

# Neutron slowing-down and resonance self-shielding

Alain Hébert

`alain.hebert@polymtl.ca`

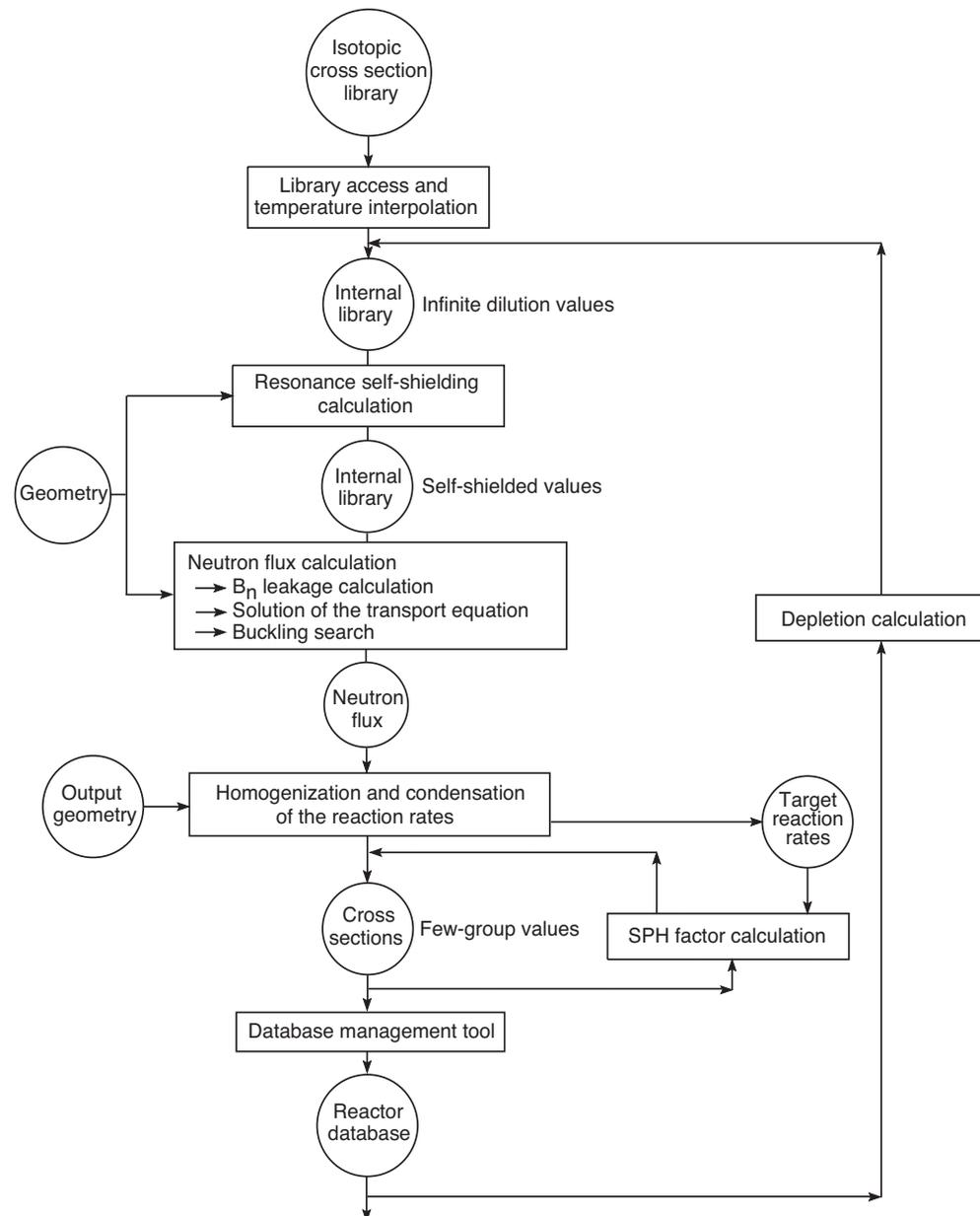
Institut de génie nucléaire  
École Polytechnique de Montréal

- Elements of lattice calculation
- Neutron slowing-down
  - elastic slowing-down operator and slowing-down current
  - the Placzek transients
- Resonance self-shielding
  - Livolant-Jeanpierre approximations
  - equivalence in dilution approach
  - subgroup approach

- A few first-generation lattice codes based of the **four-factor formula** are still in production use today.
- The second generation lattice codes features a consistent multigroup (between 50 and 400 groups) representation of the neutron energies.

The main components of a typical second generation lattice code are the following:

1. Library access and temperature interpolation.
2. Resonance self-shielding calculation.
3. Main flux calculation.
4. Homogenization and condensation of the reaction rates.
5. SPH factor calculation.
6. Isotopic depletion calculation.





