
POLYTECHNIQUE
MONTRÉAL

# Libraries and resonance self-shielding calculations

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# Outline



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# Elements of lattice calculation



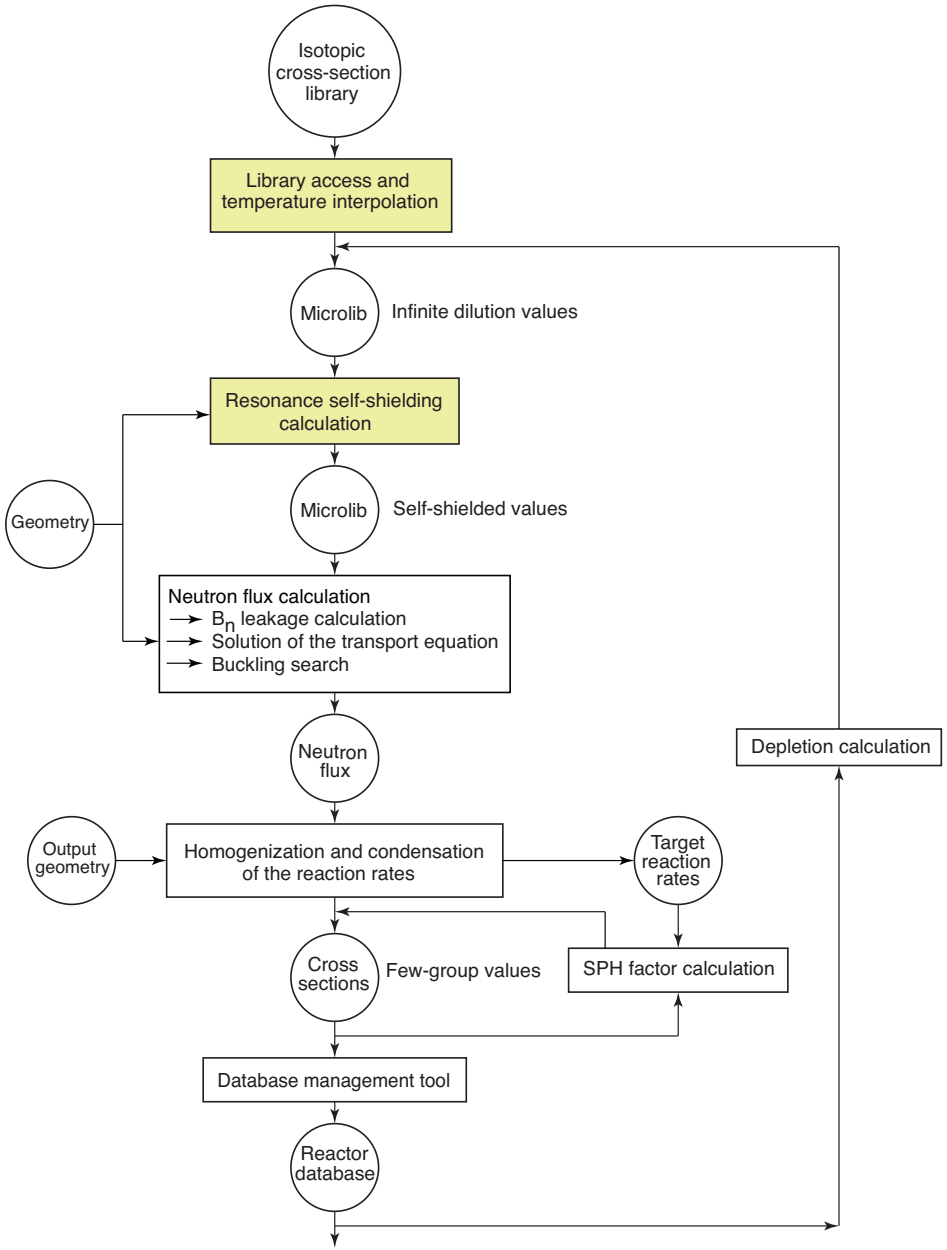
- A few first-generation lattice codes based of the four-factor formula are still in production use today.
- The second generation lattice codes features a consistent multigroup (between 50 and 400 groups) representation of the neutron energies.

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.

# Elements of lattice calculation





# Cross-section libraries



- Cross section libraries are generally produced by external applications such as NJOY-99 or NJOY-2012.
- They contain multigroup data (processed by the groupr module of NJOY) formatted according to a specific energy mesh (commonly used in DRAGON5):
  - IAEA-69: Legacy mesh used with the WIMS family of lattice codes
  - WLUP-172: Legacy mesh that can be seen as the successor of the IAEA-69 mesh. Popular in France and UK.
  - SHEM-281: New recommended mesh in France for the APOLLO2 lattice code.
  - SHEM-295: New recommended mesh for DRAGON5 calculations using advanced resonance self-shielding models.

# Cross-section libraries



- They contain most of the isotope-related data required by the lattice code:
  - cross sections
  - collision laws and emission spectra
  - radioactive decay and fission yield data
- Thek do not contain diffusion coefficient data
- A cross section library is formatted according to proprietary or public specifications (all accepted by DRAGON5)
  - WIMSLIB D4 format: Legacy format used by the WIMS Library Update Project(WLUP).
  - DRAGLIB format: Specific format for the DRAGON family of codes (LGPL license). Produced by the `dragr` module of NJOY
  - MATXS format: Specific format produced by the `matxsr` module of NJOY. Depletion data is not available.

# LIB: module data



```
LIBRARY := LIB: ::
 NMIX 6     (*MAXIMUM OF MATERIAL MIXTURES*)
 CTRA APOL  (*APOLLO TYPE TRANSPORT CORRECTION*)
 SUBG       (*HELIOS TYPE PROBABILITY TABLES*)
*
 DEPL LIB: DRAGON FIL: DLIB_J2
 MIXS LIB: DRAGON FIL: DLIB_J2
 MIX 1 293.0
    O16      = O16     4.6624E-2
    U235     = U235    7.0803E-4 1 IRSET 0.0 81
    U238     = U238    2.2604E-2 1 IRSET 0.0 81
 MIX 2 COMB 1 1.0
 MIX 3 COMB 1 1.0
 MIX 4 COMB 1 1.0
 MIX 5 293.0 NOEV
    Zrnat    = Zr0     4.3241E-2 2 IRSET 0.0 81
 MIX 6 293.0 NOEV
    H1       = H1_H2O  4.6892E-2
    O16      = O16     2.3446E-2    ;
```

# LIB: module data



`NMIX 6` Maximum number of material mixtures.

