

# Lecture Notes for the Course on NUMERICAL METHODS FOR NUCLEAR REACTORS

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## Unit-5 - Neutron Transport Theory Fundamentals and Solution Methods – Part 1

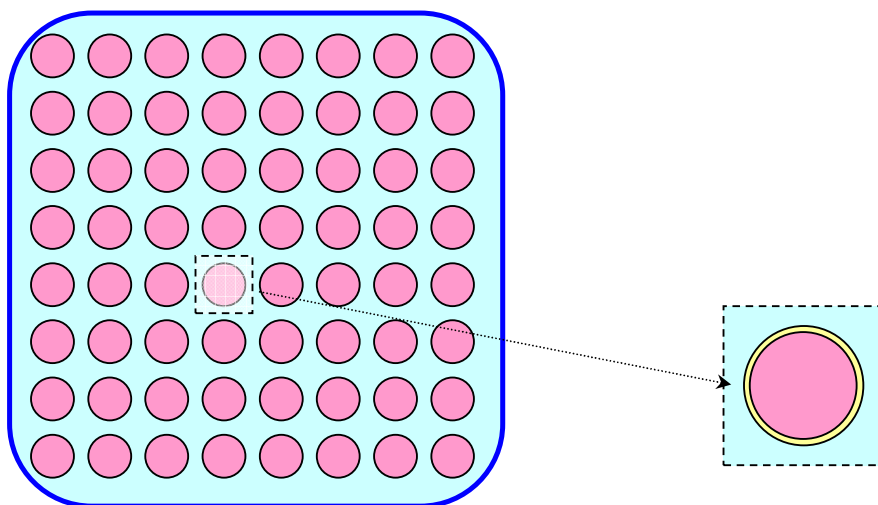
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# CELL CALCULATIONS

## General Considerations

- In heterogeneous reactors, materials are distributed in such a way that the reactor core is constituted by arrays of elementary units
- The fuel elements or “assemblies” constitute a first unit whose replication in different directions generates the entire core
- It is anyway more convenient to make reference to simpler elementary units named “cells”
- Since the number and the detail of the calculations to be performed are generally considerable, the cell must be described in such a way that the geometry will be the simplest possible
  - ◆ the height of the cell is generally considered very large with respect to the radial dimensions, in order to accept results obtained by 2D calculations
  - ◆ square or hexagonal cells can be reduced to equivalent cylindrical cells, obtained by preserving the volumes of the various regions (*Wigner-Seitz approximation*)

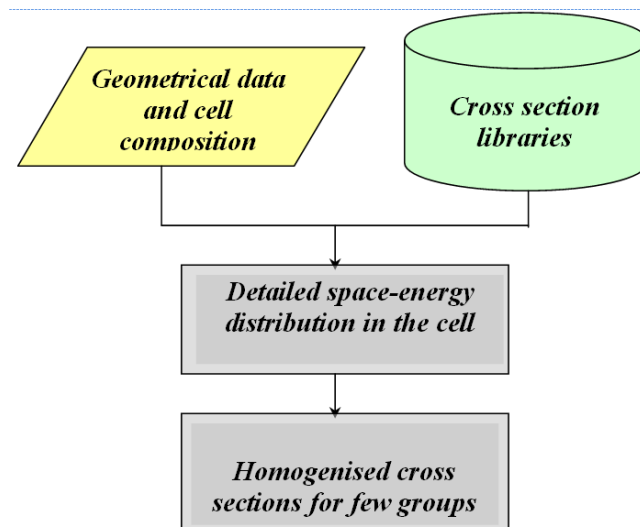


- Performing cell calculations requires to know of the exact geometry of the cell and the availability of accurate libraries of cross sections
- The calculations provide firstly the space-energy detailed trend of flux in the cell corresponding to the assigned values of material compositions and physical parameters (transport theory is used)

The number of the considered energy groups can be even relatively large, e.g. 100 - 200

The constants homogenized in few energy groups (e.g., 2 or 3) are then calculated, providing the basis for the calculation of the space-time distribution of neutron flux across the entire reactor (generally performed using diffusion)

*Elementary methods* have been applied in the past in addition to numerical ones. Some recipes used in their developments are still used nowadays in codes. We will anyway omit their discussion.



**Logical flow of cell calculations**

# NUMERICAL SCHEMES

Since elementary methods, whose discussion we omitted, make use of heavy assumptions, as flat flux profile and uniform and isotropic sources, it is necessary to make use of more adequate tools to evaluate the detailed structure (both in space and in energy) of the neutron flux

Firstly, it is necessary to discretize the addressed energy interval into a generally large number of energy groups.

The small size of the cell suggest to adopt the transport equation but, in general, examples of application of the calculation procedure can be also made making use of diffusion theory

## Calculation of the detailed energy spectrum with assigned buckling

The calculations with assigned buckling are often performed in order to consider an element of the core (cell or assembly) as belonging to a larger core with its macroscopic distribution

In fact, considering the cell or the assembly as “isolated” fails in considering the effect of leakages that do occur in finite cores: this assumed “asymptotic” spatial behavior thus improves the results of calculations including parametrical leakages effects

In this purpose, let us consider as a simple example the application of the *diffusion* theory to “macro-regions” assumed to be homogeneous

If the slowing down phase is mainly addressed, the epithermal and fast energy interval (0.65-1.3 eV to 14 MeV) is subdivided into a large number of intervals with nearly equal spacing in lethargy

In the “macro-region” the energy-space separability of the flux is assumed so that:

$$\begin{aligned} \phi(\vec{r}, E) &= \phi_{\infty}(E)\phi(\vec{r}) & \nabla^2\phi + B^2\phi &= 0 \\ B^2 &= B_{mat}^2 = (k_{\infty} - 1)/M^2 & M^2 &= L_1^2(1 - f) + \tau_t \\ L^2 &= \frac{\tilde{D}}{\tilde{\Sigma}_a} = \frac{1}{3\tilde{\Sigma}_a\tilde{\Sigma}_{tr}} = L_1^2(1 - f) \left(1 + \frac{V_0\bar{\phi}_0}{V_1\bar{\phi}_1}\right)^2 \bigg/ \left(1 + \frac{\Sigma_{tr,0}V_0\bar{\phi}_0}{\Sigma_{tr,1}V_1\bar{\phi}_1}\right) \cong L_1^2(1 - f) \end{aligned}$$

In each energy interval it is assumed that:

$$\phi_g(\vec{r}) = \int_{\Delta E_g} \phi(\vec{r}, E) dE = \phi(\vec{r}) \int_{\Delta E_g} \phi_\infty(E) dE = \phi(\vec{r}) \phi_{\infty,g}$$

**From the equations with very many energy groups**

$$\tilde{D}_g^{(h)} \nabla^2 \phi_g(\vec{r}) - \tilde{\Sigma}_{r,g}^{(h)} \phi_g(\vec{r}) + \sum_{g' < g} \tilde{\Sigma}_{s,g' \rightarrow g}^{(h)} \phi_{g'}(\vec{r}) + S_g(\vec{r}) = 0 \quad (g = 1, \dots, G)$$

**assuming that**

$$S_g(\vec{r}) = S_g \phi(\vec{r})$$

**we obtain**

$$-\left(\tilde{\Sigma}_{r,g}^{(h)} + D_g^{(h)} B^2\right) \phi_{\infty,g} + \sum_{g' < g} \tilde{\Sigma}_{s,g' \rightarrow g}^{(h)} \phi_{\infty,g'} + S_g = 0 \quad (g = 1, \dots, G)$$

**being a lower triangular system of algebraic equations**

**Generally, in order to normalize the source, it is put:**

$$S_g = \chi_g \quad (g = 1, \dots, G)$$

The vector  $\{\phi_{\infty,g}\}_1^G$  represents the *detailed asymptotic flux* in region  $h$ . Once we are in possession of its distribution, we can calculate the “few group” cross sections.

**Let us assume that we need defining three “energy macro-groups”:**

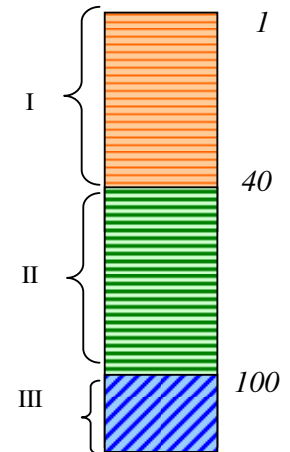
**GROUP I:** *fast group* (14 MeV → 20 keV)

**in this case we assume it involves the groups  $g = 1, \dots, 40$  in the detailed subdivision;**

**GROUP II:** *epithermal group* (20 keV → 1.3 eV)

**e.g., corresponding to  $g = 41, \dots, 100$  in the detailed subdivision;**

**GROUP III:** *thermal group* (1.3 eV → 0 eV) that is here only marginally addressed.



In this case the cross sections for the first two energy macro-groups are:

$$\tilde{\Sigma}_a^I = \frac{\sum_{g=1}^{40} \Sigma_{a,g}^{(h)} \phi_{\infty,g}}{\sum_{g=1}^{40} \phi_{\infty,g}} \quad \tilde{\Sigma}_a^{II} = \frac{\sum_{g=41}^{100} \Sigma_{a,g}^{(h)} \phi_{\infty,g}}{\sum_{g=41}^{100} \phi_{\infty,g}}$$

Similar formulations are applicable also for the other cross sections:

$$\tilde{\Sigma}_s^{I \rightarrow II} = \frac{\sum_{g=41}^{100} \sum_{g'=1}^{40} \Sigma_{s,g' \rightarrow g}^{(h)} \phi_{\infty,g'}}{\sum_{g'=1}^{40} \phi_{\infty,g'}}$$

(the index  $h$  has been momentarily omitted). Programs must supply the full scattering matrix for large groups, including the terms for transfer to the thermal group:

$$\begin{bmatrix} 0 & 0 & 0 \\ \tilde{\Sigma}_s^{I \rightarrow II} & 0 & 0 \\ \tilde{\Sigma}_s^{I \rightarrow III} & \tilde{\Sigma}_s^{II \rightarrow III} & 0 \end{bmatrix}$$

- In the case of absorption cross sections it is often necessary to start from resonance integrals calculated with analytical treatment (narrow or wide resonance) or semi-analytical treatment (intermediate resonance) or numerical treatment (Nordheim)

- We can distinguish two cases:

- ◆ *Homogeneous medium*

For the  $k$ -th resonance in group  $g$  it is

$$I_g^k = \int_{\Delta u_g} [\sigma_{a0}(u)]_{eff} du = \int_{u_g}^{u_{g+1}} \sigma_{a0}(u) \frac{\phi(u)}{\phi_{as}} du$$

So, being

$$\Sigma_{a,g} = \frac{\int_{u_g}^{u_{g+1}} N_0 \sigma_{a0}(u) \phi(u) du}{\int_{u_g}^{u_{g+1}} \phi(u) du}$$

by dividing numerator and denominator by  $\phi_{as}$ , it is therefore

$$\Sigma_{a,g} = N_0 \frac{\sum_{k=1}^{K_g} I_g^k}{\int_{\Delta u_g} \frac{\phi(u)}{\phi_{as}} du} \quad \text{or} \quad \Sigma_{a,g} = N_0 \frac{\sum_{k=1}^{K_g} I_g^k}{\Delta u_g} \quad (\text{if it is } \phi \approx \phi_{as} \text{ in } \Delta u_g)$$