At energies of the incident neutron greater than a few eV, thermal agitation of nuclides and binding effects vanishes and the elastic scattering reaction leads to a pure slowing-down effect. In this case, the transport equation simplifies to

$$(1) \quad \boldsymbol{\Omega} \cdot \nabla \phi(\mathbf{r}, u, \boldsymbol{\Omega}) + \Sigma(\mathbf{r}, u) \phi(\mathbf{r}, u, \boldsymbol{\Omega}) = \frac{1}{4\pi} \left[ S_f(\mathbf{r}, u) + \sum_{j=1}^J \mathcal{R}_j \{ \phi(\mathbf{r}, u) \} \right]$$

where  $S_f(\mathbf{r}, u)$  is the fission source and where we assumed that the scattering reaction is isotropic in the LAB.

The resonant absorption mechanism is based on different isotopes  $j$  playing antinomic roles:

- The lights isotopes are mostly responsible of the slowing-down of neutrons but are not the largest cause of absorption. This is also true for LMFBRs where the Oxygen, Sodium and structural materials are playing this role.
- The heavy isotopes are mostly responsible of the resonant absorption of neutrons but are not the largest cause of slowing-down.

We introduced  $\rho_j(\mathbf{r}, u) \equiv \mathcal{R}_j\{\phi(\mathbf{r}, u)\}$  as the **elastic slowing-down operator** of isotope  $j$ :

$$\begin{aligned}
 \rho_j(\mathbf{r}, u) \equiv \mathcal{R}_j\{\phi(\mathbf{r}, u)\} &= \int_0^u du' \Sigma_{s0,j}(\mathbf{r}, u \leftarrow u') \phi(\mathbf{r}, u') \\
 (2) \qquad \qquad \qquad &= \frac{1}{1 - \alpha_j} \int_{u-\epsilon_j}^u du' e^{u'-u} \Sigma_{s,j}(\mathbf{r}, u') \phi(\mathbf{r}, u')
 \end{aligned}$$

where  $\Sigma_{s0,j}(\mathbf{r}, u \leftarrow u')$  is the zero<sup>th</sup> Legendre moment of the differential scattering cross section and  $\epsilon_j$  is the maximum lethargy jump a neutron can make using an elastic collision with a nucleus of type  $j$  and mass ratio  $A_j$  (the ratio of the nucleus mass over the neutron mass). The parameters  $\alpha_j$  and  $\epsilon_j$  are defined as

$$(3) \qquad \qquad \alpha_j = \left( \frac{A_j - 1}{A_j + 1} \right)^2 \qquad \text{and} \qquad \epsilon_j = \ln \frac{1}{\alpha_j} .$$

$\rho_j(\mathbf{r}, u) du$  is the number of neutrons that will come out with a secondary lethargy equal to  $u$  (within a  $du$  interval) per unit time.

Note that the integration in primary lethargy  $u'$  is limited to values smaller than the secondary lethargy  $u$ .

In the case of an homogeneous media with  $J = 1$ , the elastic slowing-down equation (1) simplifies to

$$(4) \quad \Sigma(u) \phi(u) = S_f(u) + \rho(u)$$

A second form of this equation is based on the **slowing-down current**.

The **slowing-down current**  $q(u)$  defined as the number of neutrons that will cross lethargy  $u$  per unit time. The count is performed for neutrons having a primary lethargy  $u'$  smaller than  $u$  and a secondary lethargy  $u''$  greater than  $u$ . The slowing-down current is defined as

$$(5) \quad q_j(\mathbf{r}, u) \equiv \mathcal{Q}_j\{\phi(\mathbf{r}, u)\} = \int_0^u du' \int_u^\infty du'' \Sigma_{s0,j}(\mathbf{r}, u'' \leftarrow u') \phi(\mathbf{r}, u') .$$

The slowing-down operator  $\rho_j(\mathbf{r}, u)$  defined in Eq. (2) is a distribution in  $u$  although the slowing-down current  $q_j(\mathbf{r}, u)$  defined in Eq. (5) is a function of  $u$ .

The slowing-down current can be derived with respect to  $u$ , leading to

$$(6) \quad \frac{d}{du} q_j(\mathbf{r}, u) = \Sigma_{s,j}(\mathbf{r}, u) \phi(\mathbf{r}, u) - \rho_j(\mathbf{r}, u)$$

where we used the identity

$$(7) \quad \frac{d}{du} \int_0^u du' A(u, u') = A(u, u) + \int_0^u du' \frac{\partial A}{\partial u} .$$

Substituting Eq. (6) in Eq. (4), we obtain a transport equation written in terms of the slowing-down current. In the case of an homogeneous media with  $J = 1$ , we obtain the second form of the elastic slowing-down equation:

$$(8) \quad \frac{d}{du} q(u) = S_f(u) - \Sigma_a(u) \phi(u) .$$

Assuming elastic scattering, Eq. (5) can be written

$$(9) \quad \begin{aligned} q_j(\mathbf{r}, u) &= \frac{1}{1 - \alpha_j} \int_{u - \epsilon_j}^u du' \int_u^{u' + \epsilon_j} du'' e^{u' - u''} \Sigma_{s,j}(\mathbf{r}, u') \phi(\mathbf{r}, u') \\ &= \frac{1}{1 - \alpha_j} \int_{u - \epsilon_j}^u du' \left( e^{u' - u} - \alpha_j \right) \Sigma_{s,j}(\mathbf{r}, u') \phi(\mathbf{r}, u') \\ &= \rho_j(\mathbf{r}, u) - \frac{\alpha_j}{1 - \alpha_j} \int_{u - \epsilon_j}^u du' \Sigma_{s,j}(\mathbf{r}, u') \phi(\mathbf{r}, u') . \end{aligned}$$

A normalized source emits one monokinetic neutron per unit time and volume at lethargy  $u = 0$  in a non-absorbing, infinite and homogeneous material. In this case, Eqs. (4) and (8) simplify to

$$(10) \quad \rho(u) = \Sigma_s(u) \phi(u) - \delta(u)$$

and

$$(11) \quad \frac{d}{du} q(u) = \delta(u)$$

where the Dirac delta function is used to represent the source.

