A Description of the DRAGON and TRIVAC Version5 Data Structures

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64-bit

SUMMARY

This technical report contains the logical contents of the data structures used by the reactor physics codes DRAGON and TRIVAC Version5. These data structures are basically memory-resident associative tables that may contain inner structures made of associative tables and/or heterogeneous lists. These data structures are implemented using the LCM/XSM Application Programming Interface (API) described in the technical report IGE-232.

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1 Contents of a /macrolib/ directory

A /macrolib/ directory always contains the set of macroscopic multigroup cross sections associated with a set of mixtures. The structure of this directory, is quite different to that associated with an /isotope/ directory (see Section 2.9). First, it is multi-level, namely, it contains sub-directories. Moreover instead of having one directory per mixture which contains the associated multigroup cross section, one will have one directory component per group containing multi-mixture information. Finally its contents will vary depending on the operator which was used to create it. Here for convenience we will define the variable $\mathcal{M}$ to identify the creation operator:

$$\mathcal{M} = \begin{cases} 0 & \text{if the directory is created by the } \texttt{MAC:} \text{ operator} \\ 1 & \text{if the directory is created by the } \texttt{LIB:} \text{ or } \texttt{EVO:} \text{ operator} \\ 2 & \text{if the directory is created by the } \texttt{EDI:} \text{ operator} \\ 3 & \text{if the directory is created by the } \texttt{OUT:} \text{ or } \texttt{NCR:} \text{ operator} \end{cases}$$

In the case where the $\texttt{LIB:}$ or $\texttt{EDI:}$ operator is used to create this directory, it is embedded as a subdirectory in a /microlib/ or an /edition/ directory. For the other cases, it appears on the root level of the MACROLIB data structure.

1.1 State vector content for the /macrolib/ data structure

The dimensioning parameters for the /macrolib/ data structure, which are stored in the state vector $\mathcal{S}^M$, represent:

- The number of energy groups $G = \mathcal{S}_1^M$

- The number of mixtures $N_m = \mathcal{S}_2^M$

- The order for the scattering anisotropy $L = \mathcal{S}_3^M$ ($L = 1$ is an isotropic collision; $L = 2$ is a linearly anisotropic collision, etc.)

- The maximum number of fissile isotopes in a mixture $N_f = \mathcal{S}_4^M$

- The number of additional ϕ–weighted editing cross sections $N_e = \mathcal{S}_5^M$

- The transport correction option $I_{tr} = \mathcal{S}_6^M$

$$I_{tr} = \begin{cases} 0 & \text{do not use a transport correction} \\ 1 & \text{use an APOLLO-type transport correction (micro-reversibility at all energies)} \\ 2 & \text{recover a transport correction from the cross-section library} \\ 4 & \text{use a leakage correction based on } \texttt{NTOT1} \text{ data.} \end{cases}$$

- The number of precursor groups for delayed neutron $N_d = \mathcal{S}_7^M$

- The number of physical albedo $N_A = \mathcal{S}_8^M$

- The type of leakage $I_l = \mathcal{S}_9^M$

$$I_l = \begin{cases} 0 & \text{no diffusion/leakage coefficient available} \\ 1 & \text{isotropic diffusion/leakage coefficient available} \\ 2 & \text{anisotropic diffusion/leakage coefficient available.} \end{cases}$$

- The maximum Legendre order of the weighting functions $I_w = \mathcal{S}_{10}^M$

$$I_w = \begin{cases} 0 & \text{use the flux as weighting function for all cross sections} \\ 1 & \text{use the fundamental current } \mathcal{J} \text{ as weighting function for scattering cross sections with} \\ & \text{order} \geq 1 \text{ and compute both } \phi\text{– and } \mathcal{J}\text{–weighted total cross sections.} \end{cases}$$

- The number of delta cross section sets $I_{\text{step}} = \mathcal{S}_{11}^M$ used for generalized perturbation theory (GPT) or kinetics calculations:

$$I_{\text{step}} = \begin{cases} 0 & \text{no delta cross section sets} \\ > 0 & \text{number of delta cross section sets.} \end{cases}$$

- Discontinuity factor flag $I_{\text{df}} = \mathcal{S}_{12}^M$:

$$I_{\text{df}} = \begin{cases} 0 & \text{no discontinuity factor information} \\ 1 & \text{multigroup boundary current information is available} \\ 2 & \text{discontinuity factor information (see Section 1.4) is available} \\ 3 & \text{matrix } (G \times G) \text{ discontinuity factor information (see Section 1.4) is available.} \end{cases}$$

- Adjoint macrolib flag $I_{\text{adj}} = \mathcal{S}_{13}^M$:

$$I_{\text{adj}} = \begin{cases} 0 & \text{direct macrolib} \\ 1 & \text{adjoint macrolib.} \end{cases}$$

- SPH-information $I_{\text{sph}} = \mathcal{S}_{14}^M$:

$$I_{\text{sph}} = \begin{cases} 0 & \text{no SPH information available} \\ 1 & \text{SPH information is available.} \end{cases}$$

- Type of weighting in `EDI:` module $I_{\text{pro}} = \mathcal{S}_{15}^M$:

$$I_{\text{pro}} = \begin{cases} 0 & \text{use a flux weighting} \\ 1 & \text{use an adjoint–direct (a.k.a., product) flux weighting. Only available if } \mathcal{M} \geq 2 \end{cases}$$

- Group form factor index $I_{\text{gff}} = \mathcal{S}_{16}^M$:

$$I_{\text{gff}} = \begin{cases} 0 & \text{no group form factor information} \\ > 0 & \text{number of form factors per mixture and per energy group (see Section 1.5).} \end{cases}$$

- Number of companion particles in coupled sets $I_{\text{part}} = \mathcal{S}_{17}^M$:

$$I_{\text{part}} = \begin{cases} 0 & \text{the macrolib doesn't include coupled sets} \\ > 0 & \text{number of companion particles.} \end{cases}$$

1.2 The main /macrolib/ directory

The following records and sub-directories will be found on the first level of a /macrolib/ directory:

Table 1: Main records and sub-directories in /macrolib/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			Signature of the /macrolib/ data structure (SIGNA =L_MACROLIB␣␣).