◆ **Heterogeneous medium:**

**For the  $k$ -th resonance in group  $g$  it is**

$$I_g^k = \int_{\Delta u_g} [\sigma_{a0}(u)]_{eff} du = \int_{u_g}^{u_{g+1}} \sigma_{a0}(u) \frac{\phi_0(u)}{\phi_{as}} du$$

**and the macroscopic homogenized cross section in group  $g$  is:**

$$\tilde{\Sigma}_{a,g} = \frac{V_0 \int N_0 \sigma_{a0}(u) \phi_0(u) du}{V_0 \int_{\Delta u_g} \phi_0(u) du + V_1 \int_{\Delta u_g} \phi_1(u) du}$$

**where it was assumed that fluxes are spatially constant**

**If we further assume that  $\phi_1(u) \equiv \phi_{as}$ , it is:**

$$\tilde{\Sigma}_{a,g} = \frac{V_0 \int_{\Delta u_g} N_0 \sigma_{a0}(u) \frac{\phi_0(u)}{\phi_{as}} du}{V_0 \int_{\Delta u_g} \frac{\phi_0(u)}{\phi_{as}} du + V_1 \Delta u_g} = \frac{\tilde{N}_0 \sum_{k=1}^{K_g} I_g^k}{\frac{V_0}{V} \int_{\Delta u_g} \frac{\phi_0(u)}{\phi_{as}} du + \frac{V_1}{V} \Delta u_g} \quad \tilde{N}_0^{(h)} = N_0 \frac{V_0}{V}$$

**where  $V = V_0 + V_1$  is the cell volume; assuming again that  $\phi_0(u) \approx \phi_{as}$  on a large share of  $\Delta u_g$  we would again obtain**

$$\tilde{\Sigma}_{a,g} = \tilde{N}_0 \frac{\sum_{k=1}^{K_g} I_g^k}{\Delta u_g}$$

- **The few group cross sections can be therefore obtained**
- **As an alternative to the use of diffusion theory, the transport theory can be use, e.g., making use of the  $P_N$  and  $B_N$  equations with the spatial asymptotic approximation (i.e., assuming a value of the buckling)**
- **The codes normally also compute  $\sigma_{tr,g} = \sigma_{s,g}(1 - \bar{\mu})$  ( $\bar{\mu} = 2/3A$ ) and, collapsing the data into large groups, the cross sections  $\tilde{\Sigma}_{tr}^I$ ,  $\tilde{\Sigma}_{tr}^{II}$  and then  $\tilde{D}^I = 1/3\tilde{\Sigma}_{tr}^I$  e  $\tilde{D}^{II} = 1/3\tilde{\Sigma}_{tr}^{II}$  are calculated.**



- In order to obtain these results, the libraries must contain all the necessary data for the involved materials
- It is therefore possible to write the diffusion (or transport) equations for few groups. For three groups, for instance, it is:

$$\begin{cases} \tilde{D}_1^{(h)} \nabla^2 \phi_1 - \Sigma_{r,1}^{(h)} \phi_1 + \frac{1}{k} \chi_1 \left( \nu_1 \tilde{\Sigma}_{f,1}^{(h)} \phi_1 + \nu_2 \tilde{\Sigma}_{f,2}^{(h)} \phi_2 + \nu_3 \tilde{\Sigma}_{f,3}^{(h)} \phi_3 \right) = 0 \\ \tilde{D}_2^{(h)} \nabla^2 \phi_2 - \Sigma_{r,2}^{(h)} \phi_2 + \Sigma_{s,1 \rightarrow 2}^{(h)} \phi_1 + \frac{1}{k} \chi_2 \left( \nu_1 \tilde{\Sigma}_{f,1}^{(h)} \phi_1 + \nu_2 \tilde{\Sigma}_{f,2}^{(h)} \phi_2 + \nu_3 \tilde{\Sigma}_{f,3}^{(h)} \phi_3 \right) = 0 \\ \tilde{D}_3^{(h)} \nabla^2 \phi_3 - \Sigma_{r,3}^{(h)} \phi_3 + \Sigma_{s,1 \rightarrow 3}^{(h)} \phi_1 + \Sigma_{s,2 \rightarrow 3}^{(h)} \phi_2 = 0 \end{cases}$$

### Use of transport codes

- The calculation scheme for a more modern cell code is not very different from the one reported above for the simplified case of diffusion
- Traditionally, two sections of the program are considered, being *fast and epithermal*, on one side, and *thermal*, on the other

#### a) *Fast-epithermal spectrum in the cell*

- ◆ The code must have access to wide libraries in the epithermal and fast regions at several groups (hundreds)
- ◆ The resonance integrals are made making use of the Nordheim technique in a full zone approach; analytical approaches are also used
- ◆ Routines will also calculate in an automatic way the different needed coefficients (e.g., Dancoff)
- ◆ Once the homogenized cross sections are obtained for the  $G$  groups, the  $\phi_{\infty,g}$  in the homogeneous medium are calculated by transport ( $P_N$  or  $B_N$ ) with tentative buckling
- ◆ In the detailed flux analyses some codes allow to keep separate the different regions (e.g., ANISN, which is a 1D SN method, see later)
- ◆ The detailed energy distribution then allows to obtain constants with few groups

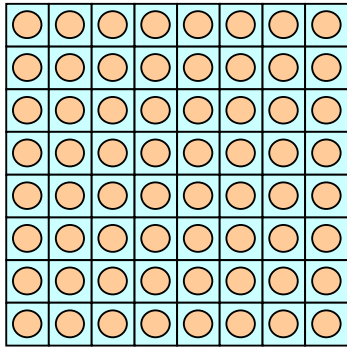
- ◆ These calculations must be repeated several times, owing to the different compositions present in the core

*b) Thermal spectrum in the cell*

- ◆ In principle the same considerations already applied for the epithermal-fast region apply
- ◆ The main difference consists in the fact that the up-scattering makes the scattering matrix to be no more triangular and it is also more complicated to be obtained
- ◆ Imposed buckling calculations can be made ( $P_N$  or  $B_N$  methods) or the method of collision probability, based on the integral equation, is also used, assuming in this case isotropic scattering
- ◆ Methods based on the integro-differential equation, fully accounting for anisotropy can be also used

*c) Assembly calculations*

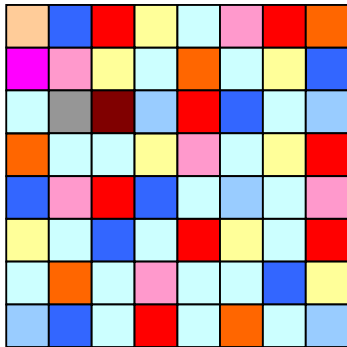
- ◆ Given the compositions of the different cells and the homogenized cross sections, there are different possible ways of making the assembly calculations
- ◆ In a traditional procedure the assembly is considered as composed of small homogenized square cells, then making use of diffusion or transport to further homogenize assuming reflective boundary conditions
- ◆ Collapsing the cross sections to fewer groups over the entire assembly must then be made
- ◆ A more up-to-date treatment involves to keep memory about the heterogeneity of the cell during further homogenization and group collapsing
- ◆ The two routes as simply illustrated in the next page



Cell calculations with many groups by transport theory



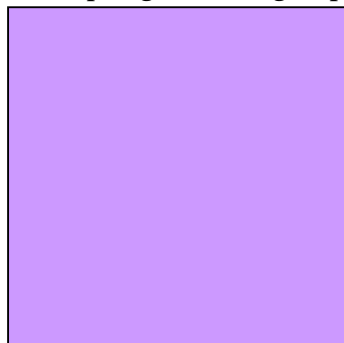
*Frist homogenization to 6 groups in each cell*



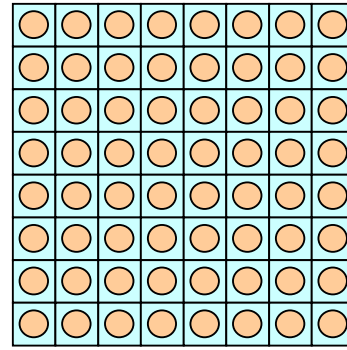
Assembly calculations with diffusion theory



*Second homogenization and collapsing to 2 or 3 groups*



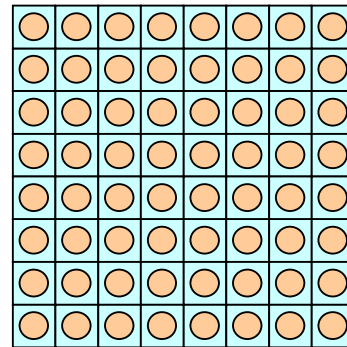
***Traditional approach***



Cell calculations with many groups by transport theory



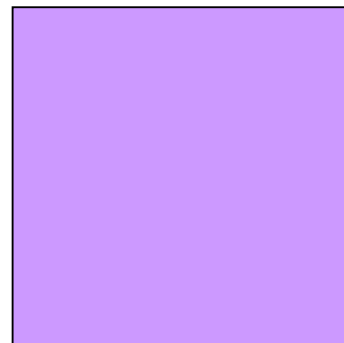
*6 or 15 group cross sections for the fuel and moderator regions*



2D assembly calculations with transport techniques



*Homogenization and collapsing to 2 or 3 groups*



***Modern approach***

**Examples of sequences of homogenization in cell and assembly calculations**

# NEUTRON TRANSPORT EQUATION

## Obtaining the integro-differential form

- We consider the change in *the number of neutrons* initially contained in an elementary volume  $dV$  around  $\vec{r}$  having direction of motion inside an elementary angle  $d\Omega$  around  $\vec{\Omega}$  and speed in an elementary interval  $dv$  around  $v$
- In one of the possible treatments, the related balance equation can be obtained “following” this bunch of neutrons initially in  $dV$ , accounting for absorptions, scattering and sources
- Since we “follow” the neutrons, in this treatment there are no explicit terms related to the leakage of neutrons through the interfaces, though what we will call “streaming” term can be also considered a “leakage” term in a control volume perspective
- The change in the number of these neutrons in the elementary time interval  $dt$  is given by

$$\delta n = \left[ n(\vec{r} + v\vec{\Omega}dt, v\vec{\Omega}, t + dt) - n(\vec{r}, v\vec{\Omega}, t) \right] dV dv d\Omega$$