Equation (11) is easily integrated in lethargy, leading to an Heaviside function:

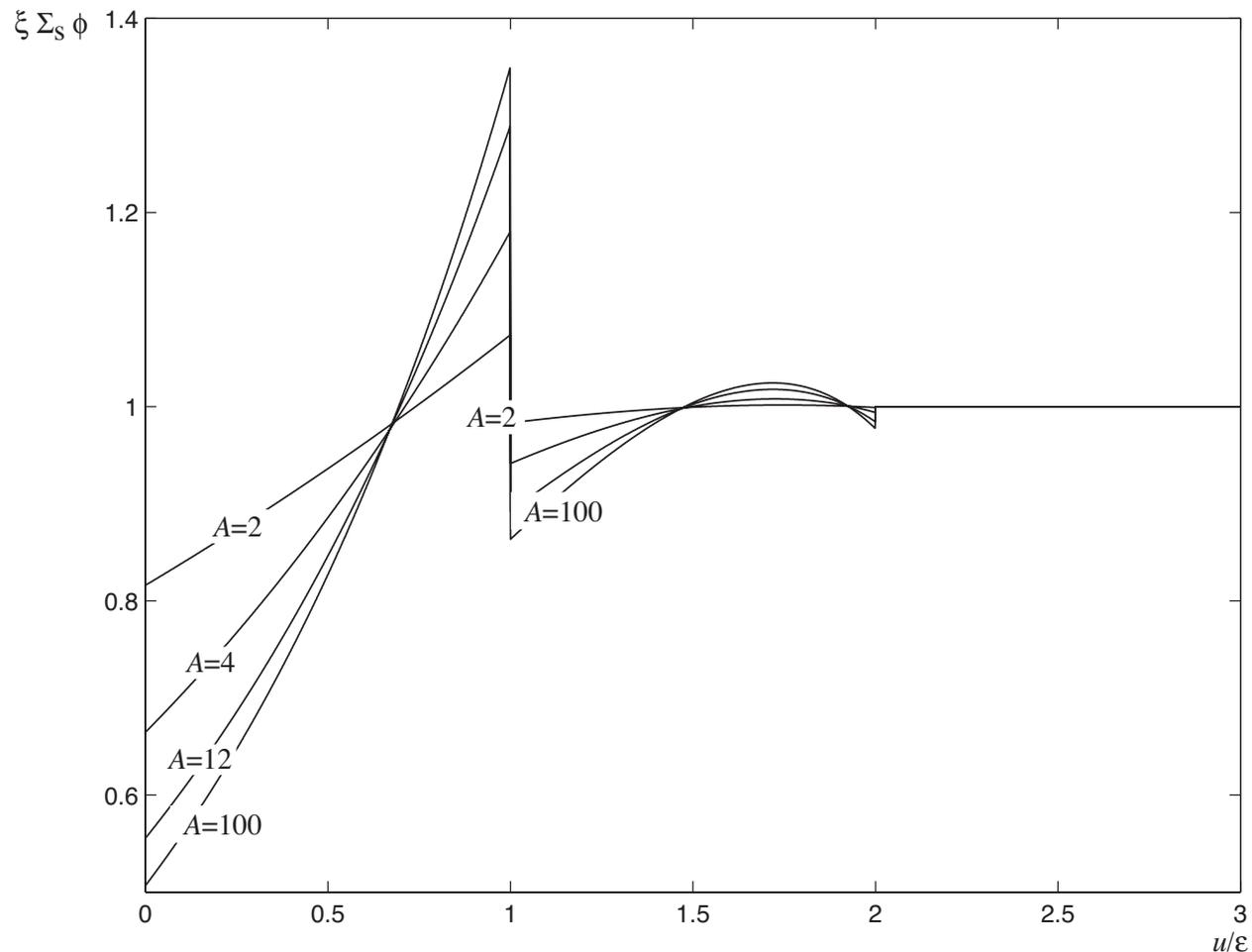
$$(12) \quad q(u) = \mathcal{H}(u) = \begin{cases} 0 & \text{if } u \leq 0 \\ 1 & \text{otherwise.} \end{cases}$$

The flux equation is obtained by substituting Eqs. (10) and (12) in Eq. (9):

$$(13) \quad \mathcal{H}(u) + \frac{\alpha}{1 - \alpha} \int_{u-\epsilon}^u du' \Sigma_s(u') \phi(u') + \delta(u) = \Sigma_s(u) \phi(u) .$$

# Placzek transients

The neutron flux, as solution of Eq. (13), presents discontinuities for values of the lethargy equal to  $\epsilon$ ,  $2\epsilon$ , etc. and its limit as  $u \rightarrow \infty$  tends toward a constant value. This behavior is typical of Placzek transients.