Main records and sub-directories in /macrolib/   continued from last page

Name	Type	Condition	Units	Comment
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^M$, as defined in Section 1.1.
ADDXSNAME-P0	C(N_e)∗8	$N_e \geq 1$		Names of the additional ϕ–weighted editing cross sections (ADDXS_k). These names should not appear in Tables 2 and 5.
FISSIONINDEX	I(N_m, N_f)	$N_f \geq 1, \mathcal{M} = 1$		For each mixture i contains the index of each fissile isotope j. The index is pointing to a component of record ISOTOPESUSED or ISOTOPERNAME of /microlib/.
ENERGY␣␣␣␣␣␣	R($G+1$)	$\mathcal{M} \geq 1$	eV	Energy group limits E_g
DELTAU␣␣␣␣␣␣	R(G)	$\mathcal{M} \geq 1$		Lethargy width of each group U_g
ALBEDO␣␣␣␣␣␣	R(N_A, G)	$N_A > 0$		Multigroup and surface ordered physical albedos. The dimension is R(N_A, G, G) in case where matrix albedos are used.
VOLUME␣␣␣␣␣␣	R(N_m)	$\mathcal{M} \geq 2$	cm^3	Volume of region containing this mixture V_m
FLUXDISAFACT	R(G)	$\mathcal{M} = 2$		Ratio of the flux in the fuel to the flux in the cell F_g after homogenization
LAMBDA-D␣␣␣␣	R(N_d, N_f)	$N_d \geq 1$	s^{-1}	Radioactive decay constants of each delayed neutron precursor group, for each fissile isotope.
BETA-D␣␣␣␣␣␣	R(N_d, N_f)	$N_d \geq 1$		Delayed-neutron fraction for each delayed neutron precursor group, for each fissile isotope.
K-EFFECTIVE␣	R(1)	$N_f \geq 1$		Effective multiplication constant k_{eff}
K-INFINITY␣␣	R(1)	$N_f \geq 1$		Infinite multiplication constant k_∞
DIFFB1HOM␣␣␣	R(G)	$\mathcal{M} = 2, I_l \geq 1$	cm	Homogeneous leakage/diffusion coefficient D^g
B2␣␣B1HOM␣␣␣	R(1)	$I_l \geq 1$	cm^{-2}	Homogeneous Buckling B_{hom}
B2␣␣HETE␣␣␣␣	R(3)	$I_l = 2$	cm^{-2}	Directional Buckling B_j
TIMESTAMP␣␣␣	R(3)	$\mathcal{M} = 1$		A vector T_j containing three elements. The first element $T_1 = t$ is the time in days, the second element $T_2 = B$ is the burnup in MW day T^{-1} and the third element $T_3 = w$ is the irradiation in Kb^{-1}
GROUP␣␣␣␣␣␣␣	Dir(G)			List of energy-group sub-directories. Each component of the list is a directory containing the reference macroscopic cross-section information associated with a specific secondary group.
PARTICLE␣␣␣␣	C∗1	$I_{\text{part}} \geq 1$		Character name of the particle associated to the macrolib. Usual names for particles are N (neutrons), G (photons), B (electrons), C (positrons) and P (protons).
PARTICLE-NAM	C($I_{\text{part}} + 1$)∗1	$I_{\text{part}} \geq 1$		Character name associated to each particle.
PARTICLE-NGR	I($I_{\text{part}} + 1$)	$I_{\text{part}} \geq 1$		Number of energy groups associated to each particle.
PARTICLE-MC2	R($I_{\text{part}} + 1$)	$I_{\text{part}} \geq 1$	eV	Rest energy associated to each particle.

Main records and sub-directories in /macrolib/   continued from last page

Name	Type	Condition	Units	Comment
{/penergy/}	$R(G_i + 1)$	$I_{\text{part}} \geq 1$	eV	Set of arrays containing energy groups limits for a companion particle. The character name of each sub-directory is the concatenation of the character*1 name of the particle with "ENERGY". For example, GENERGY contains the energy mesh of secondary photons ($G_i + 1$ values).
{/grpdir/}	Dir(G)	$I_{\text{part}} \geq 1$		List of energy-group sub-directories. Each component of the list is a directory containing scattering transition cross-section information associated with a specific secondary group. The directory {/grpdir/} name is the concatenation of GROUP- with the character*6 name of the companion particle responsible for scattering transitions.
STEP␣␣␣␣␣␣␣␣	Dir(I_{step})	$I_{\text{step}} \geq 1$		List of GPT or kinetics perturbation sub-directories. Each component of this list contains a single list of energy-group sub-directories following the GROUP specification. This GROUP list contains variations or derivatives of the reference cross-section set.
ADF␣␣␣␣␣␣␣␣␣	Dir	$I_{\text{df}} \geq 1$		ADF–related information as presented in Section 1.4.
GFF␣␣␣␣␣␣␣␣␣	Dir	$I_{\text{gff}} \geq 1$		Group form factor information as presented in Section 1.5.
SPH␣␣␣␣␣␣␣␣␣	Dir	$I_{\text{sph}} = 1$		SPH–related input data as presented in Section 1.6.