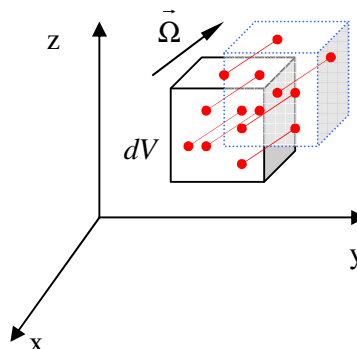
- Since in Cartesian coordinates it is by definition

$$\vec{r} \equiv \{x, y, z\} \quad \text{and} \quad \vec{\Omega} \equiv \{\Omega_x, \Omega_y, \Omega_z\}$$

we have:

$$n(\vec{r} + v\vec{\Omega}dt, v\vec{\Omega}, t + dt) \approx n(\vec{r}, v\vec{\Omega}, t) + \left[ \frac{\partial n}{\partial t} + \frac{\partial n}{\partial x} v\Omega_x + \frac{\partial n}{\partial y} v\Omega_y + \frac{\partial n}{\partial z} v\Omega_z \right] dt$$

and then



$$\delta n = \left[ \frac{\partial n}{\partial t} + \frac{\partial n}{\partial x} v \Omega_x + \frac{\partial n}{\partial y} v \Omega_y + \frac{\partial n}{\partial z} v \Omega_z \right] dV dv d\Omega dt =$$

$$= \left[ \frac{\partial n}{\partial t} + v \vec{\Omega} \cdot \text{grad}_{\vec{r}} n(\vec{r}, v \vec{\Omega}, t) \right] dV dv d\Omega dt$$

- **It is moreover:**

$$\delta n = - \left( \begin{array}{c} \text{collisions} \\ \text{extracting neutrons} \end{array} \right) + \left( \begin{array}{c} \text{inverted collisions} \\ \text{contribution} \end{array} \right) + \left( \begin{array}{c} \text{contribution} \\ \text{due to independent sources} \end{array} \right)$$

**Therefore**

$$\delta n = -v n(\vec{r}, v \vec{\Omega}, t) \Sigma_t(\vec{r}, v) \cdot dV dv d\Omega dt$$

$$+ \int_0^\infty dv' \int_{4\pi} v' n(\vec{r}, v' \vec{\Omega}', t) \Sigma_s(\vec{r}, v' \vec{\Omega}' \rightarrow v \vec{\Omega}) d\Omega' \cdot dV dv d\Omega dt$$

$$+ S(\vec{r}, v \vec{\Omega}, t) dV dv d\Omega dt$$

**and then**

$$\frac{\partial n}{\partial t} + v \vec{\Omega} \cdot \text{grad}_{\vec{r}} n(\vec{r}, v \vec{\Omega}, t) = -v n(\vec{r}, v \vec{\Omega}, t) \Sigma_t(\vec{r}, v)$$

$$+ \int_0^\infty dv' \int_{4\pi} v' n(\vec{r}, v' \vec{\Omega}', t) \Sigma_s(\vec{r}, v' \vec{\Omega}' \rightarrow v \vec{\Omega}) d\Omega' + S(\vec{r}, v \vec{\Omega}, t)$$

- **Making energy to become the independent variable in place of velocity, we have:**

$$\frac{1}{v} \frac{\partial}{\partial t} \phi(\vec{r}, E, \vec{\Omega}, t) + \vec{\Omega} \cdot \text{grad}_{\vec{r}} \phi(\vec{r}, E, \vec{\Omega}, t) + \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, \vec{\Omega}, t) =$$

$$= \iint \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \phi(\vec{r}, E', \vec{\Omega}', t) dE' d\Omega' + S(\vec{r}, E, \vec{\Omega}, t)$$

- **From left to right, we recognize the following terms in the equation:**
  - ◆ **the rate of change in neutron density**
  - ◆ **the “streaming” term (also said *leakage term*: see later for an explanation)**
  - ◆ **the collision (scattering + absorption) term**
  - ◆ **the inverted collision (“scattering”) term**
  - ◆ **the independent (assigned) source**

- If a fission source is explicitly considered, we have:

$$\begin{aligned} \frac{\partial n}{\partial t} + v\vec{\Omega} \cdot \text{grad}_{\vec{r}} n(\vec{r}, v\vec{\Omega}, t) &= -vn(\vec{r}, v\vec{\Omega}, t)\Sigma_t(\vec{r}, v) \\ + \int_0^\infty dv' \int_{4\pi} v' n(\vec{r}, v'\vec{\Omega}', t) \Sigma_s(\vec{r}, v'\vec{\Omega}' \rightarrow v\vec{\Omega}) d\Omega' &+ S(\vec{r}, v\vec{\Omega}, t) \\ + \frac{\chi(v)}{4\pi} \int_0^\infty dv' \int_{4\pi} v' n(\vec{r}, v'\vec{\Omega}', t) v \Sigma_f(\vec{r}, v') d\Omega' & \end{aligned}$$

which evidently assumes that *the fission source is isotropic*

- The transport equation is *linear*; therefore, it is possible to define (at least formally) a *Green function* that provides a solution for any given distribution of independent sources

### Initial conditions

- Assigning initial conditions does not involve special problems: an appropriate function representing the neutron flux or the angular density at  $t=0$  is sufficient

### Conditions at the interfaces

- *The angular flux [density] is spatially continuous across the interfaces, once the direction is fixed*
  - ◆ this follows from an obvious condition of continuity
  - ◆ this does not hold only if interfaces are considered as *surface sources*

### Boundary conditions

- The more frequently used ones are
  - ◆ *Free surface, i.e. interface to the void*  
it applies over the boundary  $\partial V$  of a *convex* domain  $V$  (i.e., *non-reentrant*), such that neutrons exiting from the surface have a negligible probability to reenter

$$\phi(\vec{r}, \vec{\Omega}, E, t) = 0 \quad \text{for} \quad \vec{\Omega} \cdot \vec{u}_e < 0, \vec{r} \in \partial V$$

where  $\vec{u}_e$  is the outward directed unity vector normal to the boundary

◆ *imposed incoming flux*

also this condition can be applied to the boundary  $\partial V$  of a domain  $V$  and can be expressed as

$$\phi(\vec{r}, \vec{\Omega}, E, t) = \Psi(\vec{r}, \vec{\Omega}, E, t) \quad \text{for} \quad \vec{\Omega} \cdot \vec{u}_e < 0, \vec{r} \in \partial V$$

◆ *reflection with assigned “albedo”*

it is assumed that the flux entering through  $\partial V$  in a given direction is equal to a fraction  $\alpha(E)$  (“albedo”) of the exiting one corresponding to it by a reflection condition

$$\phi(\vec{r}, \vec{\Omega}, E, t) = \alpha(E) \phi(\vec{r}, \vec{\Omega}', E, t) \quad \text{for} \quad \vec{\Omega} \cdot \vec{u}_e < 0, \vec{r} \in \partial V$$

and for

$$\vec{\Omega} \cdot \vec{u}_e = -\vec{\Omega}' \cdot \vec{u}_e \quad \mathbf{e} \quad (\vec{\Omega} \times \vec{\Omega}') \cdot \vec{u}_e = 0 \quad ;$$

with  $\alpha(E) = 1$  we have the *pure reflection*;

◆ *white or diffuse reflection*

in this case we assume that the number of neutrons exiting from any surface element is equal to that of entering neutrons and that the entering angular flux is isotropic; it is:

$$J_{u_e}^- = J_{u_e}^+ \\ \phi(\vec{r}, \vec{\Omega}, E, t) = C \quad \text{for} \quad \vec{\Omega} \cdot \vec{u}_e < 0, \vec{r} \in \partial V$$

with

$$J_{u_e}^- = |\vec{J}_{u_e}^- \cdot \vec{u}_e| = \int_{\vec{\Omega}' \cdot \vec{u}_e < 0} |\vec{u}_e \cdot \vec{\Omega}'| \phi(\vec{r}, \vec{\Omega}', E, t) d\Omega' = \int_0^{2\pi} d\phi \int_{-1}^0 |\mu| C d\mu = \pi C \\ J_{u_e}^+ = \vec{J}_{u_e}^+ \cdot \vec{u}_e = \int_{\vec{\Omega}' \cdot \vec{u}_e > 0} \vec{u}_e \cdot \vec{\Omega}' \phi(\vec{r}, \vec{\Omega}', E, t) d\Omega'$$

It is therefore:

$$\phi(\vec{r}, \vec{\Omega}, E, t) = C = \frac{1}{\pi} J_{u_e}^+ = \frac{1}{\pi} \int_{\vec{\Omega}' \cdot \vec{u}_e > 0} \vec{u}_e \cdot \vec{\Omega}' \phi(\vec{r}, \vec{\Omega}', E, t) d\Omega' \quad \vec{\Omega} \cdot \vec{u}_e < 0, \vec{r} \in \partial V$$

◆ *variable flux with space periodicity*

this situation can be obtained for instance in the case of an infinite core composed by elementary cells that are all equal and is expressed in the form

$$\phi(\vec{r}, \vec{\Omega}, E, t) = \phi(\vec{r} + m\vec{r}_l, \vec{\Omega}, E, t)$$

where  $\vec{r}_l$  is a vector whose magnitude represents the size of the cell and  $m$  is an integer number

### Transport Equation and Neutron Balance

- From the integro-differential equation, involving the angular flux, it is possible to obtain the neutron continuity equation in terms of scalar flux

$$\frac{1}{v} \frac{\partial}{\partial t} \phi(\vec{r}, E, \vec{\Omega}, t) + \vec{\Omega} \cdot \text{grad}_{\vec{r}} \phi(\vec{r}, E, \vec{\Omega}, t) + \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, \vec{\Omega}, t) = \iint \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \phi(\vec{r}, E', \vec{\Omega}', t) dE' d\Omega' + S(\vec{r}, E, \vec{\Omega}, t)$$

- In this purpose it is sufficient to integrate both sides of the integro-differential equation over the complete  $4\pi$  solid angle, i.e. over the full range of directions
- The integration over  $d\Omega$ , since it involves only the directions, can be exchanged in order of execution with space and time derivatives
- We also make use of the following straightforward results:

$$\vec{\Omega} \cdot \text{grad}_{\vec{r}} \phi(\vec{r}, \vec{\Omega}, E, t) = \vec{\Omega} \cdot \nabla \phi(\vec{r}, \vec{\Omega}, E, t) = \nabla \cdot \phi(\vec{r}, \vec{\Omega}, E, t) \vec{\Omega} = \text{div}[\phi(\vec{r}, \vec{\Omega}, E, t) \vec{\Omega}]$$

$$\int_{4\pi} \text{div}[\phi(\vec{r}, \vec{\Omega}, E, t) \vec{\Omega}] d\Omega = \text{div} \int_{4\pi} \phi(\vec{r}, \vec{\Omega}, E, t) \vec{\Omega} d\Omega = \text{div} \vec{J} = \nabla \cdot \vec{J}$$

$$\int_{4\pi} \phi(\vec{r}, \vec{\Omega}, E, t) d\Omega = \phi(\vec{r}, E, t) \quad \int_{4\pi} S(\vec{r}, \vec{\Omega}, E, t) d\Omega = S(\vec{r}, E, t)$$

- For the scattering term, it must be recognized that integrating over outgoing direction from scattering also eliminates the dependence on the incoming direction, as shown in the last of the following lines:

$$\int_{4\pi} \iint \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \phi(\vec{r}, E', \vec{\Omega}', t) dE' d\Omega' d\Omega$$

$$= \iint \left[ \int_{4\pi} \Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) d\Omega \right] \phi(\vec{r}, E', \vec{\Omega}', t) dE' d\Omega'$$

$$= \iint \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', \vec{\Omega}', t) dE' d\Omega' = \int \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', t) dE'$$