If  $0^- \leq u \leq 0^+$ , the solution of Eq. (13) is:  $\phi(u) = \delta(u)/\Sigma_s(u)$ .

For values  $0 < u \leq \epsilon$ :

$$(14) \quad 1 + \frac{\alpha}{1-\alpha} + \frac{\alpha}{1-\alpha} \int_{0^+}^u du' \Sigma_s(u') \phi(u') = \Sigma_s(u) \phi(u)$$

so that

$$(15) \quad \frac{1}{1-\alpha} + \frac{\alpha}{1-\alpha} \int_{0^+}^u du' \Sigma_s(u') \phi(u') = \Sigma_s(u) \phi(u) \quad \text{if } 0 < u \leq \epsilon .$$

Assuming a solution of the form  $\phi(u) = \frac{C}{\Sigma_s(u)} e^{\beta u}$ , Eq. (15) becomes

$$(16) \quad \frac{1}{1-\alpha} + \frac{\alpha C}{\beta(1-\alpha)} \left( e^{\beta u} - 1 \right) = C e^{\beta u}$$

so that  $\beta = \alpha/(1-\alpha)$  and  $C = 1/(1-\alpha)$ . The first Placzek transient is therefore

$$(17) \quad \phi(u) = \frac{1}{(1-\alpha)\Sigma_s(u)} e^{\frac{\alpha}{(1-\alpha)}u} \quad \text{if } 0 < u \leq \epsilon .$$

For values  $\epsilon < u \leq 2\epsilon$ , we can show that

$$1 + \frac{\alpha}{(1-\alpha)^2} \int_{u-\epsilon}^{\epsilon} du' e^{\frac{\alpha}{(1-\alpha)} u'} + \frac{\alpha}{1-\alpha} \int_{\epsilon}^u du' \Sigma_s(u') \phi(u') = \Sigma_s(u) \phi(u)$$

so that

$$1 + \frac{1}{1-\alpha} \left( e^{\frac{\alpha \epsilon}{(1-\alpha)}} - e^{\frac{\alpha}{(1-\alpha)} (u-\epsilon)} \right) + \frac{\alpha}{1-\alpha} \int_{\epsilon}^u du' \Sigma_s(u') \phi(u') = \Sigma_s(u) \phi(u) .$$

The solution of this equation is the second Placzek transient. Its analytical expression is

$$(18) \quad \phi(u) = \frac{1}{(1-\alpha) \Sigma_s(u)} \left[ e^{\frac{\alpha \epsilon}{(1-\alpha)}} - \alpha - \frac{\alpha}{1-\alpha} (u-\epsilon) \right] e^{\frac{\alpha}{(1-\alpha)} (u-\epsilon)} .$$

For values of  $u \gg \epsilon$ , the scattering density  $\Sigma_s(u) \phi(u)$  becomes regular, so that the integral in Eq. (13) can be written

$$(19) \quad \int_{u-\epsilon}^u du' \Sigma_s(u') \phi(u') = \epsilon \Sigma_s(u) \phi(u) .$$

Equation (13) simplifies to

$$(20) \quad 1 + \frac{\alpha}{1-\alpha} \epsilon \Sigma_s(u) \phi(u) = \Sigma_s(u) \phi(u)$$

and the flux tends to its asymptotic value

$$(21) \quad \phi(u) = \frac{1}{\xi \Sigma_s(u)} \quad \text{if } u \gg \epsilon$$

where we introduced the **average lethargy gain**  $\xi$  as

$$(22) \quad \xi = 1 - \frac{\alpha \epsilon}{1-\alpha} .$$

The main problem considered in the resonance self-shielding model is how to use self-shielded cross section and probability table information, as recovered from the isotopic cross-section library. The final objective is to evaluate  $\tilde{\sigma}_{\rho,g}$ , the microscopic self-shielded cross section for any reaction  $\rho$  in coarse group  $g$ , which is formally defined as

$$(23) \quad \tilde{\sigma}_{\rho,g} = \mu_g \frac{\int_{u_{g-1}}^{u_g} du \sigma_{\rho}(u) \phi(u)}{\int_{u_{g-1}}^{u_g} du \phi(u)} = \mu_g \frac{\langle \sigma_{\rho} \phi \rangle_g}{\langle \phi \rangle_g}$$

where

$u_{g-1}, u_g =$  lethargy limits of group  $g$

$\mu_g =$  **superhomogénéisation** (SPH) factor obtained from the multigroup equivalence procedure.

$\phi(u) =$  averaged neutron flux in the region where the cross section is defined

$\sigma_{\rho}(u) =$  microscopic cross section for nuclear reaction  $\rho$ .