`CTRA APOL` Select APOLLO-type transport correction.

`SUBG` Compute physical probability tables.

`DEPL LIB: DRAGON FIL: DLIB_J2` Recover depletion and energy production data from Draglib named `DLIB_J2`.

`MIXS LIB: DRAGON FIL: DLIB_J2` Recover cross-section data from Draglib named `DLIB_J2`.

`MIX 1 293.0` Mixture 1 has absolute temperature 293.0 K and is depleting.

`MIX 2 COMB 1 1.0` Mixture 2 is initially identical to mixture 1. It will be self-shielded and will deplete independently of it.

`NOEV` Indicates that a mixture is non-depleting.

`Zrnat = Zr0 4.3241E-2 2 IRSET 0.0 81` Mixture 5 contains an isotope with Dragon name `Zrnat`, library name `Zr0`, with number density 4.3241E-2 $\times 10^{-24}$ per cc and is self-shielded in zone 2. A WR model will be used if $g \geq 81$ and a ST model will be used if $g < 81$.

# Resonance self-shielding approaches



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 $\tilde{\sigma}_{\rho,i,g}$, the microscopic self-shielded cross section for any reaction $\rho$ in region $i$ and coarse group $g$, which is formally defined as

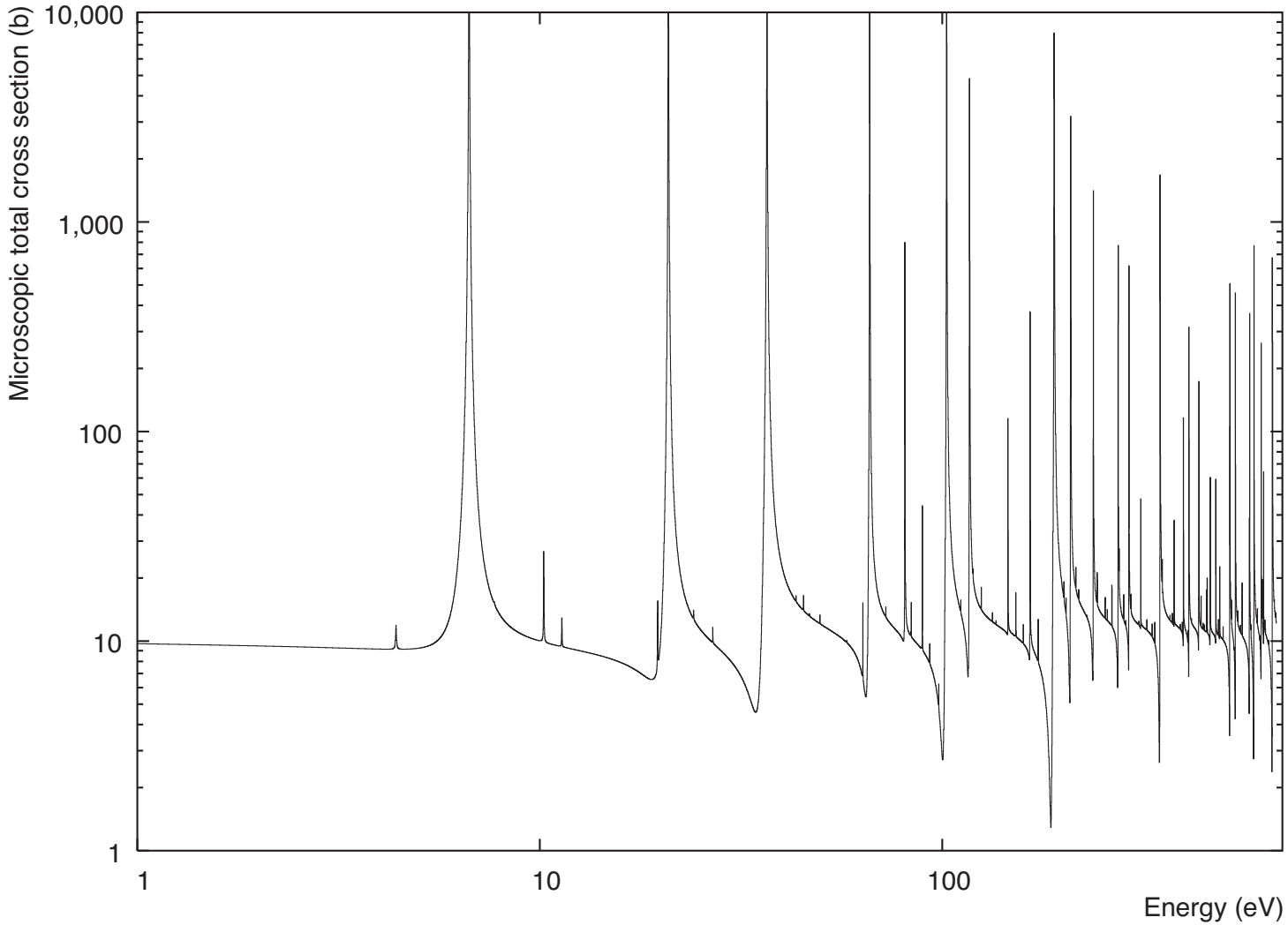
$$\tilde{\sigma}_{\rho,i,g} = \mu_{i,g} \frac{\int_{u_{g-1}}^{u_g} du\, \sigma_{\rho,i}(u)\phi_i(u)}{\int_{u_{g-1}}^{u_g} du\, \phi_i(u)} = \mu_{i,g} \frac{\langle \sigma_{\rho,i}\phi_i \rangle_g}{\langle \phi_i \rangle_g} \tag{1}$$

where

$u_{g-1}, u_g =$ lethargy limits of group $g$
$\mu_{i,g} =$ superhomogénéisation (SPH) factor in region $i$ obtained from the multigroup equivalence procedure. The SPH equivalence can be avoided in energy groups with a lethargy $\Delta u \leq 0.1$.
$\phi_i(u) =$ averaged neutron flux in region $i$ where the cross section is defined
$\sigma_{\rho,i}(u) =$ microscopic cross section for nuclear reaction $\rho$ in region $i$.