**We then obtain:**

$$\frac{1}{v} \frac{\partial}{\partial t} \phi(\vec{r}, E, t) + \nabla \cdot \vec{J}(\vec{r}, E, t) + \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, t) = \int \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', t) dE' + S(\vec{r}, E, t)$$



- As well known, by integrating over whatever finite volume  $V$  and making use of the divergence theorem the usual principle of neutron conservation is obtained

$$\int_V \frac{1}{v} \frac{\partial}{\partial t} \phi(\vec{r}, E, t) dV + \int_{\partial V} \vec{J}(\vec{r}, E, t) \cdot \vec{n} dS + \int_V \Sigma_t(\vec{r}, E) \phi(\vec{r}, E, t) dV =$$

$$= \int_V \int \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E', t) dE' dV + \int_V S(\vec{r}, E, t) dV$$

- Integrating over the complete energy spectrum, it is also possible to reach the energy-independent form of the conservation principle

$$\int_V \frac{1}{v} \frac{\partial}{\partial t} \phi(\vec{r}, t) dV + \int_{\partial V} \vec{J}(\vec{r}, t) \cdot \vec{n} dS + \int_V \Sigma_a(\vec{r}) \phi(\vec{r}, t) dV = \int_V S(\vec{r}, t) dV$$

- In summary, the “detailed” neutron balance represented by the integro-differential equation, performed direction by direction, obviously implies also the overall neutron balance (i.e., the continuity principle) that is adopted in conjunction with the Fick’s law to obtain the diffusion equation
- In this latter case, the Fick’s law, as known, represents an approximation that is not needed when using the integro-differential transport equation, being per se an “exact” equation of neutron balance and transport as well

# THE MONOKINETIC AND STEADY-STATE NEUTRON TRANSPORT EQUATION

- From the integro-differential equation, by eliminating the time dependence and assuming  $v = 1$ , it is obtained

$$\vec{\Omega} \cdot \text{grad}_{\vec{r}} n(\vec{r}, \vec{\Omega}) + \Sigma_t(\vec{r}) n(\vec{r}, \vec{\Omega}) = \int_{4\pi} \Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) n(\vec{r}, \vec{\Omega}') d\Omega' + S(\vec{r}, \vec{\Omega})$$

- Recalling the slowing down theory, it may be understood that the differential scattering macroscopic cross section, depending in general by both the incoming and outgoing neutron directions,  $\vec{\Omega}' \rightarrow \vec{\Omega}$ , can be actually expressed as a function of the angle  $\psi$  between the two directions, given by  $\vec{\Omega} \cdot \vec{\Omega}'$ :

$$\Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) = \Sigma_s(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}') = \Sigma_s(\vec{r}, \cos \psi)$$

- The scattering process, in turn, can be considered according to different assumptions

- ◆ *isotropic scattering* (in the laboratory reference frame):

$$\Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) = \frac{\Sigma_s(\vec{r})}{4\pi}$$

- ◆ *linearly anisotropic scattering* (in the laboratory reference frame):

$$\Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) = \frac{\Sigma_s(\vec{r})}{4\pi} (1 + b \vec{\Omega} \cdot \vec{\Omega}') = \frac{\Sigma_s(\vec{r})}{4\pi} (1 + b \cos \psi)$$

in which  $b$  is an appropriate non-zero constant; by integrating over the whole range of directions and recalling that it can be written

$$d\Omega = \sin \psi \, d\psi \, d\phi$$

it is

$$\int_{4\pi} \Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) d\Omega = \frac{\Sigma_s(\vec{r})}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi (1 + b \cos \psi) \sin \psi \, d\psi$$

By putting

$$\mu_0 = \vec{\Omega} \cdot \vec{\Omega}' = \cos \psi \quad \Rightarrow \quad d\mu_0 = -\sin \psi \, d\psi$$

we can check that it is:

$$\int_{4\pi} \Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) d\Omega = \frac{\Sigma_s(\vec{r})}{4\pi} \int_0^{2\pi} d\phi \int_{-1}^1 (1 + b\mu_0) d\mu_0 = \Sigma_s(\vec{r})$$

and moreover it is:

$$\begin{aligned}\bar{\mu}_0 &= \frac{\int_{4\pi} \Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) \cos \psi \, d\Omega}{\int_{4\pi} \Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) \, d\Omega} = \frac{\Sigma_s(\vec{r}) \int_0^{2\pi} d\phi \int_0^\pi (1 + b \cos \psi) \cos \psi \sin \psi \, d\psi}{\Sigma_s(\vec{r})} = \\ &= \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi (1 + b \cos \psi) \cos \psi \sin \psi \, d\psi = \frac{1}{2} \int_{-1}^1 (1 + b\mu_0) \mu_0 \, d\mu_0 = \frac{b}{3}\end{aligned}$$

or

$$b = 3\bar{\mu}_0$$

- ◆ **generally anisotropic scattering (in the laboratory reference frame):**  
in this case an expansion in series of *Legendre polynomials*

$$\Sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) = \Sigma_s(\vec{r}, \mu_0) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{s,l}(\vec{r}) P_l(\mu_0)$$

is used.

For our present purposes, it is sufficient to recall that these polynomials constitute *a complete set of orthogonal functions over the interval*  $-1 \leq \mu \leq 1$ ; a further meaning of this choice will be reported later.

These polynomials are defined as

$$P_0(\mu_0) = 1, \quad P_1(\mu_0) = \mu_0 \quad P_{l+1}(\mu_0) = \frac{2l+1}{l+1} \mu_0 P_l(\mu_0) - \frac{l}{l+1} P_{l-1}(\mu_0) \quad (l \geq 1)$$

It is therefore:

$$P_2(\mu_0) = \frac{1}{2}(3\mu_0^2 - 1), \quad P_3(\mu_0) = \frac{1}{2}(5\mu_0^3 - 3\mu_0), \quad \dots$$

The orthogonality relation between these polynomials is defined as:

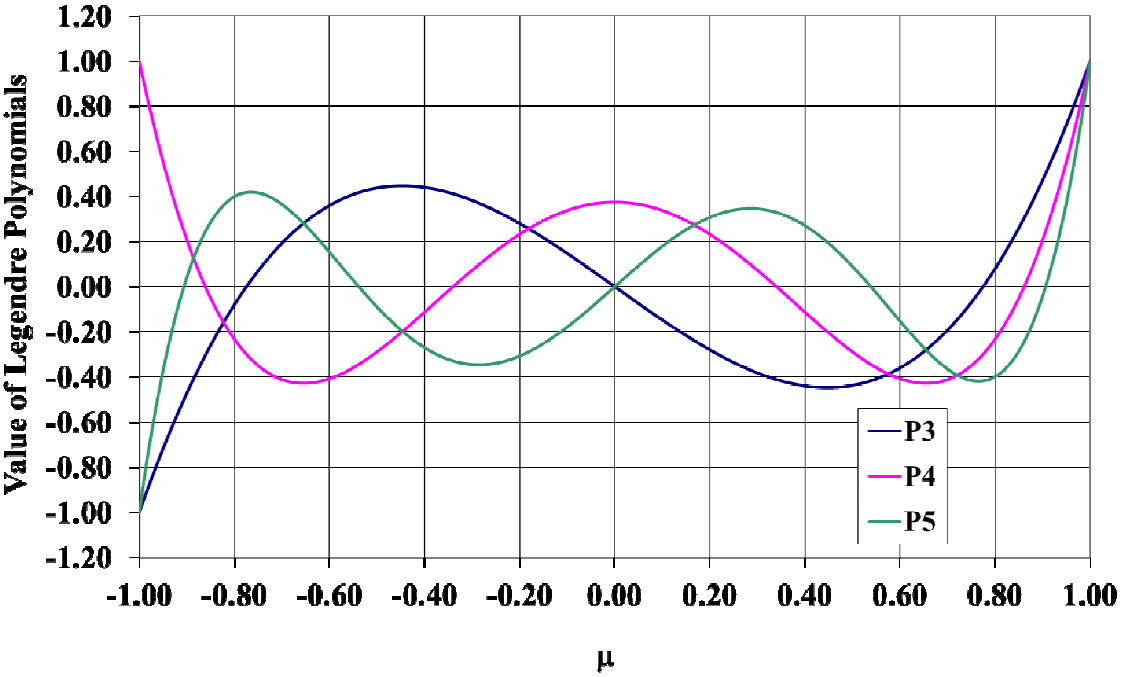
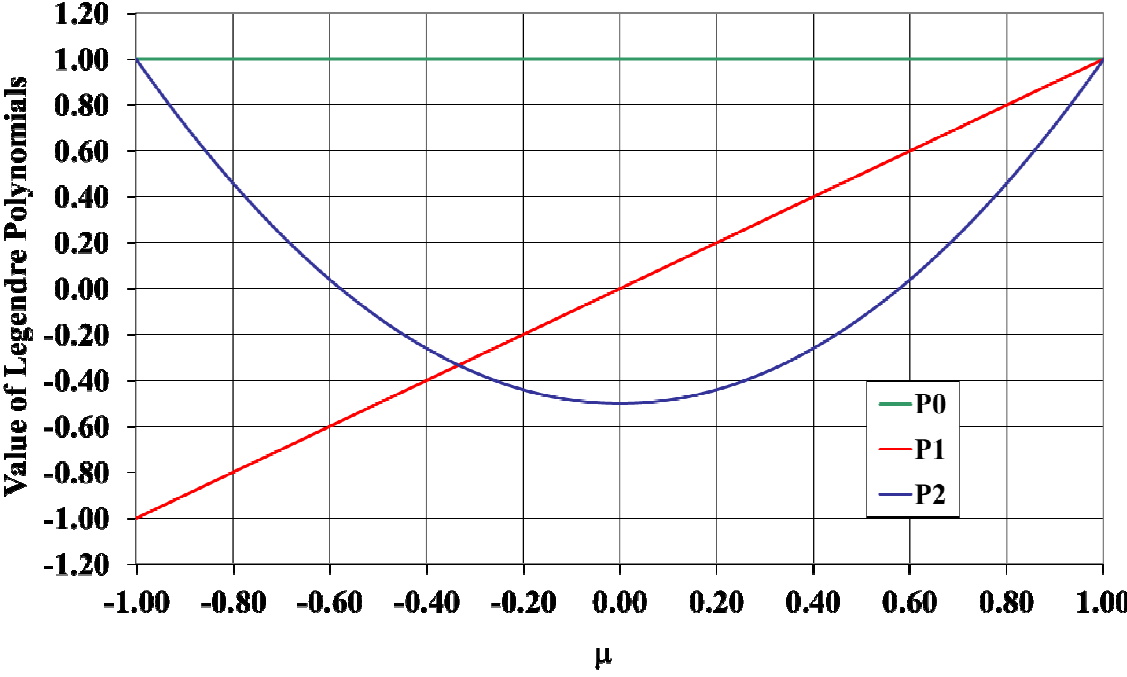
$$\int_{-1}^1 P_n(\mu_0) P_m(\mu_0) \, d\mu_0 = \frac{2}{2n+1} \delta_{nm}$$

From this relation, the following expression for the coefficients of the series can be obtained:

$$\Sigma_{s,l}(\vec{r}) = 2\pi \int_{-1}^1 \Sigma_s(\vec{r}, \mu_0) P_l(\mu_0) \, d\mu_0$$

Obviously enough, the case of the linearly anisotropic scattering correspond to truncate the series of Legendre polynomials at  $l = 1$ .