1.3   The group sub-directory GROUP in /macrolib/

Each component of the list GROUP is a directory containing cross-section information corresponding to a single energy group. Inside each groupwise directory, the following records associated with vectorial cross sections will be found:

Table 2: Vectorial cross section records and directories in GROUP

Name	Type	Condition	Units	Comment
NTOTO␣␣␣␣␣␣␣	$R(N_m)$		cm^{-1}	The ϕ–weighted total cross section $\Sigma_{0,m}^g$
NTOT1␣␣␣␣␣␣␣	$R(N_m)$	$\mathcal{M} = 2;\ I_w \geq 1$	cm^{-1}	The $\mathcal{J}$–weighted total cross section $\Sigma_{1,m}^g$
TRANC␣␣␣␣␣␣␣	$R(N_m)$	$I_{tr} = 2$	cm^{-1}	The transport correction $\Sigma_{tc,m}^g$
FIXE␣␣␣␣␣␣␣␣	$R(N_m)$		cm^{-3}s^{-1}	Fixed sources S_m^g.
NUSIGF␣␣␣␣␣␣	$R(N_m, N_f)$	$N_f \geq 1$	cm^{-1}	The product of $\Sigma_{f,m}^g$, the fission cross section with $\nu_m^{\text{ss},g}$, the steady-state number of neutron produced per fission, $\nu\Sigma_{f,m}^g$
CHI␣␣␣␣␣␣␣␣␣	$R(N_m, N_f)$	$N_f \geq 1$		The steady-state energy spectrum of the neutron emitted by fission $\chi_m^{\text{ss},g}$

Vectorial cross section records and directories in `GROUP`

Name	Type	Condition	Units	Comment
{*nusid*}	$R(N_m, N_f)$	$N_d \geq 1$	cm^{-1}	The product of $\Sigma_{f,m}^g$, the fission cross section with $\nu_{m,\ell}^{D,g}$, the averaged number of fission–emitted delayed neutron produced in the precursor group ℓ, $\nu\Sigma_{f,m,\ell}^{D,g}$
{*chid*}	$R(N_m, N_f)$	$N_d \geq 1$		The energy spectrum of the fission–emitted delayed neutron in the precursor group ℓ, $\chi_{m,\ell}^{D,g}$
FLUX-INTG␣␣␣	$R(N_m)$	$\mathcal{M} \geq 2$	cm s^{-1}	The volume-integrated flux Φ_m^g
FLUX-INTG-P1	$R(N_m)$	$\mathcal{M} \geq 2$; $I_w \geq 1$	cm s^{-1}	The volume-integrated fundamental current $\mathcal{J}_m^g$
NWAT0␣␣␣␣␣␣␣	$R(N_m)$	$I_{pro} = 1$	1	The multigroup neutron adjoint flux spectrum ϕ_m^{*g}
NWAT1␣␣␣␣␣␣␣	$R(N_m)$	$I_w \geq 1$; $I_{pro} = 1$	1	The multigroup fundamental adjoint current spectrum $\mathcal{J}_m^{*g}$
OVERV␣␣␣␣␣␣␣	$R(N_m)$		cm^{-1}s	The average of the inverse neutron velocity $< 1/v >_m^g$
DIFF␣␣␣␣␣␣␣␣	$R(N_m)$	$\mathcal{M} = 2$; $I_l = 1$	cm	The isotropic diffusion coefficient D_m^g
DIFFX␣␣␣␣␣␣␣	$R(N_m)$	$\mathcal{M} = 2$; $I_l = 2$	cm	The x-directed diffusion coefficient $D_{x,m}^g$
DIFFY␣␣␣␣␣␣␣	$R(N_m)$	$\mathcal{M} = 2$; $I_l = 2$	cm	The y-directed diffusion coefficient $D_{y,m}^g$
DIFFZ␣␣␣␣␣␣␣	$R(N_m)$	$\mathcal{M} = 2$; $I_l = 2$	cm	The z-directed diffusion coefficient $D_{z,m}^g$
NSPH␣␣␣␣␣␣␣␣	$R(N_m)$	$\mathcal{M} = 2$	1	SPH equivalence factors μ_m^g. By default, these factors are set equal to 1.0. Otherwise, all the cross sections, diffusion coefficients and integrated fluxes stored on the MACROLIB are SPH–corrected.
H-FACTOR␣␣␣␣	$R(N_m)$	$\mathcal{M} = 2$	J cm^{-1}	Energy production coefficients H_m^g (product of each macroscopic cross section times the energy emitted by this reaction).
ESTOPW␣␣␣␣␣␣	$R(N_m, 2)$	*	MeV cm^{-1}	Initial and final stopping power. Information provided if `PARTICLE`=B, C or P.
EMOMTR␣␣␣␣␣␣	$R(N_m)$	*	cm^{-1}	Restricted momentum transfer cross section. Information provided if `PARTICLE`=B, C or P.
C-FACTOR␣␣␣␣	$R(N_m)$	*	electron cm^{-1}	Charge deposition cross section. Information provided if `PARTICLE`=B, C or P.
{*/xsname/*}	$R(N_m)$	$N_e \geq 1$	cm^{-1}	Set of cross section records specified by ADDXS$_k$

The set of delayed neutron records {*nusid*} and {*chid*} will be composed, using the following FORTRAN instructions, as NUSID and CHID, respectively

WRITE(NUSID,$'$(A6,I2.2)$'$) $'$NUSIGF$'$, *ell*

WRITE(CHID,$'$(A3,I2.2)$'$) $'$CHI$'$, *ell*

for $1 \leq ell \leq N_d$. For example, in the case where two group cross sections are considered ($N_d = 2$), the following records would be generated:

Table 3: Example of delayed–neutron records in `GROUP`

Name	Type	Condition	Units	Comment
NUSIGF01␣␣␣␣	$R(N_m, N_f)$	$N_d \geq 1$	cm^{-1}	The product of $\Sigma^g_{f,m}$, the fission cross section with $\nu^{D,g}_{m,1}$, the averaged number of fission–emitted delayed neutron produced in the precursor group $\ell = 1$, $\nu\Sigma^{D,g}_{f,m,1}$
CHI01␣␣␣␣␣␣	$R(N_m, N_f)$	$N_d \geq 1$		The energy spectrum of the fission–emitted delayed neutron in the precursor group $\ell = 1$, $\chi^{D,g}_{m,1}$
NUSIGF02␣␣␣␣	$R(N_m, N_f)$	$N_d \geq 2$	cm^{-1}	The product of $\Sigma^g_{f,m}$, the fission cross section with $\nu^{D,g}_{m,2}$, the averaged number of fission–emitted delayed neutron produced in the precursor group $\ell = 2$, $\nu\Sigma^{D,g}_{f,m,2}$
CHI02␣␣␣␣␣␣	$R(N_m, N_f)$	$N_d \geq 2$		The energy spectrum of the fission–emitted delayed neutron in the precursor group $\ell = 2$, $\chi^{D,g}_{m,2}$

In the case where $N_e = 3$ and

$$\text{ADDXS}_k = \begin{cases} \text{NG} & \text{for} \quad k = 1 \\ \text{N2N} & \text{for} \quad k = 2 \\ \text{NFTOT} & \text{for} \quad k = 3 \end{cases}$$

the following reactions will be available in the data structure described in Table 2:

Table 4: Additional cross section records

Name	Type	Condition	Units	Comment
NG␣␣␣␣␣␣␣␣␣	$R(N_m)$		cm^{-1}	The neutron capture cross section $\Sigma^g_{c,m}$
N2N␣␣␣␣␣␣␣␣	$R(N_m)$		cm^{-1}	The cross section $\Sigma^g_{(n,2n),m}$ for the reaction $^A_Z X + n \rightarrow^{A-1}_Z X + 2n$
NFTOT␣␣␣␣␣␣	$R(N_m)$		cm^{-1}	The neutron fission cross section $\Sigma^g_{f,m}$

The information associated with the multigroup scattering matrix, which gives the probability for a neutron in group h to appear in group g after a collision with an isotope in mixture m is represented by the form:

$$\Sigma^{h \to g}_{s,m}(\vec{\Omega} \to \vec{\Omega}') = \sum_{l=0}^{L} \frac{2l+1}{4\pi} P_l(\vec{\Omega} \cdot \vec{\Omega}') \Sigma^{h \to g}_{l,m} = \sum_{l=0}^{L} \sum_{m=-l}^{l} Y^m_l(\vec{\Omega}) Y^m_l(\vec{\Omega}') \Sigma^{h \to g}_{l,m}$$

using a series expansion to order L in spherical harmonic. Assuming that the spherical harmonic are

orthonormalized, we can define $\Sigma_{l,m}^{h \to g}$ in terms of $\Sigma_{s,m}^{h \to g}(\vec{\Omega} \to \vec{\Omega}')$ using the following integral:

$$\Sigma_{l,m}^{h \to g} = \int_{4\pi} d^2\Omega \ \Sigma_{s,m}^{h \to g}(\vec{\Omega} \to \vec{\Omega}')P_l(\vec{\Omega} \cdot \vec{\Omega}')$$

Note that this definition of $\Sigma_{l,m}^{h \to g}$ is not unique and some authors include the factor $2l+1$ directly in the different angular moments of the scattering cross section.

Here instead of storing the $G \times M$ matrix $\Sigma_{l,m}^{h \to g}$ associated with each final energy group g, a vector which contains a compress form of the scattering matrix will be considered. We will first define three integer vectors $n_{l,m}^g$, $h_{l,m}^g$ and $p_{l,m}^g$ for order l in the scattering cross section, final energy group g and mixture m. They will contain respectively the number of initial energy groups h for which the scattering cross section to group g does not vanish, the maximum energy group index for which scattering to the final group g does not vanishes and the position in the compressed scattering vector where the data associated with mixture m for each energy group g can be found. Here $p_{l,m}^g$ is directly related to $n_{l,m}^g$ by

$$p_{l,m}^g = 1 + \sum_{k=1}^{m-1} n_{l,k}^g$$
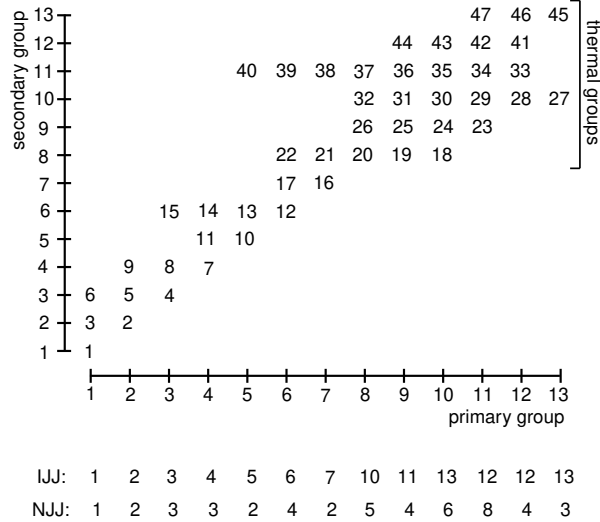
Figure 1: Numbering of scattering elements in 'SCAT' matrices.