# Uranium-238 total cross section





# The Livolant-Jeanpierre fine-structure



At energies of the incident neutron greater than a few eV the elastic scattering reaction leads to a pure slowing-down effect. 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.
- The heavy isotopes are mostly responsible of the resonant absorption of neutrons but are not the largest cause of slowing-down.

The Livolant-Jeanpierre model assumes that the neutron flux in each region is factorized as the product of a resonant fine-structure function $\varphi(\boldsymbol{r}, u)$ with a regular distribution in lethargy $\psi(\boldsymbol{r}, u)$:

$$\phi(\boldsymbol{r}, u, \boldsymbol{\Omega}) = \varphi(\boldsymbol{r}, u, \boldsymbol{\Omega})\, \psi(\boldsymbol{r}, u) \quad . \tag{2}$$

A second assumption consists to process a single resonant isotope at each self-shielding iteration, all other isotopes been assumed to be non-resonant (and taken equal to their self-shielded values).

# The Livolant-Jeanpierre fine-structure



In this case, the transport equation simplifies to (see Applied Reactor Physics):

$$\boldsymbol{\Omega}\cdot\nabla\varphi(\boldsymbol{r},u,\boldsymbol{\Omega})+\Sigma(\boldsymbol{r},u)\,\varphi(\boldsymbol{r},u,\boldsymbol{\Omega})=\frac{1}{4\pi}\left[\Sigma_s^+(\boldsymbol{r},u)+\mathscr{R}^*\{\varphi(\boldsymbol{r},u)\}\right] \tag{3}$$

- where we assumed that the scattering reaction if the resonant isotope is isotropic in the LAB and is purely elastic:

$$\mathscr{R}^*\{\varphi(\boldsymbol{r},u)\}=\int_0^\infty du'\,\Sigma_{s0}^*(\boldsymbol{r},u\leftarrow u')\,\varphi(\boldsymbol{r},u') \tag{4}$$

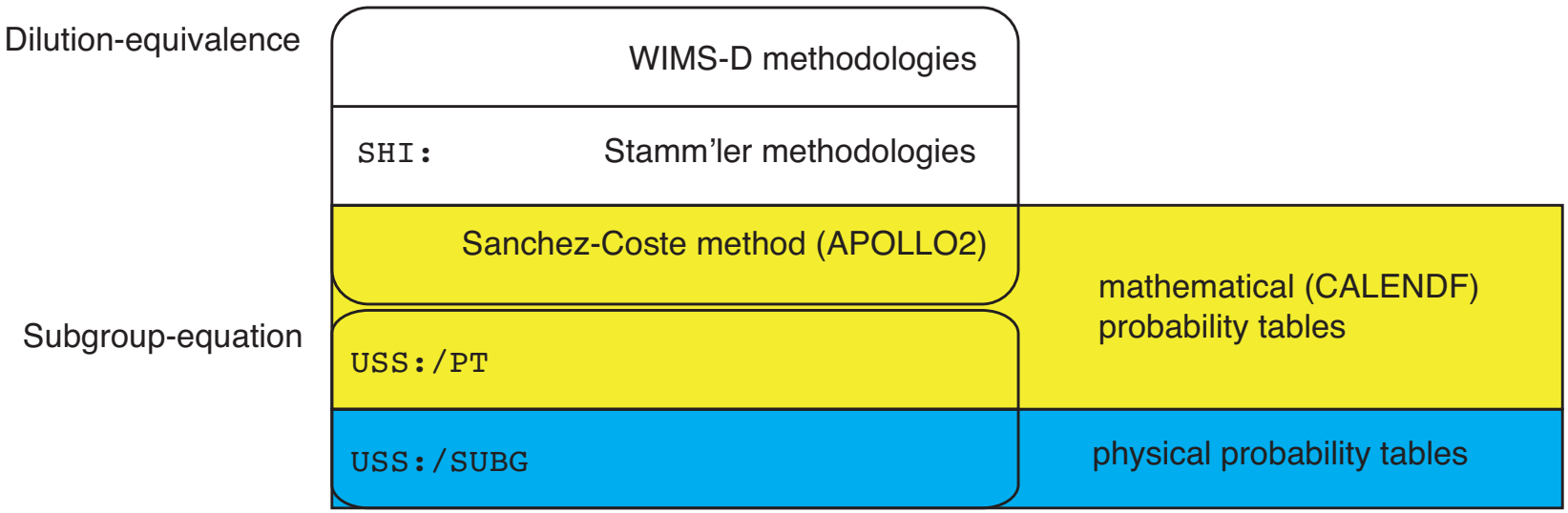
- and where $\Sigma_s^+(\boldsymbol{r},u)$ is the scattering cross section of all non-resonant cross sections at point $\boldsymbol{r}$.

Equation (3) must be solved for $\varphi(\boldsymbol{r},u)$ and used to compute $\langle\varphi\rangle_g$ and $\langle\sigma_\rho\varphi\rangle_g$.

# Two main methodologies



- Dilution-equivalence methodology
  `SHI:` Available in DRAGON3, DRAGON4 and DRAGON5
- Subgroup-equation methodology
  `USS:` Available in DRAGON4 and DRAGON5
- Note: Probability tables can by used with both methodologies.