The following plots of the first few Legendre polynomials help in understanding the reasons for their *orthogonality* (check graphically) and the fact that *odd or even numbered polynomials are odd or even functions, having symmetric positive and negative roots*.



# THE MONOKINETIC AND STEADY-STATE CASE IN PLANE 1D GEOMETRY

## Obtaining the equation

- It is assumed that the characteristics of the region depend only of the single spatial coordinate  $x$
- Both the angular density and the source will depend, in addition, by  $\Omega_x \equiv \mu = \cos \theta$ . It is:

$$n = n(x, \Omega_x) = n(x, \mu) \quad \vec{\Omega} \cdot \text{grad}_{\vec{r}} n(x, \mu) = \mu \frac{\partial n}{\partial x} \quad S = S(x, \Omega_x) = S(x, \mu)$$

$$\Sigma_t = \Sigma_t(x) \quad \Sigma_s = \Sigma_s(x, \Omega_x) = \Sigma_s(x, \mu)$$

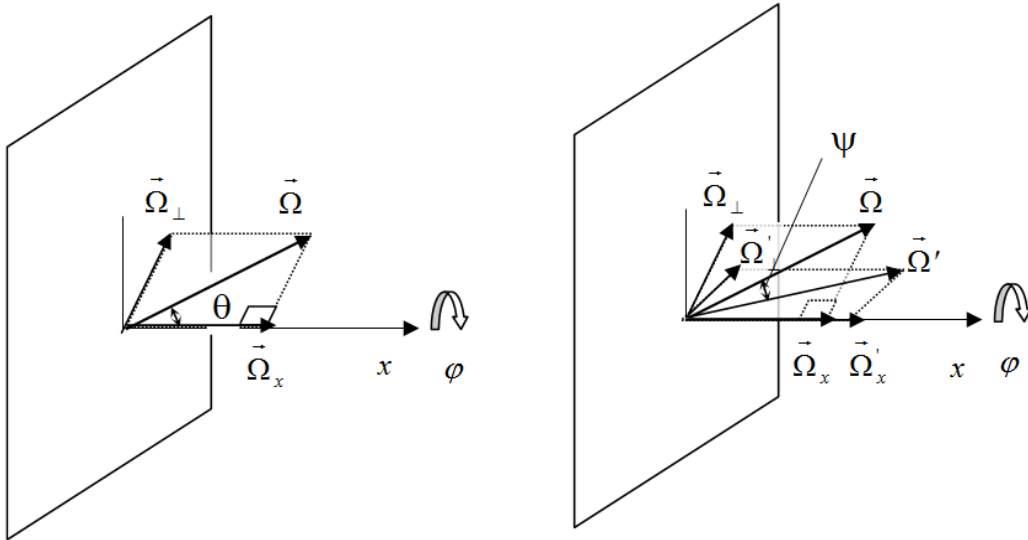
- We assume that the scattering source is linearly anisotropic in the laboratory reference frame. It is:

$$\mu \frac{\partial n(x, \mu)}{\partial x} + \Sigma_t(x) n(x, \mu) = \frac{\Sigma_s(x)}{4\pi} \int_{4\pi} (1 + b \cos \psi) n(x, \mu') d\Omega' + S(x, \mu) \quad (^\circ)$$

$$\cos \psi = \vec{\Omega} \cdot \vec{\Omega}' = \mu_0 \quad \mu' \equiv \Omega'_x$$

- Considering the Figure below, it is:

$$\begin{aligned} \mu_0 &= \vec{\Omega} \cdot \vec{\Omega}' = (\vec{\Omega}_x + \vec{\Omega}_\perp) \cdot (\vec{\Omega}'_x + \vec{\Omega}'_\perp) = \Omega_x \Omega'_x + |\Omega_\perp| |\Omega'_\perp| \cos(\varphi - \varphi') = \\ &= \mu \mu' + \sqrt{1 - \mu^2} \sqrt{1 - \mu'^2} \cos(\varphi - \varphi') \end{aligned}$$



By integrating both sides of (°) on  $0 \leq \varphi \leq 2\pi$  and making use of the definitions:

$$\tilde{n}(x, \mu) = \int_0^{2\pi} n(x, \mu) d\varphi = 2\pi n(x, \mu) \quad \tilde{S}(x, \mu) = \int_0^{2\pi} S(x, \mu) d\varphi = 2\pi S(x, \mu)$$

we obtain

$$\mu \frac{\partial \tilde{n}}{\partial x} + \Sigma_t(x) \tilde{n}(x, \mu) = \frac{\Sigma_s(x)}{4\pi} \int_0^{2\pi} d\varphi \int_{4\pi} (1 + b\mu_0) n(x, \mu') d\Omega' + \tilde{S}(x, \mu)$$

and then

$$\mu \frac{\partial \tilde{n}}{\partial x} + \Sigma_t(x) \tilde{n}(x, \mu) = \frac{\Sigma_s(x)}{2} \int_{4\pi} (1 + b\mu\mu') n(x, \mu') d\Omega' + \tilde{S}(x, \mu) \quad (^\circ\circ)$$

In the above, use is made of the relationship

$$\int_0^{2\pi} (1 + b\mu_0) d\varphi = \int_0^{2\pi} \left[ 1 + b\mu\mu' + b\sqrt{1-\mu^2} \sqrt{1-\mu'^2} \cos(\varphi - \varphi') \right] d\varphi = 2\pi(1 + b\mu\mu')$$

- Considering that  $d\Omega' = d\mu' d\varphi'$ , it is then:

$$\int_{4\pi} (1 + b\mu\mu') n(x, \mu') d\Omega' = \int_0^{2\pi} d\varphi' \int_{-1}^1 (1 + b\mu\mu') n(x, \mu') d\mu' = \int_{-1}^1 (1 + b\mu\mu') \tilde{n}(x, \mu') d\mu'$$

and Eq. (°°) becomes:

$$\mu \frac{\partial \tilde{n}}{\partial x} + \Sigma_t(x) \tilde{n}(x, \mu) = \frac{\Sigma_s(x)}{2} \int_{-1}^1 (1 + b\mu\mu') \tilde{n}(x, \mu') d\mu' + \tilde{S}(x, \mu)$$

Finally, dropping the “tilde” (i.e., dividing by  $2\pi$ ), we have:

$$\mu \frac{\partial n}{\partial x} + \Sigma_t(x) n(x, \mu) = \frac{\Sigma_s(x)}{2} \int_{-1}^1 (1 + b\mu\mu') n(x, \mu') d\mu' + S(x, \mu) \quad (^\circ\circ\circ)$$

### Spherical harmonics

- Even the angular density of neutrons can be expressed in the form of a series of Legendre polynomials with coefficients depending on the spatial coordinate

$$n(x, \mu) = \sum_{k=0}^{\infty} \frac{2k+1}{2} n_k(x) P_k(\mu)$$

with

$$n_k(x) = \int_{-1}^1 n(x, \mu) P_k(\mu) d\mu$$

- In particular, we note that it is:

$$n_0(x) = \int_{-1}^1 n(x, \mu) P_0(\mu) d\mu = \int_{-1}^1 n(x, \mu) d\mu = \rho(x)$$

$$n_1(x) = \int_{-1}^1 n(x, \mu) P_1(\mu) d\mu = \int_{-1}^1 n(x, \mu) \mu d\mu = \int_{-1}^1 n(x, \vec{\Omega}) \Omega_x d\mu = J_x(x) = J(x)$$

- Also the source, that is generally anisotropic, can be expressed in terms of a series of Legendre polynomials

$$S(x, \mu) = \sum_{k=0}^{\infty} \frac{2k+1}{2} s_k(x) P_k(\mu) \quad s_k(x) = \int_{-1}^1 S(x, \mu) P_k(\mu) d\mu$$

- If we substitute this equation into (°°°), we have

$$\begin{aligned} \sum_{k=0}^{\infty} \frac{2k+1}{2} \frac{dn_k}{dx} \mu P_k(\mu) + \Sigma_t(x) \sum_{k=0}^{\infty} \frac{2k+1}{2} n_k(x) P_k(\mu) = \\ = \frac{\Sigma_s(x)}{2} \int_{-1}^1 (1 + b\mu\mu') \sum_{k=0}^{\infty} \frac{2k+1}{2} n_k(x) P_k(\mu') d\mu' + \sum_{k=0}^{\infty} \frac{2k+1}{2} s_k(x) P_k(\mu) \end{aligned}$$

Making use of the recurrence formulation of Legendre polynomials, written in the form

$$(2k+1)\mu P_k(\mu) = (k+1)P_{k+1}(\mu) + kP_{k-1}(\mu)$$

for the first term of the balance equation it is

$$\sum_{k=0}^{\infty} \frac{2k+1}{2} \frac{dn_k}{dx} \mu P_k(\mu) = \frac{1}{2} \sum_{k=0}^{\infty} \frac{dn_k}{dx} [(k+1)P_{k+1}(\mu) + kP_{k-1}(\mu)]$$

- Considering the already seen form of the Legendre polynomials of order 0 and 1 (respectively,  $P_0(\mu')=1$  and  $P_1(\mu')=\mu'$ ), and making use of the orthogonality relation

$$\int_{-1}^1 P_n(\mu_0) P_m(\mu_0) d\mu_0 = \frac{2}{2n+1} \delta_{nm}$$

we have (follow the chain of equalities):

$$\begin{aligned} \int_{-1}^1 (1 + b\mu\mu') \sum_{k=0}^{\infty} \frac{2k+1}{2} n_k(x) P_k(\mu') d\mu' = \sum_{k=0}^{\infty} \frac{2k+1}{2} n_k(x) \int_{-1}^1 [P_0(\mu') + b\mu P_1(\mu')] P_k(\mu') d\mu' \\ = \sum_{k=0}^{\infty} \frac{2k+1}{2} n_k(x) \left[ \frac{2}{2k+1} \delta_{0k} + b\mu \frac{2}{2k+1} \delta_{1k} \right] = n_0(x) + b\mu n_1(x) = n_0(x) P_0(\mu) + b n_1(x) P_1(\mu) \end{aligned}$$

- It is therefore

$$\begin{aligned} \frac{1}{2} \sum_{k=0}^{\infty} \frac{dn_k}{dx} [(k+1)P_{k+1}(\mu) + kP_{k-1}(\mu)] + \Sigma_t(x) \sum_{k=0}^{\infty} \frac{2k+1}{2} n_k(x) P_k(\mu) \\ = \frac{\Sigma_s(x)}{2} [n_0(x) P_0(\mu) + b n_1(x) P_1(\mu)] + \sum_{k=0}^{\infty} \frac{2k+1}{2} s_k(x) P_k(\mu) \end{aligned}$$