Now consider the following 4 groups isotropic scattering cross section matrix associated with mixture 1 and 2 ($N_m = 2$) respectively:

$\sigma_{0,m}^{h \to g}$	Mixture $m = 1$				Mixture $m = 2$			
	$g = 1$	$g = 2$	$g = 3$	$g = 4$	$g = 1$	$g = 2$	$g = 3$	$g = 4$
$h = 1$	a_1	a_2	0	0	b_1	b_2	0	0
$h = 2$	0	a_3	a_4	a_5	b_3	b_4	b_5	0
$h = 3$	0	a_6	a_7	0	0	b_6	b_7	0
$h = 4$	0	a_8	0	a_9	0	0	b_8	b_9
$h_{0,m}^g$	1	4	3	4	2	3	4	4
$n_{0,m}^g$	1	4	2	3	2	3	3	1
$p_{0,m}^g$	1	1	1	1	2	5	3	4

The compressed scattering matrix will then take the following form for each final group g:

$$\Sigma_{0,k,c}^1 = (a_1, b_3, b_1)$$
$$\Sigma_{0,k,c}^2 = (a_8, a_6, a_3, a_2, b_6, b_4, b_2)$$
$$\Sigma_{0,k,c}^3 = (a_7, a_4, b_8, b_7, b_5)$$
$$\Sigma_{0,k,c}^4 = (a_9, 0, a_5, b_9)$$

Finally, we will also save the total scattering cross section vector of order l which is defined as

$$\Sigma_{l,m,s}^g = \sum_{h=1}^{G} \Sigma_{l,m}^{g \to h}$$

and the diagonal element of the scattering matrix:

$$\Sigma_{l,m,w}^g = \Sigma_{l,m}^{g \to g}$$

In the case where only the order $l = 0$ and $l = 1$ moment of scattering cross section are non vanishing (isotropic and linearly anisotropic scattering) the following records can be found on the group directory.

Table 5: Scattering cross section records in `GROUP`

Name	Type	Condition	Units	Comment
`SIGS00␣␣␣␣␣␣`	$R(N_m)$		cm^{-1}	The isotropic component ($l = 0$) of the total scattering cross section $\Sigma_{0,m,s}^g$
`SIGW00␣␣␣␣␣␣`	$R(N_m)$		cm^{-1}	The isotropic component ($l = 0$) of the within group scattering cross section $\Sigma_{0,m,w}^g$
`IJJS00␣␣␣␣␣␣`	$I(N_m)$			Highest energy group number for which the isotropic component of the scattering cross section to group g does not vanish, $h_{0,m}^g$
`NJJS00␣␣␣␣␣␣`	$I(N_m)$			Number of energy groups for which the isotropic component of the scattering cross section to group g does not vanish, $n_{0,m}^g$
`IPOS00␣␣␣␣␣␣`	$I(N_m)$			Location in the isotropic compressed scattering matrix where information associated with mixture m begins $p_{0,m}^g$
`SCAT00␣␣␣␣␣␣`	$R(\sum_{m=1}^{N_m} n_{0,m}^g)$		cm^{-1}	Compressed isotropic component of the scattering matrix $\Sigma_{0,k,c}^g$
`SIGS01␣␣␣␣␣␣`	$R(N_m)$	$L \geq 1$	cm^{-1}	The linearly anisotropic component of the total scattering cross section $\Sigma_{1,m,s}^g$
`SIGW01␣␣␣␣␣␣`	$R(N_m)$	$L \geq 1$	cm^{-1}	The linearly anisotropic component of the within group scattering cross section $\Sigma_{1,m,w}^g$
`IJJS01␣␣␣␣␣␣`	$I(N_m)$	$L \geq 1$		Highest energy group number for which the linearly anisotropic component of the scattering cross section to group g does not vanish, $h_{1,m}^g$
`NJJS01␣␣␣␣␣␣`	$I(N_m)$	$L \geq 1$		Number of energy groups for which the linearly anisotropic component of the scattering cross section to group g does not vanish, $n_{1,m}^g$

Scattering cross section records in `GROUP` continued from last page

Name	Type	Condition	Units	Comment
`IPOS01`␣␣␣␣␣␣	$I(N_m)$	$L \geq 1$		Location in the linearly anisotropic compressed scattering matrix where information associated with mixture m begins $p_{1,m}^g$
`SCAT01`␣␣␣␣␣␣	$R(\sum_{m=1}^{N_m} n_{1,m}^g)$	$L \geq 1$	cm^{-1}	Compressed linearly anisotropic component of the scattering matrix $\Sigma_{1,k,c}^g$

1.4 The /`ADF`/ sub-directory in /macrolib/

Sub-directory containing ADF-type boundary flux edition information. This information can be used to compute discontinuity factors or to perform Selengut-type normalization with the *superhomogénéisation* (SPH) method.

Table 6: Records in the /`ADF`/ sub-directory

Name	Type	Condition	Units	Comment
`NTYPE`␣␣␣␣␣␣	$I(1)$	$I_{\text{df}} \geq 2$		Number of ADF-type boundary flux edits.
`HADF`␣␣␣␣␣␣␣	$C(\text{NTYPE})*8$	$I_{\text{df}} \geq 2$		Name of each ADF-type boundary flux edit. Any name can be used, but some names are standard. Standard names are: $=$ `FD_C`: corner flux edition; $=$ `FD_B`: surface (assembly gap) flux edition; $=$ `FD_H`: row flux edition (these are the first row of surrounding cells in the assembly).
`ALBS00`␣␣␣␣␣␣	$R(G,2)$	$I_{\text{df}} = 1$		Multigroup boundary currents J_{out}^g and J_{in}^g. These values correspond to surfaces where a `VOID` or `ALBE` boundary condition is set in DRAGON.
{/*type*/}	$R(N_m,G)$	$I_{\text{df}} = 2$		Averaged fluxes in boundary regions or discontinuity factors in a material mixture. Name *type* is a component of `HADF` array.
{/*type*/}	$R(N_m,G,G)$	$I_{\text{df}} = 3$		Matrix discontinuity factors in a material mixture. Name *type* is a component of `HADF` array.