# The dilution-equivalence approach



In each resonant region and each resonant energy group, find a dilution parameter $\sigma_e$ such as the following two equations are leading to the same absorption reaction rate:

$$\boldsymbol{\Omega}\cdot\nabla\varphi(\boldsymbol{r},u,\boldsymbol{\Omega})+\Sigma(\boldsymbol{r},u)\,\varphi(\boldsymbol{r},u,\boldsymbol{\Omega})=\frac{1}{4\pi}\left[\Sigma_s^+(\boldsymbol{r},u)+\mathscr{R}^*\{\varphi(\boldsymbol{r},u)\}\right]$$

$$\Updownarrow$$

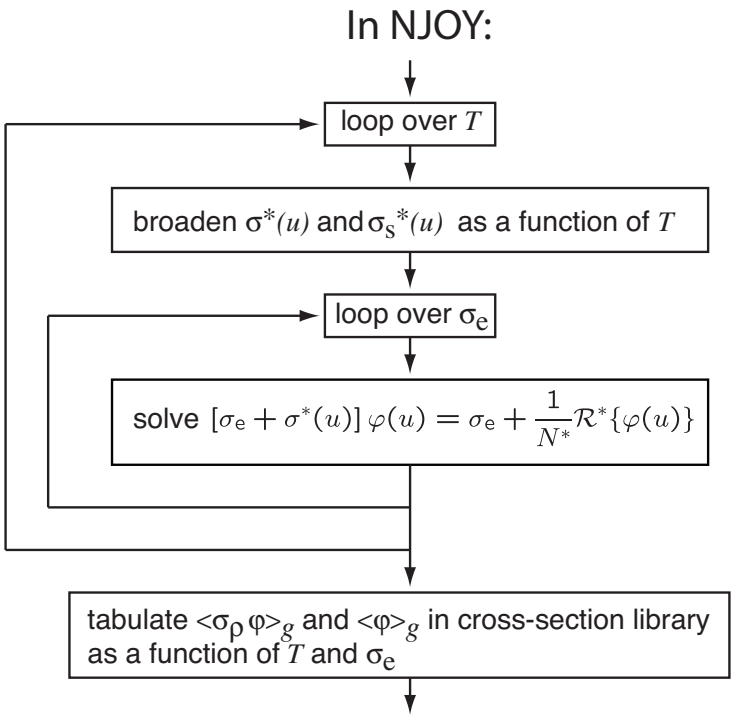
$$\left[\sigma_e+\sigma^*(u)\right]\varphi(u)=\gamma\,\sigma_e+\frac{1}{N^*}\mathscr{R}^*\{\varphi(u)\} \tag{5}$$

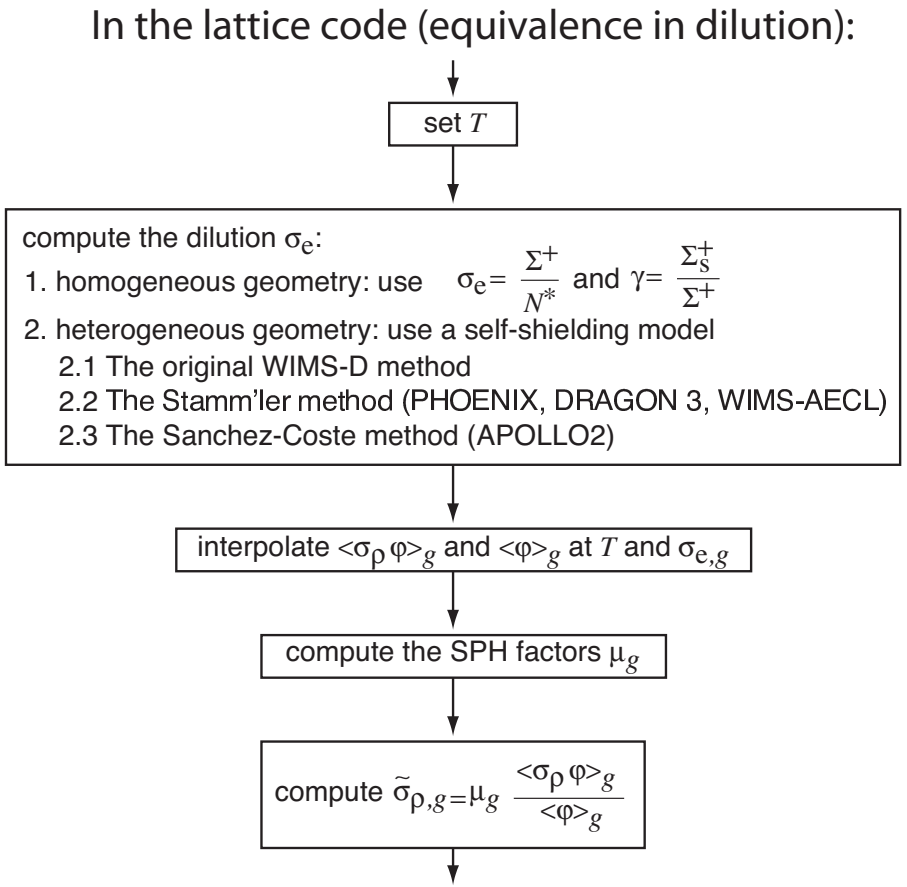
Next, interpolate $\langle\varphi\rangle_g$ and $\langle\sigma_\rho\varphi\rangle_g$ from existing solutions of Eq. (5) obtained in `groupr` module of NJOY.

# The dilution-equivalence approach



The DRAGON3 (module `SHI:`), APOLLO2 (module `AUTOP:`) and WIMS-D families of lattice codes are using successful models for representing an heterogeneous lattice geometry by one or many equivalent homogeneous media.

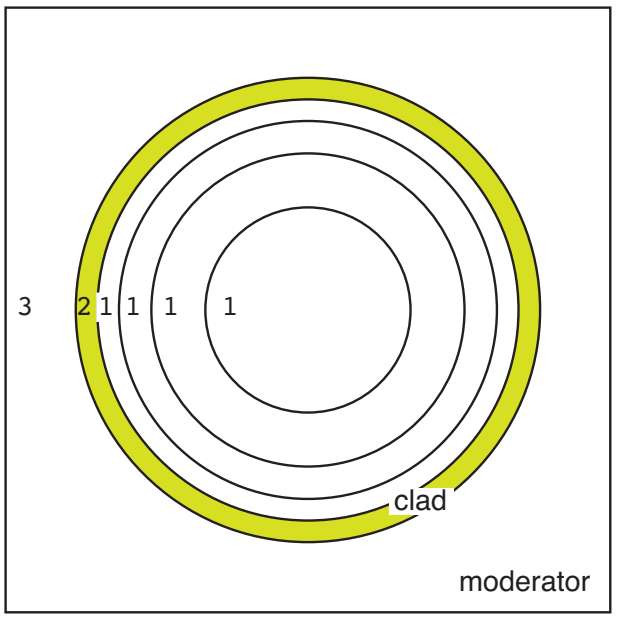


# The dilution-equivalence approach



- Legacy module SHI : is used
- No distributed self-shielding (LEVEL 0 default option)
- No need to subdivide the moderator in self-shelding calculations