- Now, by multiplying both sides of the previous equations by  $P_l(\mu)$  and integrating on  $-1 \leq \mu \leq 1$ , it can be found:

$$\boxed{\frac{l}{2l+1} \frac{dn_{l-1}}{dx} + \frac{l+1}{2l+1} \frac{dn_{l+1}}{dx} + \Sigma_t(x)n_l(x) = \Sigma_s(x) \left[ n_0(x)\delta_{0l} + \frac{b}{3}n_1(x)\delta_{1l} \right] + s_l(x)}$$

$(l = 0, 1, \dots)$

- ◆ In fact, it can be noted that:

$$\begin{aligned} & \frac{1}{2} \int_{-1}^1 \sum_{k=0}^{\infty} \frac{dn_k}{dx} [(k+1)P_{k+1}(\mu) + kP_{k-1}(\mu)] P_l(\mu) d\mu \\ &= \frac{1}{2} \int_{-1}^1 \sum_{k=0}^{\infty} \frac{dn_k}{dx} [(k+1)P_{k+1}(\mu)] P_l(\mu) d\mu + \frac{1}{2} \int_{-1}^1 \sum_{k=0}^{\infty} \frac{dn_k}{dx} [kP_{k-1}(\mu)] P_l(\mu) d\mu \\ &= \frac{1}{2} \int_{-1}^1 \frac{dn_{l-1}}{dx} (l) P_l(\mu) P_l(\mu) d\mu + \frac{1}{2} \int_{-1}^1 \frac{dn_{l+1}}{dx} [(l+1)P_l(\mu)] P_l(\mu) d\mu \\ &= \frac{1}{2} \frac{dn_{l-1}}{dx} (l) \frac{2}{2l+1} + \frac{1}{2} \frac{dn_{l+1}}{dx} (l+1) \frac{2}{2l+1} = \frac{dn_{l-1}}{dx} \frac{l}{2l+1} + \frac{dn_{l+1}}{dx} \frac{l+1}{2l+1} \end{aligned}$$

Moreover, it is:

$$\begin{aligned} \int_{-1}^1 \Sigma_t(x) \sum_{k=0}^{\infty} \frac{2k+1}{2} n_k(x) P_k(\mu) P_l(\mu) d\mu &= \int_{-1}^1 \Sigma_t(x) \frac{2l+1}{2} n_l(x) P_l(\mu) P_l(\mu) d\mu \\ &= \Sigma_t(x) \frac{2l+1}{2} n_l(x) \frac{2}{2l+1} = \Sigma_t(x) n_l(x) \end{aligned}$$

and

$$\begin{aligned} & \int_{-1}^1 \frac{\Sigma_s(x)}{2} [n_0(x)P_0(\mu) + bn_1(x)P_1(\mu)] P_l(\mu) d\mu \\ &= \frac{\Sigma_s(x)}{2} \left[ n_0(x) \frac{2}{2 \times (0) + 1} \delta_{0l} + bn_1(x) \frac{2}{2 \times (1) + 1} \delta_{1l} \right] = \Sigma_s(x) \left[ n_0(x) \delta_{0l} + \frac{b}{3} n_1(x) \delta_{1l} \right] \end{aligned}$$

and finally

$$\int_{-1}^1 \sum_{k=0}^{\infty} \frac{2k+1}{2} s_k(x) P_k(\mu) P_l(\mu) d\mu = \frac{2l+1}{2} s_l(x) \frac{2}{2l+1} = s_l(x)$$

- ◆ The obtained one is a system of infinite ordinary differential equations completely equivalent to the original partial differential equation
- ◆ The single assumption introduced in their development is related to the fact that linear anisotropy of the scattering source
- ◆ The use of Legendre polynomials in place of the more general “spherical harmonics” has been possible owing to the symmetry that is obtained in the planar geometry around the  $x$  axis



◆ In fact, the *spherical harmonics*, in their most general form constitute an orthonormal basis of functions that can be used to express in the form of a series any other sufficiently regular function of *colatitude* and *azimuth*,  $\theta$  and  $\varphi$ .

◆ They have the form

$$Y_{lm}(\theta, \varphi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\varphi} \text{ and it is } Y_{l,-m}(\theta, \varphi) = (-1)^m Y_{l,m}^*(\theta, \varphi)$$

where  $Y_{lm}^*(\theta, \varphi)$  represents the complex conjugate of  $Y_{lm}(\theta, \varphi)$  and the *Legendre associated functions* are defined as

$$P_l^m(\mu) = (-1)^m (1-\mu^2)^{m/2} \frac{d^m P_l(\mu)}{d\mu^m} \quad (m = 0, 1, \dots, l)$$

◆ In other words, they can represent any function defined on a sphere having unit radius and depending only on the above angles (as on an ideal spherical earth would be for the geological corrugations)

◆ Given a function  $f(\theta, \varphi)$ , it is therefore

$$f(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l f_{lm} Y_{lm}(\theta, \varphi) \quad f_{lm} = \int_0^{2\pi} d\varphi \int_{-1}^1 f(\theta, \varphi) Y_{lm}^*(\theta, \varphi) d(\cos\theta)$$

where use was made of the orthogonality relationship

$$\int_0^{2\pi} d\varphi \int_{-1}^1 Y_{lm}(\theta, \varphi) Y_{l'm'}^*(\theta, \varphi) d(\cos\theta) = \delta_{ll'} \delta_{mm'}$$

◆ As the Legendre polynomials, to which they are identical when  $m=0$  (i.e.,  $P_l^0(\mu) = P_l(\mu)$ ), also the Legendre associated functions possess an orthogonality property

$$\int_{-1}^1 P_l^m(\mu) P_{l'}^m(\mu) d\mu = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{ll'}$$

and can be obtained by a recurrence relationship as

$$\mu P_l^m(\mu) = \frac{1}{2l+1} \left[ (l-m+1) P_{l+1}^m(\mu) + (l+m) P_{l-1}^m(\mu) \right]$$

Assuming  $\mu = \cos\theta$ , the first Legendre associated functions are

$$P_1^1(\mu) = -(1-\mu^2)^{1/2} = -\sin\theta \quad P_2^1(\mu) = -3(1-\mu^2)^{1/2} \mu = -3\sin\theta \cos\theta$$

$$P_2^2(\mu) = 3(1-\mu^2) = 3\sin^2\theta$$

**$P_N$  approximations and the particular case of  $P_1$**

**a) The  $P_N$  equations and the related boundary conditions**

- An approximate solution of the system of infinite equations reached in terms of spherical harmonics can be obtained by truncating the series
- In particular, truncating the development at  $N+1$ -th term ( $l=0,1,\dots,N$ ) the  $P_N$  approximation is obtained
- Concerning the  $N+1$  boundary conditions to be imposed, a difficulty arises in the case of a medium facing the void, since the angular flux is discontinuous while passing from  $\mu < 0$  to  $\mu > 0$ ; in fact:

$$\begin{aligned} \phi(\vec{r}, \vec{\Omega}, E, t) &= 0 & \text{for} & \quad \vec{\Omega} \cdot \vec{u}_e < 0, \vec{r} \in \partial V \\ \phi(\vec{r}, \vec{\Omega}, E, t) &\neq 0 & \text{for} & \quad \vec{\Omega} \cdot \vec{u}_e > 0, \vec{r} \in \partial V \end{aligned}$$

- It is obvious that a relatively low order polynomial cannot adequately represent this angular discontinuity in the angular flux
- Some practical rules that allow for an approximation of the true boundary conditions were proposed. We will express them in term of flux, since in our one-velocity case we have  $n \equiv \phi$
- The first rule, with reference to an isolated layer with  $0 \leq x \leq a$ , is known as the *Marshak boundary conditions* and consists in choosing an odd  $N$  and imposing:

$$\int_0^1 P_i(\mu) \phi(0, \mu) d\mu = \int_{-1}^0 P_i(\mu) \phi(a, \mu) d\mu = 0 \quad (i = 1, 3, 5, \dots, N) \text{ } N \text{ odd}$$

In the case  $i = 1$ , we have, in fact, the condition of zero entering current which is the one actually used in diffusion cases:

$$\int_0^1 \mu \phi(0, \mu) d\mu = \int_{-1}^0 \mu \phi(a, \mu) d\mu = 0$$

- A second rule is the one under the name of *Mark boundary conditions*, consisting in imposing that it is:

$$\begin{aligned} \phi(0, \mu_i^+) &= 0 & \mu_i^+ &> 0 \quad (i = 1, 2, 3, \dots, (N+1)/2) \text{ } N \text{ odd} \\ \phi(a, \mu_i^-) &= 0 & \mu_i^- &< 0 \quad (i = 1, 2, 3, \dots, (N+1)/2) \text{ } N \text{ odd} \end{aligned}$$

where  $\mu_i^+$  and  $\mu_i^-$  identify respectively the positive and negative roots of the equation

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

(remember the shape of the Legendre polynomials)

- It has been shown that the Mark boundary conditions imply the substitution of the void space with a purely absorbing medium
- In the case of “pure reflection” at a boundary, we have instead no problem. In fact, the conditions

$$\phi(0, \mu) = \phi(0, -\mu) \quad (0 < \mu < 1) \quad \text{e} \quad \phi(a, \mu) = \phi(a, -\mu) \quad (-1 < \mu < 0)$$

immediately translate into requiring that

$$\phi_i(0) = \phi_i(a) = 0 \quad i \text{ odd}$$

i.e., the angular flux at the boundary must be an even function of  $\mu$ .

### b) $P_1$ Approximation

In this case it is:

$$n(x, \mu) \cong \sum_{k=0}^1 \frac{2k+1}{2} n_k(x) P_k(\mu) = \frac{1}{2} n_0(x) + \frac{3}{2} n_1(x) \mu$$

- The related differential equations are:

$$(l=0) \quad \frac{dn_0}{dx} + \Sigma_t(x) n_0(x) = \Sigma_s(x) n_0(x) + s_0(x)$$

$$(l=1) \quad \frac{1}{3} \frac{dn_0}{dx} + \frac{2}{3} \frac{dn_1}{dx} + \Sigma_t(x) n_1(x) = \frac{b}{3} \Sigma_s(x) n_1(x) + s_1(x)$$

(check the correctness of this form as a simple exercise)

- Putting  $n_2(x) = 0$ , as it must be for  $P_1$ , and assuming that the source is independent and isotropic ( $s_1(x) = 0$ ) from the second equation we get the following one

$$n_1(x) = - \frac{1}{3(\Sigma_t - \bar{\mu}\Sigma_s)} \frac{dn_0}{dx}$$

which, remembering that  $n_0(x) = \rho(x)$  and  $n_1(x) = J(x)$ , expresses the Fick's law of diffusion:

$$J(x) = -D \frac{d\rho}{dx} \quad D(x) = \frac{1}{3(\Sigma_t - \bar{\mu}\Sigma_s)} \approx \frac{1}{3\Sigma_s(1 - \bar{\mu})}$$

- **By introducing this result in the equation for  $l=0$ , having the role of a continuity equation, it is:**

$$\frac{d}{dx} \left( D(x) \frac{d\rho}{dx} \right) - \Sigma_a(x) \rho(x) + s_0(x) = 0$$

**So, it is quite interesting to see that, in the limit of the considered assumptions, *the  $P_1$  approximation coincides with the diffusion equation with the transport correction for the diffusion coefficient***

