphi_g(\mu) = \sum_{lm} \frac{2l+1}{2} \varphi_g^{lm} P_{lm}(\mu)$$

$$\Sigma_{g'g}^{s}(\Omega' \to \Omega) = \sum_{lm} \frac{2l+1}{2} \Sigma_{g'g}^{l} P_l(\Omega.\Omega')$$

Bn Solution

- The variable A is given by

$$A_{lk}^{g} = \frac{1}{2}\int_{-1}^{1}\frac{P_l(\mu)P_k(\mu)}{\Sigma_g + iB\mu}d\mu$$

Simplified Solution

- Only P1 terms - Only equations in scalar and first moment of flux

$$\Phi_g = \varphi_g^0, J_g = -i\varphi_g^1$$

- This gives the following equations

Simplified Solution

- 2 Equations are

$$\left\{\Sigma_g - \Sigma^0_{gg} + \frac{B^2}{\left(3\alpha_g\Sigma_g - \Sigma^1_{gg}\right)}\right\}\Phi_g = \left\{\sum_{g'\neq g}\Sigma^0_{g'g}\Phi_{g'} + \lambda\chi_g\sum_{g'}\upsilon\Sigma_{fg'}\Phi_{g'}\right\}$$

$$-\frac{|B|}{\left(3\alpha_g\Sigma_g - \Sigma^1_{gg}\right)}\sum_{g'\neq g}\Sigma^1_{g'g}J_{g'}$$

$$J_g = \frac{\frac{B^2}{|B|}\Phi_g + \sum_{g'\neq g}\Sigma^1_{g'g}J_{g'}}{\left(3\alpha_g\Sigma_g - \Sigma^1_{gg}\right)}$$

Simplified Solution

- Note new form of diffusion coefficient

$$D_g = \frac{1}{3\alpha_g \Sigma_g - \Sigma^1_{gg}}$$

LEAKAGE OPTIONS in CHAIN 14

Homogeneous solutions based on:

- Diagonal Transport Corrected Flux Solution
- B1 Flux Solution

Diffusion Coefficients based on:

- Benoist 3-region model
- Transport cross sections
- Ariadne method

NUMERICAL INTEGRATION OF COLLISION PROBABILITIES

PIJ

COLLISION PROBABILITIES

Integral Transport Equation

$$\underbrace{\Sigma(\underline{\mathbf{r}}, E)\,\phi(\underline{\mathbf{r}}, E)} = \int_{\underline{\mathbf{r}}'} \underbrace{P(\underline{\mathbf{r}}' \rightarrow \underline{\mathbf{r}}, E)}\,\underbrace{\psi(\underline{\mathbf{r}}', E)}\, d\underline{\mathbf{r}}'$$

- **Reaction rate at position $\underline{\mathbf{r}}$**
- **Integrate over all positions $\underline{\mathbf{r}}'$**
- **First flight probability that neutrons produced at energy E and position $\underline{\mathbf{r}}'$ will have next collision at position $\underline{\mathbf{r}}$**
- **Neutron source at position $\underline{\mathbf{r}}'$ and energy E**

COLLISION PROBABILITIES (Continued)

$$\psi(\underline{r}', E) = \int_{E'} \left[\Sigma_s(\underline{r}', E' \to E) + \frac{\chi(E)}{k} \nu \Sigma_f(\underline{r}', E') \right] \phi(\underline{r}', E')\, dE'$$

- Neutron source at position $\underline{r}'$ and Energy E
- Integrate over all energies E′
- Neutron source at $\underline{r}'$ due to scattering
- Neutron source at Energy E due to fission at position $\underline{r}'$ and energy E′

COLLISION PROBABILITIES (Continued)

In group form

$$V_j \Sigma_j^g \phi_j^g = \sum_i V_i P_{ij}^g \sum_h \Sigma_i (h \rightarrow g) \phi_i^h + \sum_i V_i P_{ij}^g S_i^g$$

where the □'s are average fluxes in regions i and j.