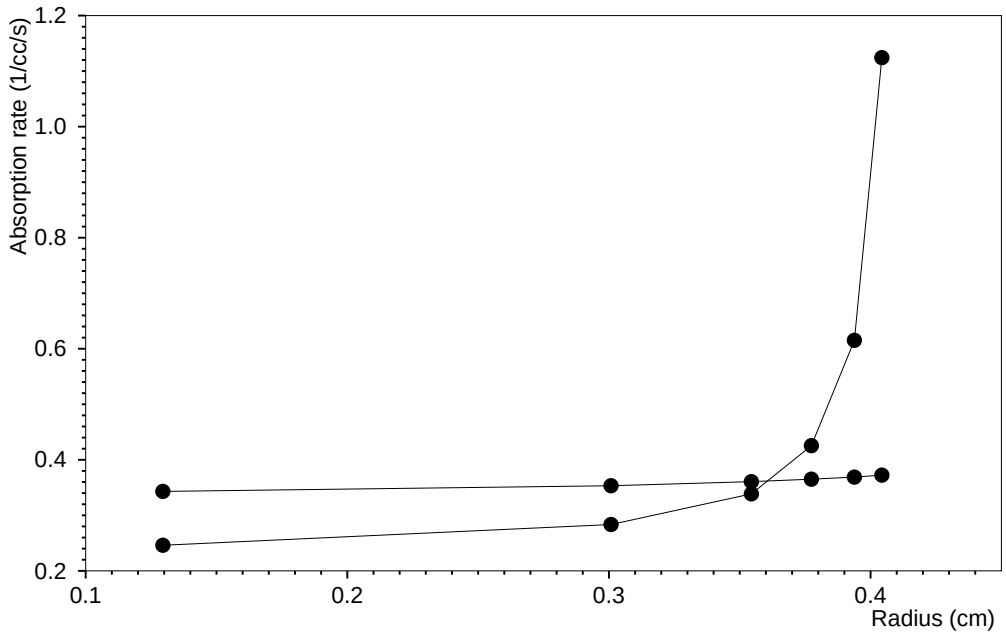

```
LIBRARY := LIB: ::
  EDIT 1
  NMIX 3    (*MAXIMUM OF MATERIAL MIXTURES*)
  MIXS LIB: DRAGON FIL: DLIB_J2        XMAS-172 library
  MIX 1 293.0
    U235    = U235   7.0803E-4 1
    U238    = U238   2.2604E-2 1      first self-shielding domain
    O16     = O16    4.6624E-2
  MIX 2 293.0
    Zr0     = Zr0    4.3241E-2 2      second self-shielding domain
  MIX 3 293.0
    H1      = H1_H2O 6.6988E-2
    O16     = O16    3.3494E-2
  ;
LIBRARY := SHI: LIBRARY TRACK :: EDIT 1 LJ ;

                                       compute a SPH factor
```

# The dilution-equivalence approach



## Distributed self-shielding effects

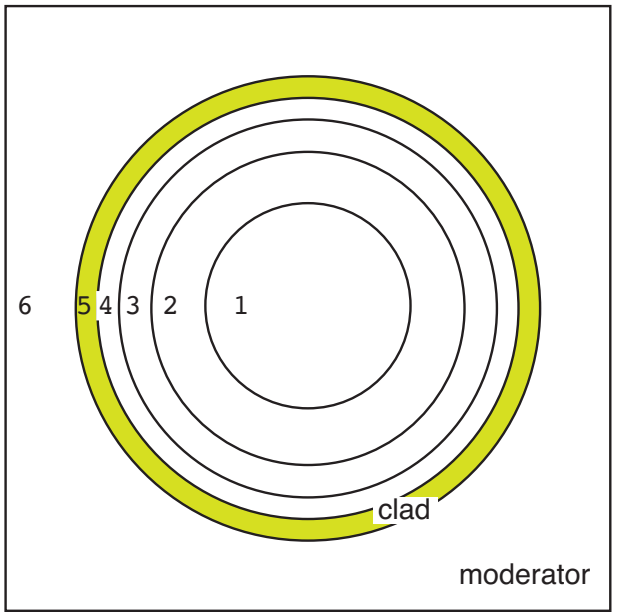
- The principle is to assign many sub-regions $V_i$ to the resonant part of the geometry and to consider many resonant regions in the self-shielding calculation.
- This possibility allows the subdivision of a fuel rod into annulus and to represent the Plutonium build-up in the outer ring with a better 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.
- This capability is a characteristic of advanced self-shielding models.



# The dilution-equivalence approach



- Legacy module SHI : is used
- Distributed self-shielding with the Nordheim model (LEVEL 1)
- Fuel is divided in four volumes: 50% (region 1), 30% (region2), 15% (region 3) and 5% (region 4)




```
LIBRARY := LIB: ::
 EDIT 1
 NMIX 6    (*MAXIMUM OF MATERIAL MIXTURES*)
 MIXS LIB: DRAGON FIL: DLIB_J2
 MIX 1 293.0
    O16      = O16     4.6624E-2
    U235     = U235    7.0803E-4 1
    U238     = U238    2.2604E-2 1
 MIX 2 COMB 1 1.0
 MIX 3 COMB 1 1.0
 MIX 4 COMB 1 1.0
 MIX 5 293.0
    Zr0      = Zr0     4.3241E-2 2
 MIX 6 293.0
    H1       = H1_H2O 6.6988E-2
    O16      = O16     3.3494E-2
;
LIBRARY2 := SHI: LIBRARY TRACK :: EDIT 1 LJ LEVEL 1 ;
```