# INTEGRAL EQUATION

## Derivation

- The transport equation in integral form (Perierls equation) can be obtained directly on the basis of simple considerations or even from the integro-differential equation
- For the sake of simplicity, let us consider the steady-state case, bring of greatest interest for applications. The transient treatment, anyway, is not too complex (see Bell & Glasstone, 1979, Par. 1.2).
- The integro-differential equation for transport in steady-state

$$v\vec{\Omega} \cdot \text{grad}_{\vec{r}} n(\vec{r}, v\vec{\Omega}) + v\Sigma_t(\vec{r}, v) n(\vec{r}, v\vec{\Omega}) = \iint v'\Sigma_s(\vec{r}, v'\vec{\Omega}' \rightarrow v\vec{\Omega}) n(\vec{r}, v'\vec{\Omega}') dv' d\Omega' + S(\vec{r}, v\vec{\Omega})$$

can be rewritten in terms of *emission density*

$$q(\vec{r}, v\vec{\Omega}) = \iint v'\Sigma_s(\vec{r}, v'\vec{\Omega}' \rightarrow v\vec{\Omega}) n(\vec{r}, v'\vec{\Omega}') dv' d\Omega' + S(\vec{r}, v\vec{\Omega})$$

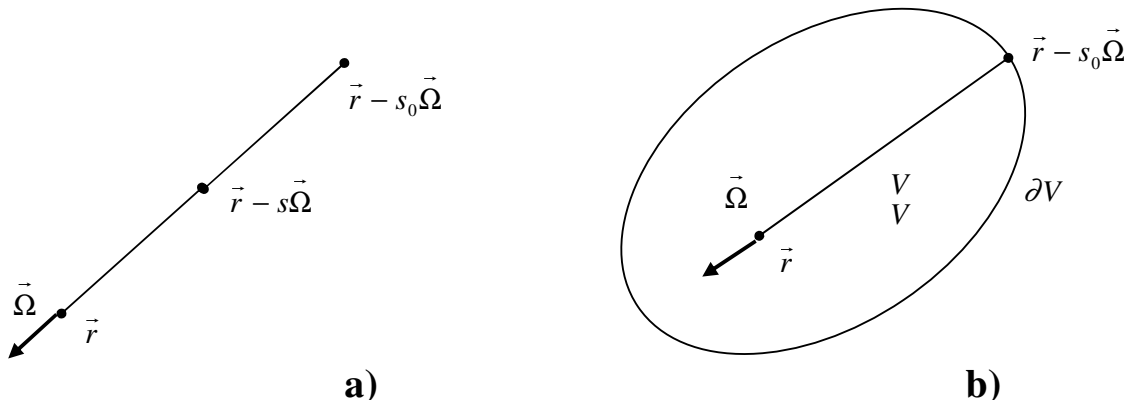
and expressing the first term in the left hand side as a local (directional) derivative of angular density along the direction of motion of neutrons; it is:

$$-v \frac{d}{ds} n(\vec{r} - s\vec{\Omega}, v\vec{\Omega}) \Big|_{s=0} = v\vec{\Omega} \cdot \text{grad}_{\vec{r}} n(\vec{r}, v\vec{\Omega})$$

We have then:

$$-v \frac{d}{ds} n(\vec{r} - s\vec{\Omega}, v\vec{\Omega}) \Big|_{s=0} + v\Sigma_t(\vec{r}, v) n(\vec{r}, v\vec{\Omega}) = q(\vec{r}, v\vec{\Omega})$$

Now we can note that in *every* points of the trajectory of neutrons, a similar equation can be written for any  $\vec{\Omega}$  and  $\vec{r}$



## Definizione di vettori rilevanti nella derivazione

- Therefore, considering a generic location “upstream” the considered location, identified by the coordinate  $s$ , we have

$$-v \frac{d}{ds} n(\vec{r} - s\vec{\Omega}, v\vec{\Omega}) + v \Sigma_t(\vec{r} - s\vec{\Omega}, v) n(\vec{r} - s\vec{\Omega}, v\vec{\Omega}) = q(\vec{r} - s\vec{\Omega}, v\vec{\Omega})$$

this relationship, once  $\vec{r}$  and  $\vec{\Omega}$  are assigned, gives rise to a differential equation in terms of ordinary derivatives

- This equation can be integrated between  $\vec{r} - s_0\vec{\Omega}$  and the generic location  $\vec{r} - s\vec{\Omega}$  through a usual variable separation technique

$$\frac{d}{ds} n(\vec{r} - s\vec{\Omega}, v\vec{\Omega}) = \Sigma_t(\vec{r} - s\vec{\Omega}, v) n(\vec{r} - s\vec{\Omega}, v\vec{\Omega}) - \frac{1}{v} q(\vec{r} - s\vec{\Omega}, v\vec{\Omega})$$

providing the solution

$$n(\vec{r} - s\vec{\Omega}, v\vec{\Omega}) = n(\vec{r} - s_0\vec{\Omega}, v\vec{\Omega}) e^{-\int_s^{s_0} \Sigma_t(\vec{r} - s'\vec{\Omega}, v) ds'} + \int_s^{s_0} e^{-\int_s^{s'} \Sigma_t(\vec{r} - s''\vec{\Omega}, v) ds''} \frac{1}{v} q(\vec{r} - s'\vec{\Omega}, v\vec{\Omega}) ds'$$

- Since the objective of this process is to evaluate the angular density at  $\vec{r}$ , i.e. for  $s = 0$ , from the previous one we obtain

$$n(\vec{r}, v\vec{\Omega}) = n(\vec{r} - s_0\vec{\Omega}, v\vec{\Omega}) e^{-\int_0^{s_0} \Sigma_t(\vec{r} - s'\vec{\Omega}, v) ds'} + \int_0^{s_0} e^{-\int_0^{s'} \Sigma_t(\vec{r} - s''\vec{\Omega}, v) ds''} \frac{1}{v} q(\vec{r} - s'\vec{\Omega}, v\vec{\Omega}) ds'$$

- The angular density in  $\vec{r}$  is obtained by the summation of two contributions:
  - ◆ the one due to the neutrons that at the location  $\vec{r} - s_0\vec{\Omega}$  have a velocity  $v$  and direction of motion  $\vec{\Omega}$ , times the probability of experiencing no collisions between  $\vec{r} - s_0\vec{\Omega}$  and  $\vec{r}$
  - ◆ the summation of the elementary contributions due to emission density,  $q$  at locations  $\vec{r} - s'\vec{\Omega}$ , with  $s' \in [0, s_0]$  times the probability of experiencing no collisions before reaching  $\vec{r}$

### The isolated body

- Selecting the coordinate  $s_0$  on the boundary of domain  $V$ , we impose that

$$n(\vec{r}, v\vec{\Omega}) = 0 \quad \text{for any } \vec{\Omega} \cdot \vec{u}_e < 0, \vec{r} \in \partial V$$

as it must be for an isolated body, and it is

$$n(\vec{r} - s_0 \vec{\Omega}, v \vec{\Omega}) = 0$$

thus obtaining

$$n(\vec{r}, v \vec{\Omega}) = \int_0^{s_0(\vec{r}, \vec{\Omega})} e^{-\int_0^{s'} \Sigma_t(\vec{r} - s'' \vec{\Omega}, v) ds''} \frac{1}{v} q(\vec{r} - s' \vec{\Omega}, v \vec{\Omega}) ds'$$

where the dependence of  $s_0$  on  $\vec{r}$  and  $\vec{\Omega}$ , in relation to the particular geometry of the volume  $V$ , has been pointed out

- We now assume that the scattering reactions are isotropic in the laboratory reference frame and that the independent sources are also isotropic; it is

$$\Sigma_s(\vec{r}, v' \vec{\Omega}' \rightarrow v \vec{\Omega}) = \frac{1}{4\pi} \Sigma_s(\vec{r}, v' \rightarrow v) \quad e \quad S(\vec{r}, v \vec{\Omega}) = \frac{1}{4\pi} S(\vec{r}, v)$$

and therefore

$$q(\vec{r}, v \vec{\Omega}) \equiv q(\vec{r}, v)$$

- Integrating over the complete solid angle, we have

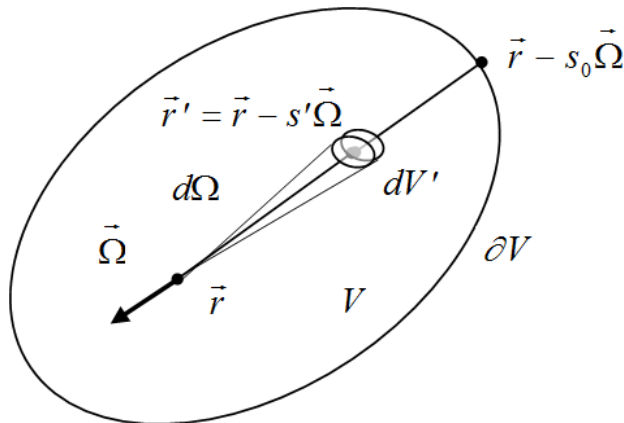
$$\rho(\vec{r}, v) = \int_{4\pi} n(\vec{r}, v \vec{\Omega}) d\Omega = \int_{4\pi} d\Omega \int_0^{s_0(\vec{r}, \vec{\Omega})} e^{-\int_0^{s'} \Sigma_t(\vec{r} - s'' \vec{\Omega}, v) ds''} \frac{1}{v} q(\vec{r} - s' \vec{\Omega}, v) ds'$$

- We then make use of useful definitions

$$\vec{r}' = \vec{r} - s' \vec{\Omega} \Rightarrow \quad s' = |\vec{r} - \vec{r}'| \quad e \quad dV' = s'^2 d\Omega ds'$$

recognising that

$$\vec{\Omega} = \frac{\vec{r} - \vec{r}'}{s'} = \frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|} \quad d\Omega ds' = \frac{dV'}{s'^2} = \frac{dV'}{|\vec{r} - \vec{r}'|^2} \cdot$$



**Definition of the volume of integration around  $\vec{r}'$**

- We also define the *optical path*

$$\tau(\vec{r}, \vec{r}', v) \equiv \int_0^{s'} \Sigma_t(\vec{r} - s'' \vec{\Omega}, v) ds''$$

representing *the number of mean free paths for any type of collisions covered by the integration distance*

- In the case of an homogeneous body, it is

$$\tau(\vec{r}, \vec{r}', v) = \Sigma_t(v) s' = \Sigma_t(v) |\vec{r} - \vec{r}'|$$

- The exponential  $e^{-\tau(\vec{r}, \vec{r}', v)}$  represents therefore the probability that a neutron emitted in  $\vec{r}'$  with velocity  $v$  (in the direction of  $\vec{r}$ ) has of reaching  $\vec{r}$  without colliding along the path

- Making use of these definitions, it is

$$\rho(\vec{r}, v) = \int_V e^{-\tau(\vec{r}, \vec{r}', v)} \frac{1}{v} q(\vec{r}', v) \frac{dV'}{|\vec{r} - \vec{r}'|^2}$$