The flux used in Equation (23) is the solution of the slowing-down equation:

$$\boldsymbol{\Omega} \cdot \nabla \phi(\mathbf{r}, u, \boldsymbol{\Omega}) + \Sigma(\mathbf{r}, u) \phi(\mathbf{r}, u, \boldsymbol{\Omega}) = \frac{1}{4\pi} \left[ S_f(\mathbf{r}, u) + \sum_{j=1}^J \mathcal{R}_j \{ \phi(\mathbf{r}, u) \} \right]$$

This equation is first simplified using the [Livolant-Jeanpierre approximations](#)

Consider the neutron slowing-down equation. We will first assume that the domain contains a single resonant isotope. The neutron flux is the solution of Eq. (1):

$$(24) \quad \boldsymbol{\Omega} \cdot \nabla \phi(\mathbf{r}, u, \boldsymbol{\Omega}) + \Sigma(\mathbf{r}, u) \phi(\mathbf{r}, u, \boldsymbol{\Omega}) = \frac{1}{4\pi} [\mathcal{R}^+ \{\phi(\mathbf{r}, u)\} + \mathcal{R}^* \{\phi(\mathbf{r}, u)\}]$$

where

$\mathcal{R}^+ \{\phi(\mathbf{r}, u)\} =$  slowing-down operator for nuclear reactions with non-resonant isotopes

$\mathcal{R}^* \{\phi(\mathbf{r}, u)\} =$  slowing-down operator for nuclear reactions with a single heavy isotope and it is assumed that neutron sources originating from inelastic, (n,xn) and fission nuclear reactions vanish over the slowing-down energy domain.

The two slowing-down operators can be written:

$$(25) \quad \mathcal{R}^+ \{\phi(\mathbf{r}, u)\} = \int_0^\infty du' \Sigma_{s0}^+(\mathbf{r}, u \leftarrow u') \phi(\mathbf{r}, u')$$

and

$$(26) \quad \mathcal{R}^* \{\phi(\mathbf{r}, u)\} = \int_0^\infty du' \Sigma_{s0}^*(\mathbf{r}, u \leftarrow u') \phi(\mathbf{r}, u') .$$

We next simplify Eq. (24) by using a set of approximations proposed by Livolant and Jeanpierre. We first assume that the neutron flux in each region is factorized as the product of a resonant fine-structure function  $\varphi(\mathbf{r}, u)$  with a regular distribution in lethargy  $\psi(\mathbf{r}, u)$ :

$$(27) \quad \phi(\mathbf{r}, u, \boldsymbol{\Omega}) = \varphi(\mathbf{r}, u, \boldsymbol{\Omega}) \psi(\mathbf{r}, u) \quad .$$

and

$$(28) \quad \phi(\mathbf{r}, u) = \varphi(\mathbf{r}, u) \psi(\mathbf{r}, u) \quad .$$

The distribution  $\psi(\mathbf{r}, u)$  is called the macroscopic flux and represents the asymptotic behavior of the neutron flux between the resonances. This distribution is defined in terms of  $\mathcal{R}^+\{\phi(\mathbf{r}, u)\}$ , which acts as a smoothing operator on the neutron flux:

$$(29) \quad \psi(\mathbf{r}, u) = \frac{1}{\Sigma_s^+(\mathbf{r}, u)} \mathcal{R}^+\{\phi(\mathbf{r}, u)\}$$

where  $\Sigma_s^+(\mathbf{r}, u)$  is the macroscopic scattering cross section of the non-resonant isotopes.

The first assumption is based on the fact that the resonant isotope is heavy and that  $\mathcal{R}^* \{\phi(\mathbf{r}, u)\}$ , the slowing-down operator for the resonant isotope, is acting over a short lethargy range. This results in

$$(30) \quad \mathcal{R}^* \{\phi(\mathbf{r}, u)\} = \psi(\mathbf{r}, u) \mathcal{R}^* \{\varphi(\mathbf{r}, u)\} \quad .$$

A second approximation consists of assuming a spatially flat value for distribution  $\psi(\mathbf{r}, u)$  across the domain. The substitution of Eqs. (27), (29) and (30) in slowing-down Eq. (24) and the simplification of the  $\psi(\mathbf{r}, u)$  distribution leads to

$$(31) \quad \boldsymbol{\Omega} \cdot \nabla \varphi(\mathbf{r}, u, \boldsymbol{\Omega}) + \Sigma(\mathbf{r}, u) \varphi(\mathbf{r}, u, \boldsymbol{\Omega}) = \frac{1}{4\pi} [\Sigma_s^+(\mathbf{r}, u) + \mathcal{R}^* \{\varphi(\mathbf{r}, u)\}] \quad .$$

Equation (31) is a simplified transport equation that is solved in the resonance self-shielding calculation module of the lattice code. This is a source equation that is defined only over resonant energy groups. The cross sections  $\Sigma(\mathbf{r}, u)$  and  $\Sigma_{s0}^*(\mathbf{r}, u)$  are resonant functions of the lethargy.