additional mixtures for distributed self-shielding

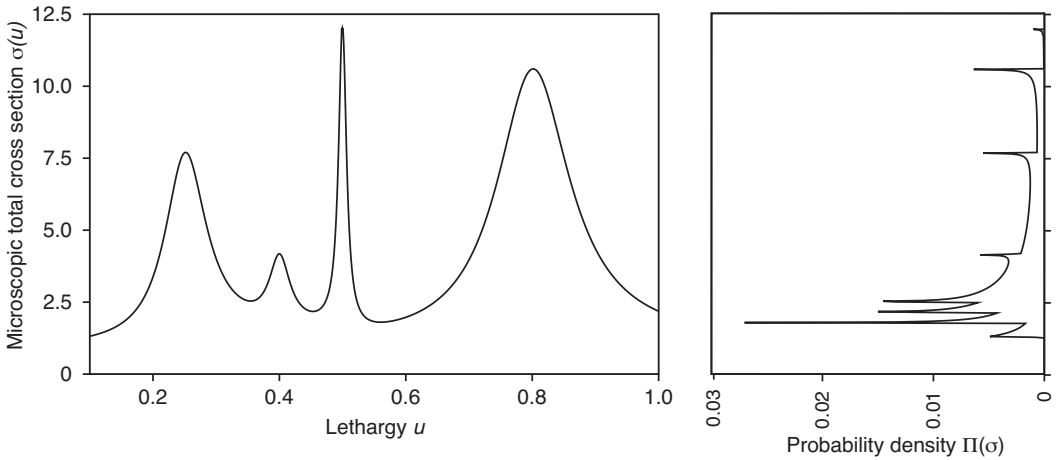
distributed self-shielding flag

# Calculation of the probability tables



Probability tables corresponding to the microscopic total cross section $\sigma(u)$ with $u_{g-1} \leq u \leq u_g$ can be defined from the probability density $\Pi(\sigma)$.

$\Pi(\sigma)d\sigma$ is the probability for the microscopic total cross section of the resonant isotope, to have a value between $\sigma$ and $\sigma + d\sigma$. $\{u_g\ ;\ 1 \leq g \leq N_g + 1\}$ is the multigroup structure containing $N_g + 1$ lethargy limits.




As might be expected, the probability density $\Pi(\sigma)$ is normalized to unity:

$$\int_0^{\max(\sigma)} d\sigma\, \Pi(\sigma) = 1 \quad . \tag{6}$$

# Calculation of the probability tables



The probability density $\Pi(\sigma)$ is represented by a series of $K$ Dirac distributions centered at discrete values $\sigma_k$ of the microscopic total cross section for the resonant isotope. Each discrete level is called a subgroup and is also characterized by a discrete weight $\omega_k$. This approach leads to an approximative expression of $\Pi(\sigma)$ written as

$$\Pi(\sigma) = \sum_{k=1}^{K} \delta(\sigma - \sigma_k)\,\omega_k \quad \text{with} \quad \sum_{k=1}^{K} \omega_k = 1 \quad . \tag{7}$$

Using this definition, any Riemann integral in lethargy, with a $\sigma$–dependent integrand, can be replaced by an equivalent Lebesgue integral:

$$\frac{1}{\Delta u_g} \int_{u_{g-1}}^{u_g} du\, f\,[\sigma(u)] = \int_0^{\max(\sigma)} d\sigma\, \Pi(\sigma)\, f(\sigma) \tag{8}$$

Substitution of Eq. (7) into Eq. (8) leads to the following discretization:

$$\frac{1}{\Delta u_g} \int_{u_{g-1}}^{u_g} du\, f\,[\sigma(u)] = \sum_{k=1}^{K} \omega_k\, f(\sigma_k) \quad . \tag{9}$$

# Calculation of the probability tables



We can also compute partial cross section information. $\sigma_x(\sigma)$ is the average value of the microscopic partial cross section $\sigma_x(u)$ corresponding to the value $\sigma(u)$ of the total microscopic cross section. The following discretization is used:

$$\Pi(\sigma)\,\sigma_x(\sigma) = \sum_{k=1}^{K} \delta(\sigma - \sigma_k)\,\sigma_{x,k}\,\omega_k \quad . \tag{10}$$

Partial cross section information can also be used to discretize the Riemann integral:

$$\frac{1}{\Delta u_g} \int_{u_{g-1}}^{u_g} du\,\sigma_x(u)\,f\left[\sigma(u)\right] = \sum_{k=1}^{K} \omega_k\,\sigma_{x,k}\,f(\sigma_k) \quad . \tag{11}$$

The set of values $\{\omega_k, \sigma_k, \sigma_{x,k};\ k = 1, K\}$ corresponding to energy group $g$ is the probability table describing the resonant behavior of the cross sections.

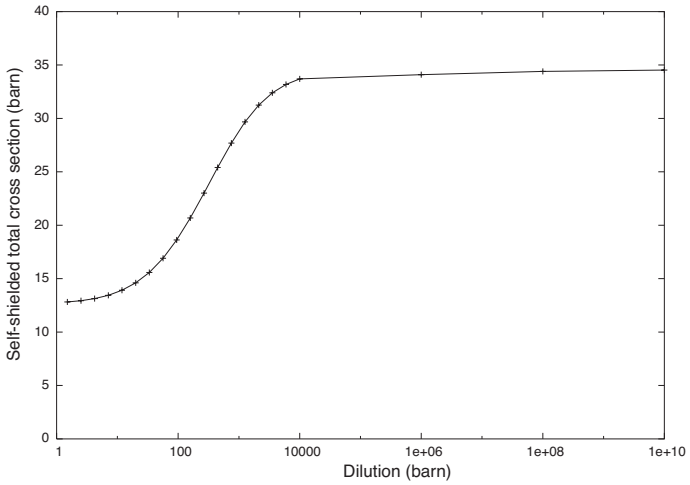
# Calculation of the probability tables



- Computing physical probability tables:
  - Use a root mean square (RMS) fitting to preserve the dilution tabulation in NJOY

$$\overline{\sigma}_\rho(\sigma_e) = \frac{\left\langle \frac{\sigma_\rho}{\sigma+\sigma_e} \right\rangle_g}{\left\langle \frac{1}{\sigma+\sigma_e} \right\rangle_g} = \frac{\sum_{k=1}^{K} \frac{\omega_k \sigma_{\rho,k}}{\sigma_k+\sigma_e}}{\sum_{k=1}^{K} \frac{\omega_k}{\sigma_k+\sigma_e}}$$

  - Described in Sect. 4.2.4 of Applied Reactor Physics
  - The correlation between the diffusion source and the collision term is automatically taken into account
  - No guaranties that the probability table is consistent
  - Used in HELIOS, WIMS9 and DRAGON4/DRAGON5.