Remembering the definition of emission density, it is:

$$\rho(\vec{r}, v) = \int_V \frac{e^{-\tau(\vec{r}, \vec{r}', v)}}{4\pi |\vec{r} - \vec{r}'|^2} \left[ \frac{1}{v} S(\vec{r}', v) + \int_0^\infty \frac{v'}{v} \Sigma_s(\vec{r}', v' \rightarrow v) \rho(\vec{r}', v') dv' \right] dV'$$

- In a mono-energetic case ( $v = 1, \Sigma_s(\vec{r}, v' \rightarrow v) \equiv \Sigma_s(\vec{r})$ ) it is:

$$\rho(\vec{r}) = \int_V \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi |\vec{r} - \vec{r}'|^2} [S(\vec{r}') + \Sigma_s(\vec{r}') \rho(\vec{r}')] dV'$$

- We note that:

- ◆ The formulations obtained *involve a volume integral over the domain  $V$  (and, possibly, one over velocity)*
- ◆ They express the density of neutrons in the generic location  $\vec{r}$  *as a result of the contributions of the emission density in elementary volumes  $dV'$*
- ◆ *The contributions are weighted according to the probability to have no collisions during the path and to the geometric attenuation expressed by the factor  $1/(4\pi |\vec{r} - \vec{r}'|^2)$*

### Numerical solution for the isolated body

- The above interpretation suggests an algorithm for the approximate solution of the transport problem for an isolated body in steady conditions, called the *collision probability method*
- The integration domain  $V$  is subdivided into a number  $N_V$  of control volumes in which it is assumed that neutron density and sources are uniform



- Each volume is assigned a value of neutron density that represents the averaged actual values

$$\rho_i \equiv \frac{1}{V_i} \int_{V_i} \rho(\vec{r}) dV \cong \rho(\vec{r}) \quad \vec{r} \in V_i, \quad (i = 1, \dots, N_V)$$

- Making use of the relationship

$$\rho(\vec{r}) = \int_V \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi|\vec{r} - \vec{r}'|^2} [S(\vec{r}') + \Sigma_s(\vec{r}')\rho(\vec{r}')] dV'$$

the previous formulation can be rephrased as

$$\rho_i \equiv \frac{1}{V_i} \int_{V_i} dV \int_V \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi|\vec{r} - \vec{r}'|^2} [S(\vec{r}') + \Sigma_s(\vec{r}')\rho(\vec{r}')] dV' \quad (i = 1, \dots, N_V)$$

- It is therefore possible to write

$$\rho_i \equiv \frac{1}{V_i} \int_{V_i} dV \sum_{j=1}^{N_V} \int_{V_j} \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi|\vec{r} - \vec{r}'|^2} [S_j + \Sigma_{s,j}\rho_j] dV' \quad (i = 1, \dots, N_V)$$

- Finally, putting

$$A_{i,j} \equiv \frac{1}{V_i} \int_{V_i} dV \int_{V_j} \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi|\vec{r} - \vec{r}'|^2} dV' \quad (i, j = 1, \dots, N_V)$$

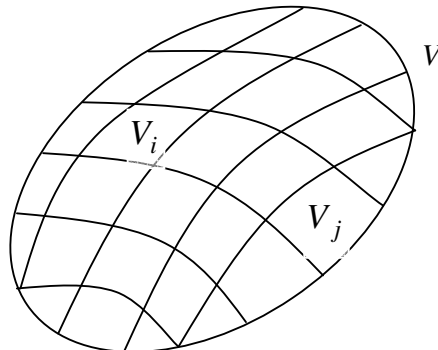
a linear system in nodal densities is obtained

$$\rho_i = \sum_{j=1}^{N_V} A_{i,j} \Sigma_{s,j} \rho_j + q_i \quad (i = 1, \dots, N_V)$$

where

$$q_i = \sum_{j=1}^{N_V} A_{i,j} S_j \quad (i = 1, \dots, N_V)$$

- The system can be solved with any of the already seen usual techniques
- It can be found that the constants  $A_{i,j}$  are related to the probability



**Subdivision of volume  $V$  in control volumes**

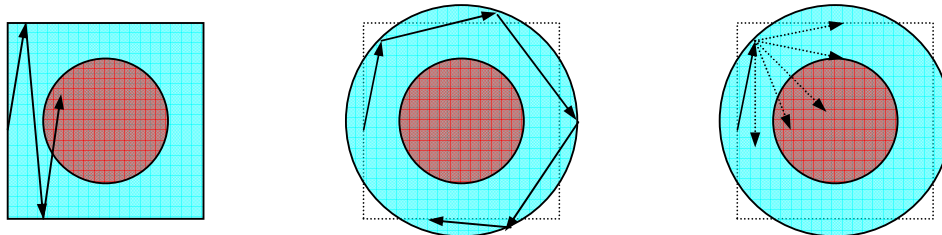
of “first collision” in  $V_i$  of neutrons emitted in  $V_j$ . In fact, by definition, it is:

$$P_{j \rightarrow i}^{(0)} \equiv \int_{V_i} \Sigma_{ti} dV \int_{V_j} \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi|\vec{r} - \vec{r}'|^2} \frac{1}{V_j} dV' = \Sigma_{ti} \frac{V_i}{V_j} \frac{1}{V_i} \int_{V_j} dV \int_{V_i} \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi|\vec{r} - \vec{r}'|^2} dV' = \Sigma_{ti} \frac{V_i}{V_j} A_{i,j}$$

- Therefore, the solution of the problem requires the evaluation of the collision probabilities  $P_{j \rightarrow i}^{(0)}$

### Numerical solution in the case of the cell

- In the case of the cell, the appropriate boundary condition is a “white” (i.e., diffuse) reflection at the cell surface
- White reflection is generally preferred to pure reflection in cell calculations because, in the case of a cylindrical cell, neutrons having a small angle of incidence on the external cylindrical surface will be hardly reflected towards the fuel rod (case b), contrary to what would happen in the original square cell (case a). This would lead to overestimate the neutron flux in the peripheral part of the cell. The selection of a “diffuse” reflection (case c), instead, restores a reasonable probability that neutrons reflected from the external surface can intercept the fuel.



a) Pure reflection      b) Pure reflection      c) Diffuse reflection

- However, the introduction of reflection would change completely the development of the integral transport equation, with the need to consider incoming currents corresponding to outgoing ones at the surface
- It is here shown that it is possible to modify the previous treatment concerning the “collision probability method”, by including reflections at the cell surface

- In the single energy case ( $\phi = \rho$  since we chose  $\nu = 1$ ) with an external surface facing the void, the approximate solution  $\phi_i$  is given by the linear system

$$\phi_i = \sum_j A_{i,j} (\sum_{s,j} \phi_j + S_j)$$

where

$$A_{i,j} = \frac{1}{V_i} \int_{V_i} \int_{V_j} \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi|\vec{r} - \vec{r}'|^2} dV dV'$$

**Introducing the collision probability**

$$P_{j \rightarrow i} = \frac{V_i}{V_j} \sum_{ii} A_{i,j} = \frac{\sum_{ii}}{V_j} \int_{V_i} \int_{V_j} \frac{e^{-\tau(\vec{r}, \vec{r}')}}{4\pi|\vec{r} - \vec{r}'|^2} dV dV'$$

the system can be interestingly rewritten as

$$V_i \sum_{ii} \phi_i = \sum_j V_j P_{j \rightarrow i} (\sum_{sj} \phi_j + S_j)$$

having an obvious meaning: *collisions in volume  $V_i$  are due to the emissions in all the  $V_j$  multiplied by the collision probability from volume  $j$  to volume  $i$ .*

- We can generalize the algorithm considering a multi-group energy approach

$$V_i \sum_{ii}^g \phi_i^g = \sum_j V_j P_{j \rightarrow i}^g (\sum_{g'} \sum_{sj}^{g' \rightarrow g} \phi_j^{g'} + S_j^g)$$

- In the case of white reflective boundary, a similar calculation scheme is possible, avoiding complications due to the consideration of incoming and outgoing currents
- We now define

$$P_{j \rightarrow S}^g = 1 - \sum_i P_{j \rightarrow i}^g = \left( \begin{array}{l} \text{probability that a neutron of the energy} \\ \text{group } g \text{ produced in } V_j \\ \text{reaches the boundary } S \text{ at its first flight} \end{array} \right)$$

$$P_{S \rightarrow i}^g = \frac{4V_i \sum_{ii}}{S} P_{i \rightarrow S}^g = \left( \begin{array}{l} \text{probability that a neutron of the energy} \\ \text{group } g \text{ reflected by } S \\ \text{collides in } V_i \text{ at its first flight} \end{array} \right) \quad (1)$$

<sup>(1)</sup> We accept this formulation without demonstration.

$$P_{S \rightarrow S}^g = 1 - \sum_i P_{S \rightarrow i}^g = \left( \begin{array}{c} \text{probability that a neutron of the energy} \\ \text{group } g \text{ reflected by } S \\ \text{reaches again } S \end{array} \right)$$

- **We put therefore**

$$\tilde{P}_{j \rightarrow i}^g = P_{j \rightarrow i}^g + P_{j \rightarrow S}^g P_{S \rightarrow i}^g + P_{j \rightarrow S}^g P_{S \rightarrow S}^g P_{S \rightarrow i}^g + P_{j \rightarrow S}^g (P_{S \rightarrow S}^g)^2 P_{S \rightarrow i}^g + \dots$$

**that can be read as:**

$$\left( \begin{array}{c} \text{total probability that a neutron of the group } g \\ \text{emitted in } V_j \\ \text{collides in } V_i \end{array} \right) =$$

$$= \left( \begin{array}{c} \text{probability that a neutron of group } g \\ \text{emitted in } V_j \\ \text{collides directly at the first flight in } V_i \end{array} \right)$$

$$+ \left( \begin{array}{c} \text{probability that a neutron of group } g \\ \text{emitted in } V_j \text{ collides} \\ \text{in } V_i \text{ after a reflection in } S \end{array} \right)$$

$$+ \left( \begin{array}{c} \text{probability that a neutron of group } g \\ \text{emitted in } V_j \text{ collides} \\ \text{in } V_i \text{ after two reflections in } S \end{array} \right)$$

$$+ \left( \begin{array}{c} \text{probability that a neutron of group } g \\ \text{emitted in } V_j \text{ collides} \\ \text{in } V_i \text{ after three reflections in } S \end{array} \right) + \dots$$

- **Considering the above geometric progression, it is therefore**

$$\tilde{P}_{j \rightarrow i}^g = P_{j \rightarrow i}^g + \frac{P_{j \rightarrow S}^g P_{S \rightarrow i}^g}{1 - P_{S \rightarrow S}^g}$$

**and the solution scheme for the cell with diffuse reflection is formally the same found for the isolated body, provided we substitute the “first flight” collision probabilities with the ones combined with reflection**

$$V_i \Sigma_{ii}^g \phi_i^g = \sum_j V_j \tilde{P}_{j \rightarrow i}^g \left( \sum_{g'} \Sigma_{sj}^{g' \rightarrow g} \phi_j^{g'} + S_j^g \right)$$

- **The calculation of  $\tilde{P}_{j \rightarrow i}^g$  (and of  $P_{j \rightarrow i}^g$ ) represents an heavy task to be performed, for which specific techniques have been developed**