A first class of resonant self-shielding models is based on **equivalence in dilution** in which an heterogeneous case is represented by an **equivalent** homogeneous case. Two techniques currently exist to compute the **equivalent dilution** of the homogeneous case:

- Use rational expansions of fuel-to-fuel collision probabilities, either in close or open cell (or assembly).
  - In its simplest form, this technique reduces to the Bell-factor approximation applied on a cylindrical fuel pin. This class of models originates from WIMS-D and is still used in many legacy codes in some advanced form.
  - Helpful extensions have been proposed by Stamm'ler (code PHOENIX) and later by Hébert and Marleau (code DRAGON, module `SHI` : ) to increase the number of terms in the rational expansions.
- Use the Sanchez-Coste method. Both the heterogeneous and homogeneous cases are solved using **probability tables**. Many implementations exist
  - the APOLLO1 original technique is a simplified Sanchez-Coste method where a unique hard-coded probability table covers the complete epithermal domain
  - the APOLLO2 module `AUTOP` : is the official implementation.

We assume an infinite and homogeneous medium and represent as  $\Sigma^+$  the macroscopic total cross section of the non-resonant isotopes in the coarse energy group  $g$  under consideration. Eq. (31) simplifies to

$$(32) \quad [\Sigma^+ + N^* \sigma^*(u)] \varphi(u) = \Sigma_s^+ + \mathcal{R}^* \{ \varphi(u) \}$$

where  $\sigma^*(u)$  is the microscopic total cross section of the resonant isotope.

Equation (32) is similar to the **flux calculator** in the `groupR` module of NJOY:

$$(33) \quad [\sigma_e + \sigma^*(u)] \varphi(u) = \gamma \sigma_e + \frac{1}{N^*} \mathcal{R}^* \{ \varphi(u) \}$$

where we defined the **dilution**  $\sigma_e$  and **gamma factor**  $\gamma$  as

$$(34) \quad \sigma_e = \frac{\Sigma^+}{N^*} \quad \text{and} \quad \gamma = \frac{\Sigma_s^+}{\Sigma^+} .$$

The equation solved in NJOY is identical to Eq. (33) if we set  $\gamma = 1$ . The solution of Eq. (33) is therefore identical to the solution  $\phi(u)$  of the `groupR` flux calculator, taken at a dilution  $\sigma_e$ , multiplied by  $\gamma$ :

$$(35) \quad \varphi(u) = \gamma \phi(u) .$$

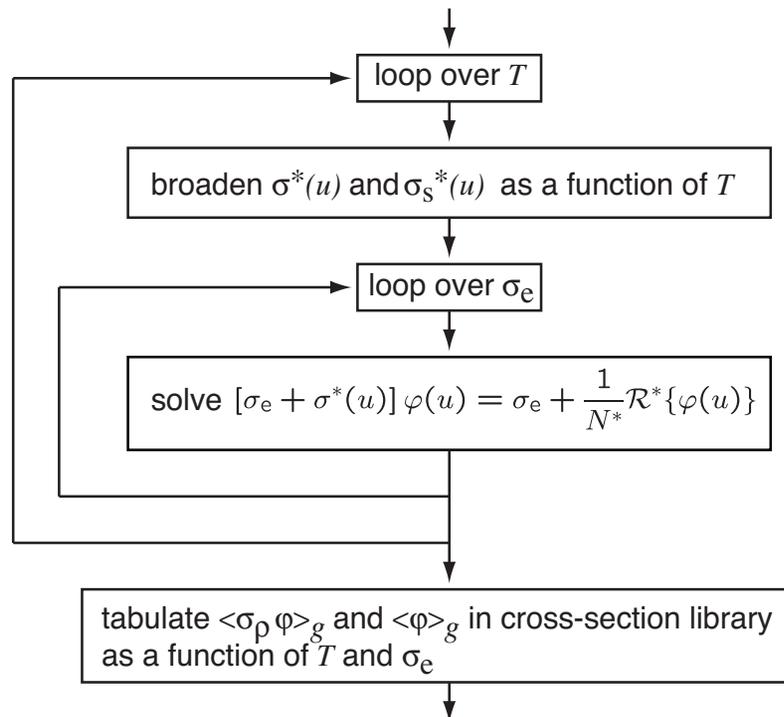
Equation (35) is the justification for self-shielding models based on an **equivalence in dilution**. All averaged quantities such as  $\langle \phi \rangle_g$  or  $\langle \sigma_\rho^* \phi \rangle_g$  can be **interpolated** from the tabulation produced by NJOY, as soon as we know the dilution parameter  $\sigma_e$  of the actual problem. It is then sufficient to multiply these interpolated values by  $\gamma$  to obtain the actual averaged quantities.

The **equivalence in dilution** method consists to compute in the lattice code an **equivalent dilution** characterizing the heterogeneous geometry so that an **equivalent homogeneous geometry** is going to have similar absorption reaction rates.