# Calculation of the probability tables



## Computing mathematical probability tables:

- The CALENDF approach is the more straightforward approach
- NJOY-generated data is not used.
- The correlation between the diffusion source and the collision term is generally not taken into account ⇒ More than 150 energy groups must be used in the resolved energy domain.
- The probability table is compute so as to preserve negative and positive moments of the microscopic total cross section:

$$\mathcal{M}_\ell = \frac{1}{\Delta u_g}\int_{u_{g-1}}^{u_g} du\,\sigma(u)^\ell = \sum_{k=1}^{K}\omega_k\sigma_k^\ell\,;\quad 1-K\le\ell\le K \tag{12}$$

and

$$\mathcal{M}_{\ell,\rho} = \frac{1}{\Delta u_g}\int_{u_{g-1}}^{u_g} du\,\sigma_\rho(u)\sigma(u)^\ell = \sum_{k=1}^{K}\omega_k\sigma_{\rho,k}\sigma_k^\ell\,;\quad (1-K)/2\le\ell\le K/2 \tag{13}$$

- $\sigma(u)$ and $\sigma_\rho(u)\ \forall\rho$ is recovered from Autolib records, present in Draglibs.
- CALENDF guaranty that the probability table is consistent. The base points are constrained as follows: $\min(\sigma(u))\le\sigma_k\le\max(\sigma(u))$; the values of the probability table are real, the weights are positive, and their sum is equal to one.
- Used in codes APOLLO2, ECCO and DRAGON4/DRAGON5.

# The subgroup-equation approach



The space-dependent Livolant-Jeanpierre transport equation is replaced by a subgroup equation in lethargy:

$$\boldsymbol{\Omega}\cdot\nabla\varphi(\boldsymbol{r},u,\boldsymbol{\Omega})+\Sigma(\boldsymbol{r},u)\,\varphi(\boldsymbol{r},u,\boldsymbol{\Omega})=\frac{1}{4\pi}\left[\Sigma_{\mathrm{s}}^{+}(\boldsymbol{r},u)+\mathscr{R}^{*}\{\varphi(\boldsymbol{r},u)\}\right]$$

$$\Updownarrow$$

$$\boldsymbol{\Omega}\cdot\nabla\phi_k(\boldsymbol{r},\boldsymbol{\Omega})+\Sigma_k(\boldsymbol{r})\,\phi_k(\boldsymbol{r},\boldsymbol{\Omega})=\frac{1}{4\pi}\left[\Sigma_{\mathrm{s}}^{+}(\boldsymbol{r},u)+\sum_{k'=1}^{K}\frac{\mathscr{W}_{k,k'}}{\omega_k}\Sigma_{\mathrm{s},k'}(\boldsymbol{r})\,\phi_{k'}(\boldsymbol{r})\right] \tag{14}$$

where $1\leq k\leq K$ is the subgroup index of the probability table.

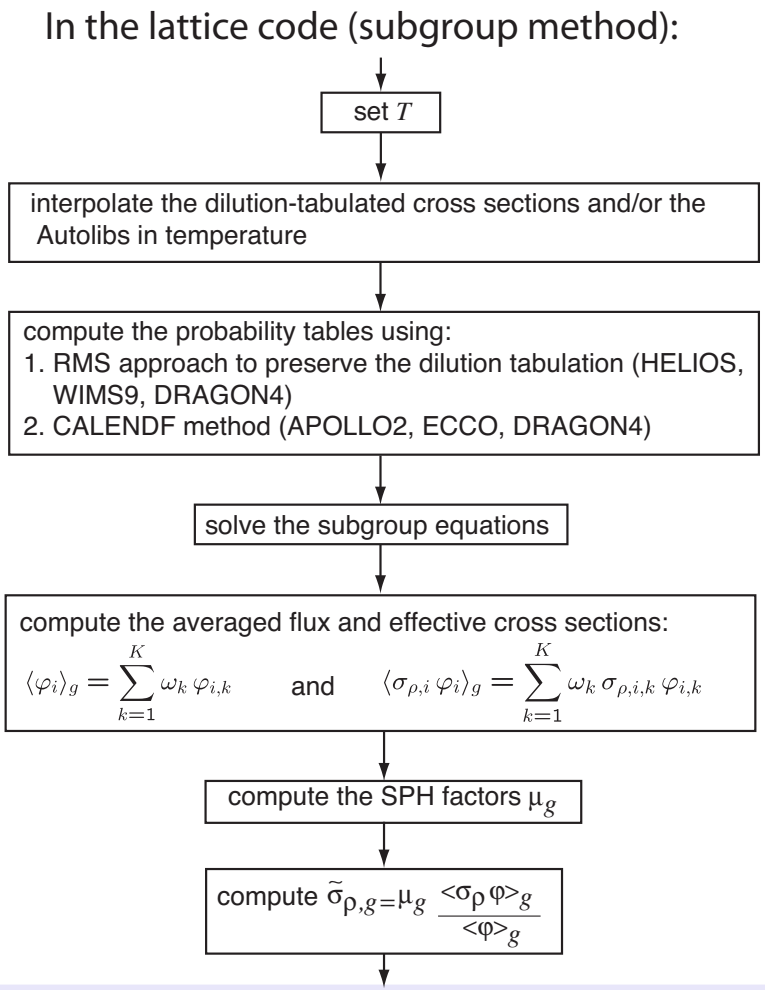
$\mathscr{W}_{k,k'}$ is a correlated weight matrix taking into account the correlation between the diffusion source and the collision term.