1.5 The /`GFF`/ sub-directory in /macrolib/

Sub-directory containing group form factor information. This information can be used to perform *fine power reconstruction* over a fuel assembly.

Table 7: Records in the `/GFF/` sub-directory

Name	Type	Condition	Units	Comment
`GFF-GEOM␣␣␣␣`	Dir			Macro–geometry directory. This geometry corresponds to an unfolded fuel assembly and is compatible for a discretization with TRIVAC. This directory follows the specification presented in Section 3.2.
`VOLUME␣␣␣␣␣␣`	$R(N_m, I_{\rm gff})$		cm^3	Volumes of homogenized cells V_m
`NWTO␣␣␣␣␣␣␣␣`	$R(N_m, I_{\rm gff}, G)$		s^{-1}cm^{-2}	The multigroup neutron flux spectrum ϕ_w^g
`H-FACTOR␣␣␣␣`	$R(N_m, I_{\rm gff}, G)$		J cm^{-1}	Energy production coefficients H_m^g (product of each macroscopic cross section times the energy emitted by this reaction).
`NFTOT␣␣␣␣␣␣␣`	$R(N_m, I_{\rm gff}, G)$		cm^{-1}	The neutron fission cross section $\Sigma_{{\rm f},m}^g$
`FINF_NUMBER␣`	$I(N_{\rm ifx})$			Array containing the $N_{\rm ifx}$ ifx indices used by the user every time the multicompo were "enriched" with different options.
`{/FINF/}`	$R(N_m, I_{\rm gff}, G)$		s^{-1}cm^{-2}	The diffusion multigroup neutron flux spectrum in an infinite domain $\psi_{m,p}^{d,\infty}$. See `NAP:` module description in IGE344 user guide for details.

The set of diffusion multigroup neutron flux spectrum records {/FINF/} will be composed, using the following FORTRAN instructions as HVECT,

WRITE(HVECT,$'$(5HFINF␣,I3.3)$'$) $'$`ifx`$'$

where `ifx` is a value chosen by the user (default value is 0). A different value can be chosen every time the multicompo are "enriched" with different options (homogeneous/heterogeneous, tracking options, etc.).

1.6 The `/SPH/` sub-directory in `/macrolib/`

The first level of the macrolib directory may contains a *superhomogénéisation* (SPH) sub-directory `/SPH/` containing input data:

Table 8: Records in the `/SPH/` sub-directory

Name	Type	Condition	Units	Comment
`STATE-VECTOR`	$I(40)$			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^{\rm sph}$.
`SPH$TRK␣␣␣␣␣`	C*12	$\mathcal{S}_1^{\rm sph} \geq 2$		Name of the flux solution door.
`SPH-EPSILON␣`	$R(1)$	$\mathcal{S}_1^{\rm sph} \geq 2$	1	Convergence criterion for stopping the SPH iterations.

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}^{\mathrm{sph}}$, represent values related to the last editing step:

- Type of SPH equivalence factors: $I_{\mathrm{type}} = \mathcal{S}_1^{\mathrm{sph}}$

$$I_{\mathrm{type}} = \begin{cases} 0 & \text{no SPH correction;} \\ 1 & \text{the SPH factors are read from LCM;} \\ 2 & \text{homogeneous macro-calculation (non-iterative procedure or Hébert-Benoist} \\ & \text{SPH-5 procedure);} \\ 3 & \text{any type of } P_{ij} \text{ macro-calculation;} \\ 4 & \text{any type of diffusion, } S_n, P_n \text{ or } SP_n \text{ macro-calculation.} \end{cases}$$

- Type of SPH equivalence normalization $I_{\mathrm{norm}} = \mathcal{S}_2^{\mathrm{sph}}$

$$I_{\mathrm{norm}} = \begin{cases} < 0 & \text{asymptotic normalization with respect to homoheneous mixture} - I_{\mathrm{norm}}; \\ 1 & \text{average flux normalization;} \\ 2 & \text{Selengut normalization using } \texttt{ALBS00} \text{ information;} \\ 3 & \text{Selengut normalization using } \texttt{FD\_B} \text{ boundary fluxes;} \\ 4 & \text{Generalized Selengut normalization (EDF-type);} \\ 5 & \text{Selengut normalization with surface leakage.} \end{cases}$$

- The maximum number of SPH iterations $\mathcal{S}_3^{\mathrm{sph}}$

- The acceptable number of SPH iterations with an increase in convergence error before aborting $\mathcal{S}_4^{\mathrm{sph}}$

- Flag for forcing the production of a macrolib or microlib at LHS $I_{\mathrm{lhs}} = \mathcal{S}_5^{\mathrm{sph}}$

$$I_{\mathrm{lhs}} = \begin{cases} 0 & \text{produce an object of the type of the RHS;} \\ 1 & \text{produce an edition object;} \\ 2 & \text{produce a microlib;} \\ 3 & \text{produce a macrolib.} \end{cases}$$

- Type of SPH factors $I_{\mathrm{imc}} = \mathcal{S}_6^{\mathrm{sph}}$

$$I_{\mathrm{imc}} = \begin{cases} 1 & \text{factors compatible with diffusion theory, } P_n \text{ and } SP_n \text{ equations} \\ 2 & \text{factors compatible with other types of transport-theory macro-calculations} \\ 3 & \text{factors compatible with } P_{ij} \text{ macro-calculations and Bell acceleration.} \end{cases}$$

- The first group index where the equivalence process is applied $\mathcal{S}_7^{\mathrm{sph}}$

- The maximum group index where the equivalence process is applied $\mathcal{S}_8^{\mathrm{sph}}$

1.7 Delayed neutron information

We will present space-time kinetics equations in the context of the diffusion approximation (i.e. using the Fick law) and equations used in a lattice code to produce condensed and homogenized information. These equations will be useful to understand the information written in the MACROLIB specification. Similar expressions can be obtained in transport theory. Note that delayed neutron information β_ℓ and Λ can also be computed at the scale of the complete reactor provided that bilinear direct–adjoint condensation and homogenization relations are used.