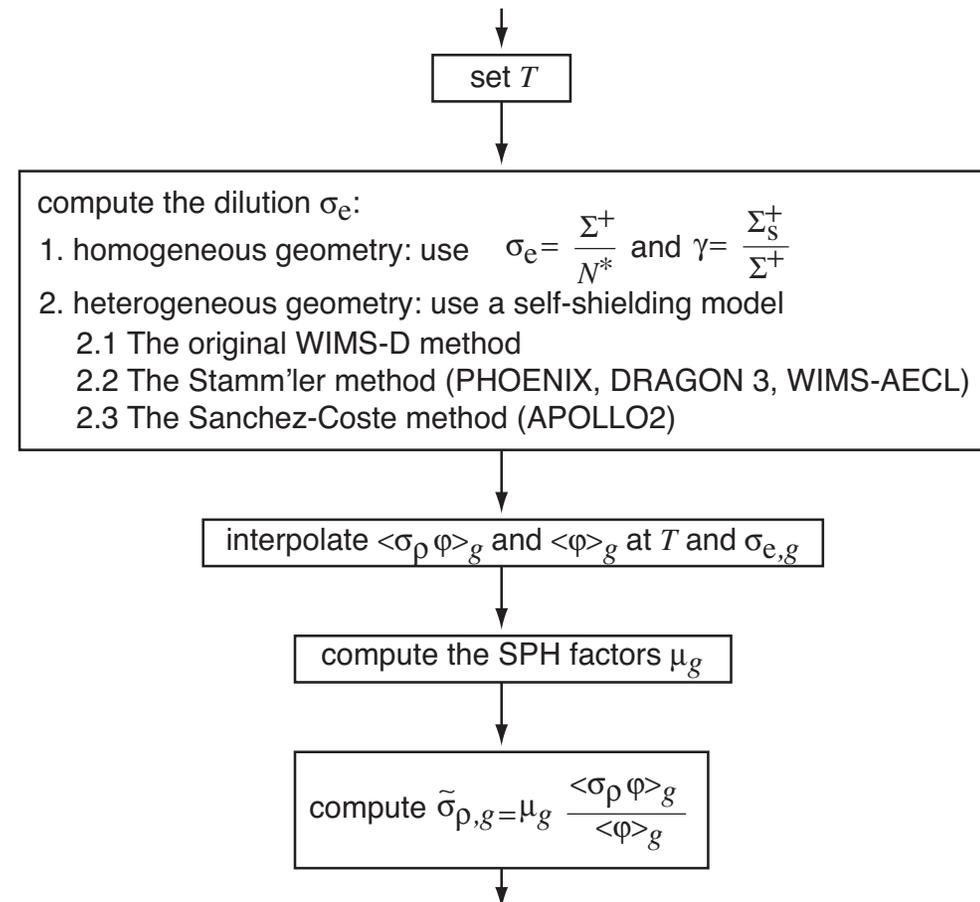
# Equivalence in dilution

The APOLLO and WIMS-D families of lattice codes are using successful models for representing an heterogeneous lattice geometry by one or many **equivalent homogeneous media**.

In NJOY:



In the lattice code (equivalence in dilution):



Another class of resonant self-shielding models relies on the subgroup (or multiband) approach:

- We replace all Riemann integrals over resonant quantities in energy with Lebesgue integrals in total cross section and to discretize these Lebesgue integrals with probability tables.
- The resulting equation is called a **subgroup equation** and has the form of an ordinary transport equation. It can be solved by classical approaches, such as the CP, discrete-ordinates or characteristics method. In a resonant group, this equation is approximated as

$$(36) \quad \boldsymbol{\Omega} \cdot \nabla \phi_k(\mathbf{r}, \boldsymbol{\Omega}) + \Sigma_k(\mathbf{r}) \phi_k(\mathbf{r}, \boldsymbol{\Omega}) = \frac{1}{4\pi} \left[ \Sigma_s^+(\mathbf{r}) + \sum_{k'=1}^K \frac{\mathcal{W}_{k,k'}}{\omega_k} \Sigma_{s,k'}(\mathbf{r}) \phi_{k'}(\mathbf{r}) \right]$$

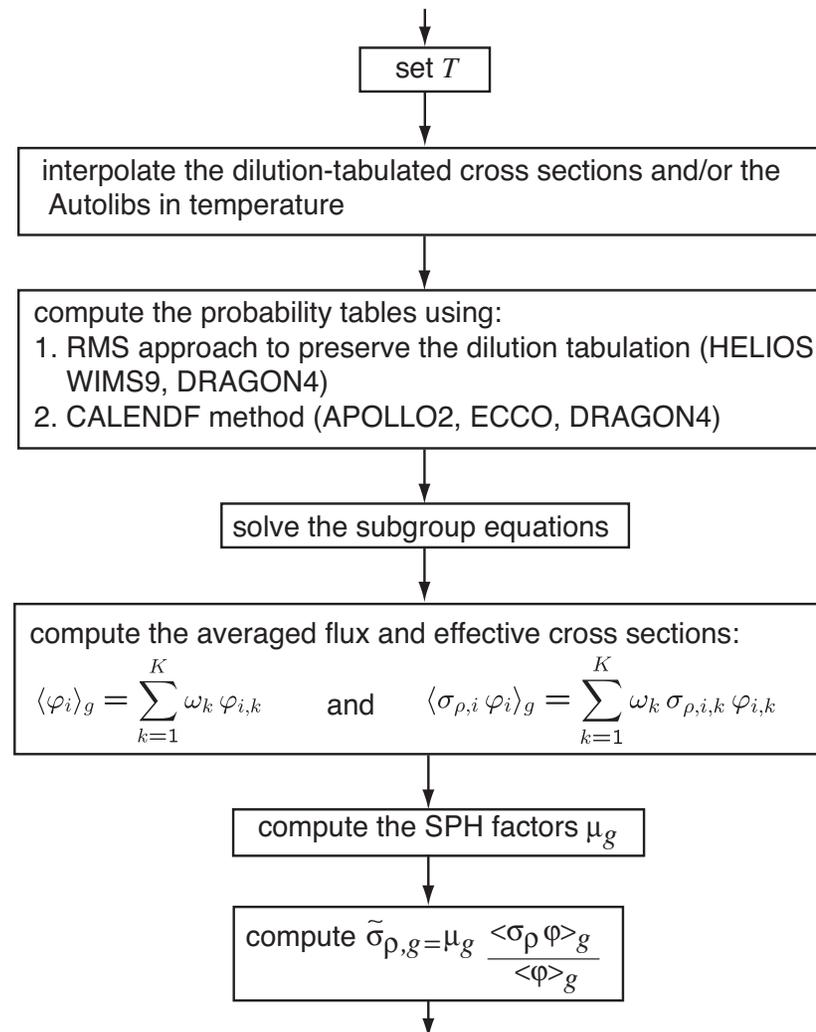
where  $1 \leq k \leq K$  is the subgroup index of the probability table.  $\mathcal{W}_{k,k'}$  is a correlated weight matrix taking into account the correlation between the diffusion source and the collision term.