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

# The subgroup-equation approach



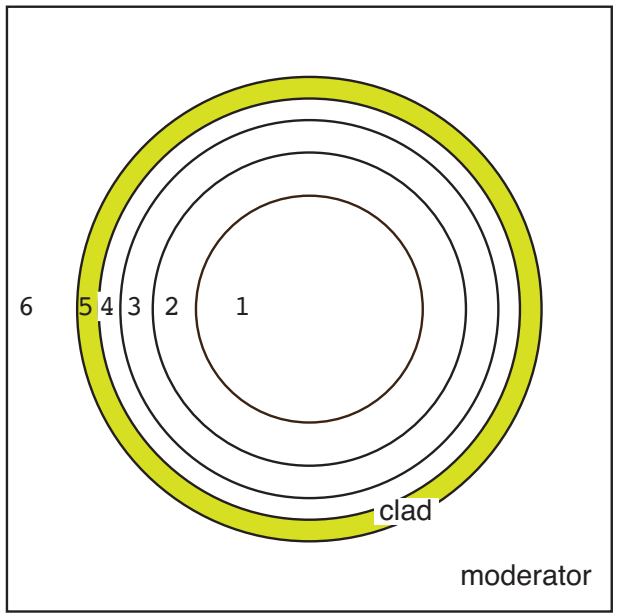
Recent codes such as HELIOS, WIMS8 and DRAGON4 are using the subgroup method (production path). The subgroup method is also available in APOLLO2 as validation path.



# The subgroup-equation approach



- Advanced USS : module with physical probability tables is used
- Distributed self-shielding with four volumes
- Only available in DRAGON4 and DRAGON5




```
LIBRARY := LIB: ::
 EDIT 1
 NMIX 6     (*MAXIMUM OF MATERIAL MIXTURES*)
 SUBG
 MIXS LIB: DRAGON FIL: DLIB_J2
 MIX 1 293.0
    O16      = O16     4.6624E-2
    U235     = U235    7.0803E-4 1 IRSET 0.0 81
    U238     = U238    2.2604E-2 1 IRSET 0.0 81
 MIX 2 COMB 1 1.0
 MIX 3 COMB 1 1.0
 MIX 4 COMB 1 1.0
 MIX 5 293.0
    Zr0      = Zr0     4.3241E-2 2 IRSET 0.0 81
 MIX 6 293.0
    H1       = H1_H2O  6.6988E-2
    O16      = O16     3.3494E-2
;
LIBRARY2 := USS: LIBRARY TRACK :: EDIT 1 PASS 2 ;
```

physical probability tables

use WR if $g \geq 81$ and ST if $g < 81$

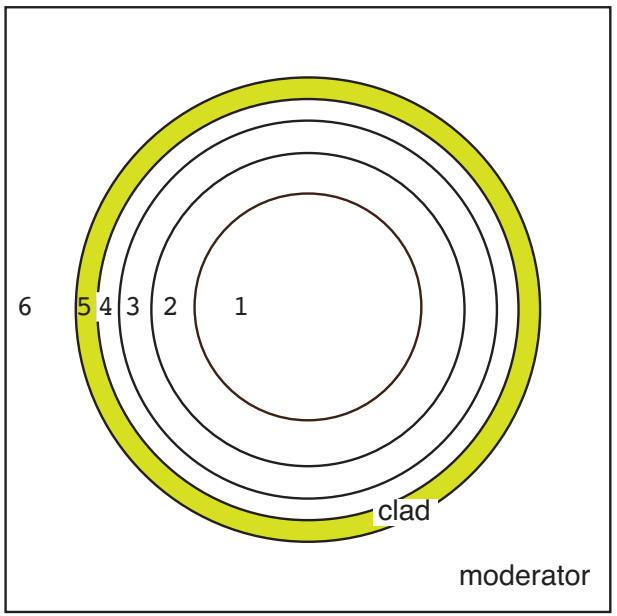
new self-shielded Microlib

2 self-shielding iterations

# The subgroup-equation approch



- Advanced USS : module with mathematical probability tables (or CALENDF tables) is used
- Distributed self-shielding with four volumes
- Only available in DRAGON4 and DRAGON5 with SHEM-361, SHEM-295 or SHEM-315 libraries.




```
LIBRARY := LIB: ::
 EDIT 1
 NMIX 6    (*MAXIMUM OF MATERIAL MIXTURES*)
 PT
*
 MIXS LIB: DRAGON FIL: DLIB_295
 MIX 1 293.0
    O16      = O16     4.6624E-2
    U235     = U235    7.0803E-4 CORR 1 IRSET PT 1
    U238     = U238    2.2604E-2 CORR 1 IRSET PT 1
 MIX 2 COMB 1 1.0
 MIX 3 COMB 1 1.0
 MIX 4 COMB 1 1.0
 MIX 5 293.0
    Zr0      = Zr0     4.3241E-2 2 IRSET PT 1
 MIX 6 293.6
    H1       = H1_H2O  6.6988E-2
    O16      = O16     3.3494E-2
;
LIBRARY2 := USS: LIBRARY TRACK :: EDIT 1 PASS 2 ;
```

CALENDF probability tables

SHEM-295 cross-section library

use CALENDF tables
remove this keyword to suppress correlation

# Datasets



Complete DRAGON5 datasets are provided for the above workshop examples

| Self-shielding | $K_{\text{eff}}$ | DRAGON5 dataset |
|---|---|---|
| `SHI: / LEVEL 0` | 1.327089 | `workshop_level0.x2m` |
| `SHI: / LEVEL 1` | 1.331646 | `workshop_level1.x2m` |
| `USS: / SUBG` | 1.331530 | `workshop_subg.x2m` |
| `USS: / PT` | 1.331575 | `workshop_pt.x2m` |
| `USS: / PT / CORR` | 1.331460 | `workshop_ptcorr.x2m` |

# Library compatibility



| | WLUP libraries | XMAS-172 | SHEM-281 | SHEM-361 | SHEM-295 | SHEM-315 |
|---|---|---|---|---|---|---|
| SHI: | | | | | | |
| USS:/SUBG | | | | | | |
| USS:/PT | Not compatible | | | | | |