The continuous-energy space-time diffusion equation is written:

$$\frac{\partial}{\partial t}\left[\frac{1}{v(E)}\,\phi(\vec{r},E,t)\right] \;=\; \sum_j \chi_j^{\mathrm{pr}}(E)\int_0^\infty dE'\;\nu_j^{\mathrm{pr}}(\vec{r},E',t)\Sigma_{\mathrm{f},j}(\vec{r},E',t)\phi(\vec{r},E',t)$$

$$+\;\sum_j\sum_\ell \chi_{\ell,j}^{\mathrm{D}}(E)\lambda_\ell c_{\ell,j}(\vec{r},t)+\nabla\cdot D(\vec{r},E,t)\nabla\phi(\vec{r},E,t)$$

$$-\;\Sigma(\vec{r},E,t)\phi(\vec{r},E,t)+\int_0^\infty dE'\;\Sigma_{\mathrm{s}0}(\vec{r},E\leftarrow E',t)\phi(\vec{r},E',t) \tag{1.1}$$

together with the set of N_d precursor equations:

$$\frac{\partial c_{\ell,j}(\vec{r},t)}{\partial t}=\int_0^\infty dE\;\nu_{\ell,j}^{\mathrm{D}}(\vec{r},E,t)\Sigma_{\mathrm{f},j}(\vec{r},E,t)\phi(\vec{r},E,t)-\lambda_\ell c_{\ell,j}(\vec{r},t)\;\;;\quad \ell=1,N_d \tag{1.2}$$

where

$\phi(\vec{r},E,t)=$ neutron flux

$\chi_j^{\mathrm{pr}}(E)=$ prompt neutron spectrum for a fission of isotope j

$\nu_j^{\mathrm{pr}}(\vec{r},E,t)=$ number of prompt neutrons for a fission of isotope j

$\Sigma_{\mathrm{f},j}(\vec{r},E,t)=$ macroscopic fission cross section for isotope j

$\chi_{\ell,j}^{\mathrm{D}}(E)=$ neutron spectra for delayed neutrons emitted by precursor group ℓ due to a fission of isotope j

$\lambda_\ell=$ radioactive decay constant for precursor group ℓ. This constant is assumed to be independent of the fissionable isotope j.

$c_{\ell,j}(\vec{r},t)=$ concentration of the ℓ–th precursor for a fission of isotope j

$D(\vec{r},E,t)=$ diffusion coefficient

$\Sigma(\vec{r},E,t)=$ macroscopic total cross section

$\Sigma_{\mathrm{s}0}(\vec{r},E\leftarrow E',t)=$ macroscopic scattering cross section

$\nu_{\ell,j}^{\mathrm{D}}(\vec{r},E,t)=$ number of delayed neutrons in precursor group ℓ for a fission of isotope j.

The neutron spectrum are normalized so that

$$\int_0^\infty dE\;\chi_j^{\mathrm{ss}}(E)=1 \tag{1.3}$$

and

$$\int_0^\infty dE\;\chi_\ell^{\mathrm{D}}(E)=1\;\;;\;\;\ell=1,N_d\;\;. \tag{1.4}$$

After condensation over energy, Eqs. (1.1) and (1.2) are written

$$<1/v>^g\;\frac{\partial}{\partial t}\phi^g(\vec{r},t) \;=\; \sum_j\chi_j^{\mathrm{pr},g}\left[1-\sum_\ell\beta_{\ell,j}\right]\sum_h\nu\Sigma_{\mathrm{f},j}^h(\vec{r},t)\phi^h(\vec{r},t)$$

$$+\;\sum_j\sum_\ell\chi_{\ell,j}^{\mathrm{D},g}\lambda_\ell c_{\ell,j}(\vec{r},t)+\nabla\cdot D^g(\vec{r},t)\nabla\phi^g(\vec{r},t)$$

$$-\;\Sigma^g(\vec{r},t)\phi^g(\vec{r},t)+\sum_h\Sigma_{\mathrm{s}0}^{g\leftarrow h}(\vec{r},t)\phi^h(\vec{r},t) \tag{1.5}$$

together with the set of N_d precursor equations:

$$\frac{\partial c_{\ell,j}(\vec{r},t)}{\partial t} = \beta_{\ell,j} \sum_h \nu\Sigma_{\mathrm{f},j}^h(\vec{r},t)\phi^h(\vec{r},t) - \lambda_\ell c_{\ell,j}(\vec{r},t) \ ; \quad \ell = 1, N_d \tag{1.6}$$

where

$\nu\Sigma_{\mathrm{f},j}^h(\vec{r},t)=$ product of the number $\nu_j^{\mathrm{ss}}(\vec{r},E)$ of secondary neutrons (both prompt and delayed) for a fission of isotope j times the macroscopic fission cross section for a fission of isotope j.

$\beta_{\ell,j}=$ delayed neutron fraction in precursor group ℓ.