Reciprocity and Conservation

Σi Vi Pij $=\Sigma j$ Vj Pji

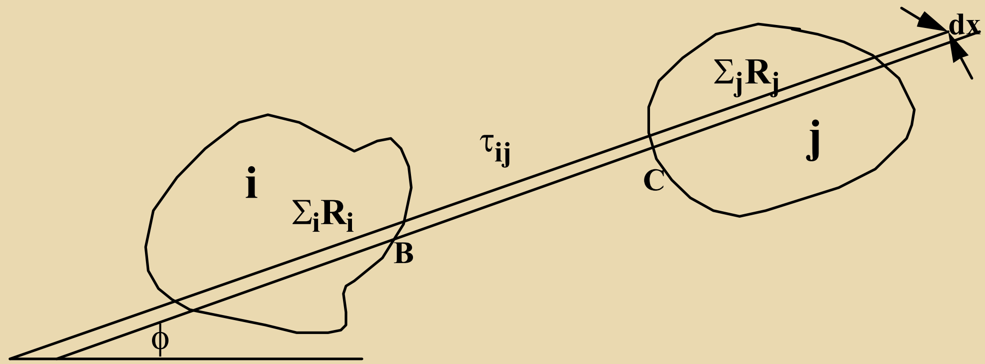
and $$\sum_j P_{ij} = 1$$

Can also show that

$$P_{si} = \frac{4\Sigma_i V_i}{S} P_{is} = \frac{4\Sigma_i V_i}{S}(1 - P_{ii})$$

where S is the surface for a single region

NUMERICAL INTEGRATION OF COLLISION PROBABILITIES



Integrate from

x =	- ∞	to	+∞
ϕ = 0	to	2π	
θ = 0	to	$\pi/2$	

$$P_{ij} = \frac{1}{2\pi V_i \Sigma_i} \int_0^{\pi/2} d\theta \int_{-\infty}^{\infty} dx \int_0^{2\pi} d\phi \left(1 - e^{(-\Sigma_i R_i)/\sin\theta}\right) e^{-\tau_{ij}/\sin\theta} \left(1 - e^{-\Sigma_j R_j/\sin\theta}\right) \sin^2\theta$$

$$P_{ij} = \frac{1}{2\pi V_i \Sigma_i} \int_0^{2\pi} d\phi \int_{-\infty}^{\infty} dx \{Ki_3(\tau_{ij}) - Ki_3(\tau_{ij} + \Sigma_i R_i) - Ki_3(\tau_{ij} + \Sigma_j R_j) + Ki_3(\tau_{ij} + \Sigma_i R_i + \Sigma_j R_j)\}$$

NUMERICAL INTEGRATION OF COLLISION PROBABILITIES

Note Symmetry

$$\Sigma_i V_i P_{ij} = \Sigma_j V_j P_{ji}$$

Collision Probability form of Transport Equation:

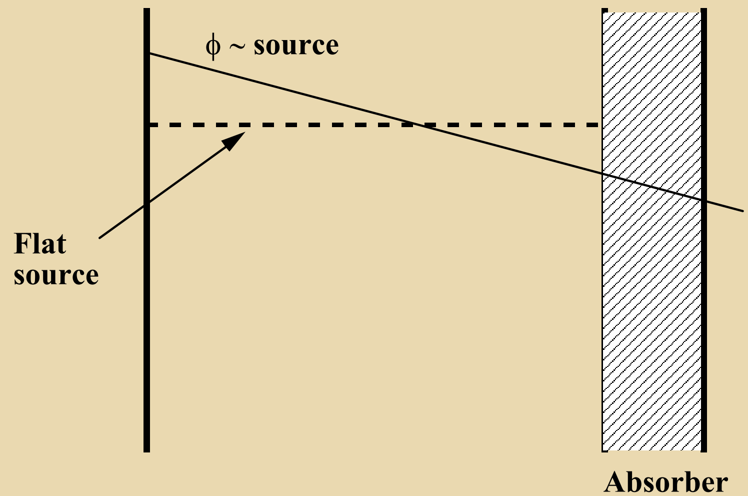
$$\Sigma\phi \sim \int_{space} P\psi$$

ASSUMPTIONS IN COLLISION PROBABILITY METHODS

Basic Assumptions:

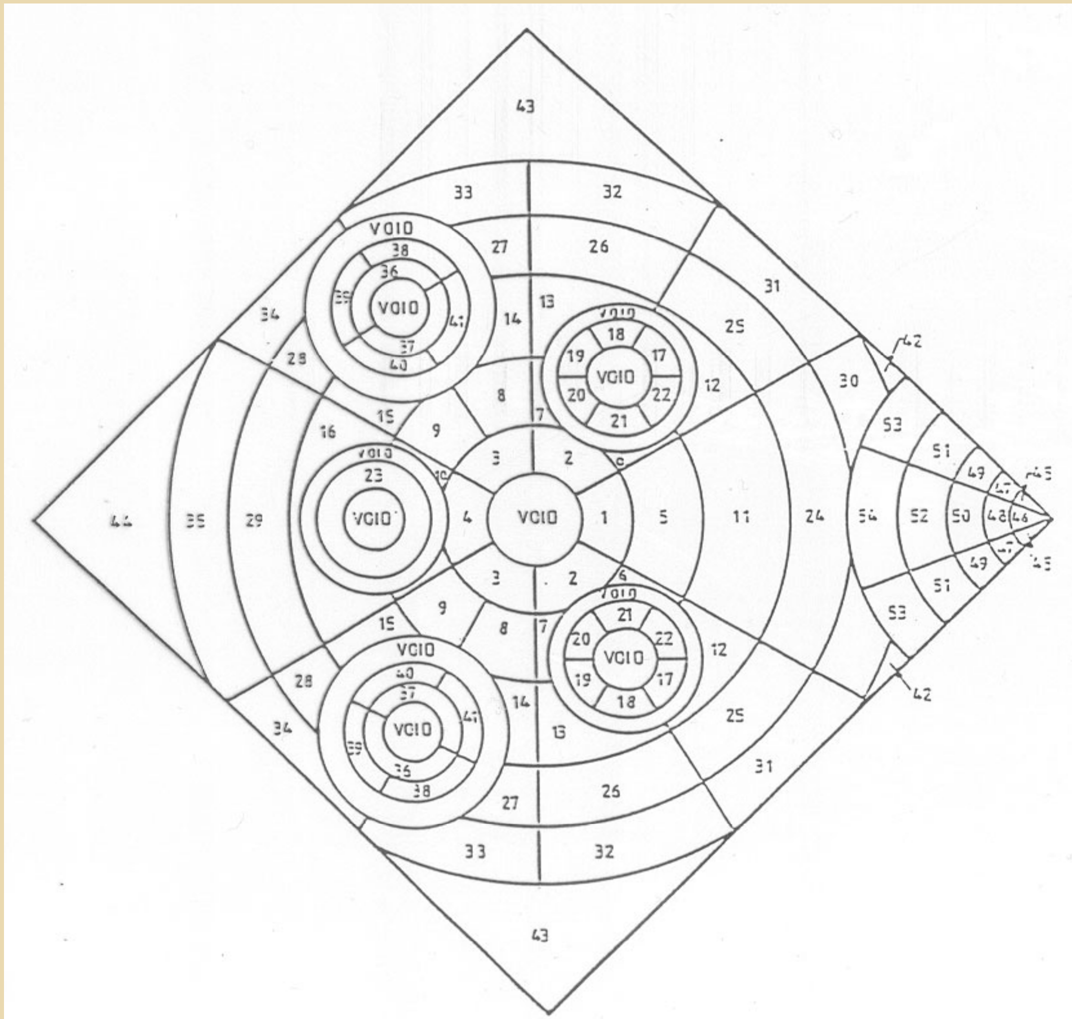
- isotropic scattering
- isotropic flux
- flat source in each region

Consequence of flat source assumption:



Flat source moves neutrons closer to absorber, which increases absorptions and reduces k.

PIJ Geometry



ANNULI IN PIJ GEOMETRY

In PIJ, ‘meshes’ in annuli cannot be defined.

Extra annuli must be defined as indicated above.

nregion defines the number of PIJ regions.

(If there are no azimuthal subdivisions of rods or annuli, nregion is the number of annuli plus the number of different ‘rodsubs’.)

Boundary Conditions

- Explicit Boundaries
  - a boundary can be dealt with explicitly by PIJ
  - Track is reflected back into problem as from a mirror
  - repeat process at number of reflections until no loss results from terminating track

Sn Methods

DSN

Boltzmann Equation

$$\vec{\Omega}_m \cdot \vec{\nabla}\varphi_m + \Sigma\varphi_m = S_m$$

Boltzmann Equation for Cylinders

$$\left[\eta\cos\phi\frac{\partial}{\partial r}-\eta\frac{\sin\phi}{r}\frac{\partial}{\partial\phi}+\Sigma\right]N(r,\omega,\phi,E)=S$$