- This approach is used in the following codes: APOLLO2 (validation path), HETAIRE, ECCO, HELIOS, WIMS8 and DRAGON4 (module `USS` :).

# Subgroup approach

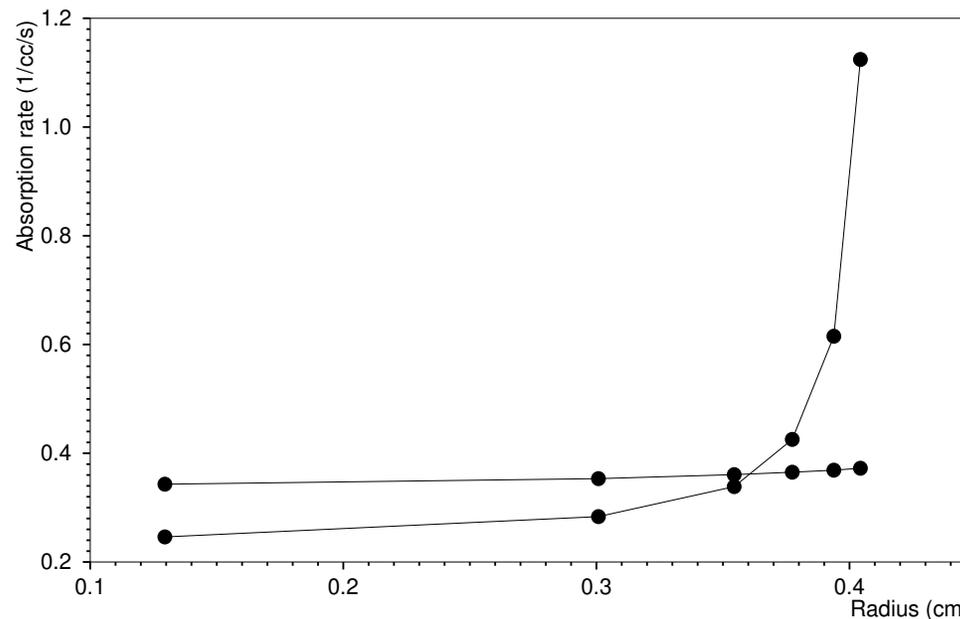
Recent codes such as HELIOS, WIMS8 and DRAGON4 are using the subgroup method (production path). The subgroup method is also available in APOLLO2 as validation path.

In the lattice code (subgroup method):



# Distributed self-shielding effects

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 The principle is to assign many sub-regions  $V_i$  to the resonant part of the geometry and to consider many resonant regions in the self-shielding calculation.
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 This possibility allows the subdivision of a fuel rod into annulus and to represent the Plutonium build-up in the outer ring with a better accuracy. The so-called **rim effect** is represented in the figure where we see the effect on the absorption rate distribution of using one or six resonant regions in the self-shielding calculation.
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 This capability is a characteristic of advanced self-shielding models.



# Many resonant isotopes case

- If the medium contains many resonant isotopes:
  - We perform a different self-shielding calculation of each of them, assuming that all the other admixed isotopes are non-resonant.
  - Any admixed resonant isotope is represented by its self-shielded cross sections that are used as components to compute  $\Sigma^+$  and  $\Sigma_s^+$ .
  - Outer iterations must be performed in order to converge on self-shielded cross sections for all the resonant isotopes present in the medium.
- This simple approach is sufficient to represent mixtures of different resonant isotopes, as long as their low-energy resonances are not overlapping. If overlapping occurs:
  - One must select a more advanced self-shielding model with capabilities to represent **mutual shielding effects**.
  - Another option is to finely discretize these overlapping resonances with the multigroup energy mesh of the main flux calculation and to avoid using a self-shielding model at these energies.