$$\eta = \sin\ \omega$$

Scalar flux

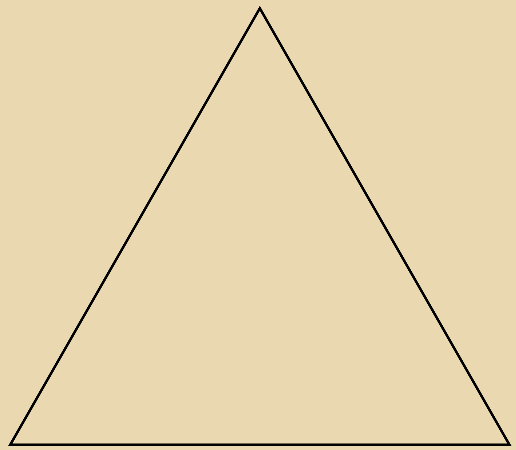
Sum over discrete directions

$$\phi = \sum_m w_m \ \varphi_m$$

Discrete Ordinates

- Set of points on the unit sphere
- Place triangular set of points on octant of unit sphere
- S_N method of order N
  - N/2 levels
  - ith level has N/2-i+1 points

S_2



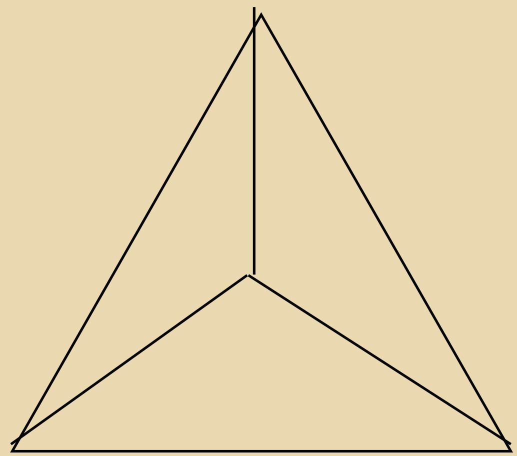
Lowest possible approximation

One direction per octant

8 equations (3D)

4 equations (2D)

S_4

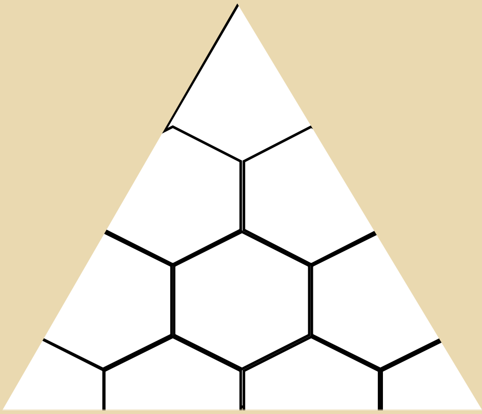


3 directions per octant

24 equations (3D)

12 equations (2D)

S_8



10 directions per octant

80 equations (3D)

40 equations (2D)

Weights

Weights proportional to angle subtended on unit sphere

$$w_m = \frac{\Delta \Omega_m}{4\pi}$$

$$\sum_m w_m = 1$$

Odd Moment Condition

For isotropic flux net current is zero

$$\vec{J} = \sum_m w_m \Omega_m \varphi_m = 0$$

$$\therefore \sum_m w_m \Omega_m = 0$$

Scattering Source

$$S_g(\vec{\Omega}) = \int \Sigma_{s,g'\to g}(\mu_0)\varphi_{g'}(\Omega')d\Omega'$$

could expand angular flux ....

$$\varphi(\vec{\Omega}) = \sum_{l=0}^{N} \sum_{m=-l}^{+l} \varphi_{lm} Y_{lm}(\vec{\Omega})$$

$$Y_{lm}(\theta,\psi) = \sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta)\exp(im\psi)$$

Linearly Anisotropic Scattering

$$S_m = \int \Sigma_{s0} \phi \, dE' + 3\hat{\Omega}_m \cdot \int \Sigma_{s1} J \, dE'$$

Use transport corrected cross sections

- scattering assumed isotropic

- correction for non isotropic effects

WIMSD DSN OPTION

GEOMETRY OPTIONS: HOMOGENEOUS
SLAB
ANNULAR
SPHERICAL
+ black or white boundary

SOLVES spatial mesh neutron balance equations by differential transport method of k-infinity and neutron flux by mesh and group.

NOT DIRECTLY APPLICABLE to complex geometries (eg. fuel clusters) without preliminary smearing of pincells into annuli.

S_N v Diffusion Theory

- S_N in principle more accurate than diffusion theory
- Difficult to calculate accurate transport cross sections in smeared geometries
- Restricted to simple geometries