The following condensation formulas have been used:

$$\nu_j^{\mathrm{ss}}(\vec{r},E) = \nu_j^{\mathrm{pr}}(\vec{r},E) + \sum_\ell \nu_{\ell,j}^{\mathrm{D}}(\vec{r},E) \tag{1.7}$$

$$\beta_{\ell,j} = \frac{\int_0^\infty dE \ \nu_{\ell,j}^{\mathrm{D}}(\vec{r},E)\Sigma_{\mathrm{f},j}(\vec{r},E)\phi(\vec{r},E)}{\int_0^\infty dE \ \nu_j^{\mathrm{ss}}(\vec{r},E)\Sigma_{\mathrm{f},j}(\vec{r},E)\phi(\vec{r},E)} = \frac{\sum_g \nu\Sigma_{\mathrm{f},\ell,j}^{\mathrm{D},g}(\vec{r})\phi^g(\vec{r})}{\sum_g \nu\Sigma_{\mathrm{f},j}^g(\vec{r})\phi^g(\vec{r})} \tag{1.8}$$

$$\left[1 - \sum_\ell \beta_{\ell,j}\right] = \frac{\int_0^\infty dE \ \nu_j^{\mathrm{pr}}(\vec{r},E)\Sigma_{\mathrm{f},j}(\vec{r},E)\phi(\vec{r},E)}{\int_0^\infty dE \ \nu_j^{\mathrm{ss}}(\vec{r},E)\Sigma_{\mathrm{f},j}(\vec{r},E)\phi(\vec{r},E)} = \frac{\sum_g \nu\Sigma_{\mathrm{f},j}^{\mathrm{pr},g}(\vec{r})\phi^g(\vec{r})}{\sum_g \nu\Sigma_{\mathrm{f},j}^g(\vec{r})\phi^g(\vec{r})} \tag{1.9}$$

$$\phi^g(\vec{r}) = \int_{E_g}^{E_{g-1}} dE \ \phi(\vec{r},E) \tag{1.10}$$

$$\chi_j^{\mathrm{pr},g} = \int_{E_g}^{E_{g-1}} dE \ \chi_j^{\mathrm{pr}}(E) \tag{1.11}$$

$$\chi_{\ell,j}^{\mathrm{D},g} = \int_{E_g}^{E_{g-1}} dE \ \chi_{\ell,j}^{\mathrm{D}}(E) \ ; \quad \ell = 1, N_d \tag{1.12}$$

$$< 1/v >^g = \frac{1}{\phi^g(\vec{r})} \int_{E_g}^{E_{g-1}} dE \ \frac{1}{v(E)} \ \phi(\vec{r},E) \tag{1.13}$$

$$\Sigma^g(\vec{r}) = \frac{1}{\phi^g(\vec{r})} \int_{E_g}^{E_{g-1}} dE \ \Sigma(\vec{r},E) \ \phi(\vec{r},E) \tag{1.14}$$

$$\Sigma_{\mathrm{s0}}^{g\leftarrow h}(\vec{r}) = \frac{1}{\phi^h(\vec{r})} \int_{E_g}^{E_{g-1}} dE \int_{E_h}^{E_{h-1}} dE' \ \Sigma_{\mathrm{s0}}(\vec{r},E\leftarrow E') \ \phi(\vec{r},E') \tag{1.15}$$

$$\nu\Sigma_{\mathrm{f},j}^g(\vec{r}) = \frac{1}{\phi^g(\vec{r})} \int_{E_g}^{E_{g-1}} dE \ \nu_j^{\mathrm{ss}}(\vec{r},E) \ \Sigma_{\mathrm{f},j}(\vec{r},E) \ \phi(\vec{r},E) \ . \tag{1.16}$$

where the variable t has been omitted in order to simplify the notation.

A steady-state fission spectrum (taking into account both prompt and delayed neutrons), for a fission of isotope j, is also required for solving the static neutron diffusion equation:

$$\chi_j^{\mathrm{ss}}(E) = \left[1 - \sum_\ell \beta_{\ell,j}\right] \chi_j^{\mathrm{pr}}(E) + \sum_\ell \beta_{\ell,j} \ \chi_{\ell,j}^{\mathrm{D}}(E) \ . \tag{1.17}$$

The group-integrated steady-state fission spectrum is therefore given as

$$\chi_j^{\text{ss},g} = \left[1 - \sum_\ell \beta_{\ell,j}\right] \chi_j^{\text{pr},g} + \sum_\ell \beta_{\ell,j}\, \chi_{\ell,j}^{\text{D},g} \quad . \tag{1.18}$$

The space-time diffusion equation is generally solved by assuming a *unique* averaged fissionable iso-tope. In this case, the variable N_f is set to 1 in the MACROLIB specification and the summations over j disapears in Eqs. (1.5) and (1.6):

$$
\begin{aligned}
< 1/v >^g \frac{\partial}{\partial t}\phi^g(\vec{r},t) \;=\;& \chi^{\text{pr},g}\left[1 - \sum_\ell \beta_\ell\right]\sum_h \nu\Sigma_{\text{f}}^h(\vec{r},t)\phi^h(\vec{r},t) \\
+\;& \sum_\ell \chi_\ell^{\text{D},g}\lambda_\ell c_\ell(\vec{r},t) + \nabla\cdot D^g(\vec{r},t)\nabla\phi^g(\vec{r},t) \\
-\;& \Sigma^g(\vec{r},t)\phi^g(\vec{r},t) + \sum_h \Sigma_{\text{s}0}^{g\leftarrow h}(\vec{r},t)\phi^h(\vec{r},t)
\end{aligned} \tag{1.19}
$$

together with the set of n_d precursor equations:

$$\frac{\partial c_\ell(\vec{r},t)}{\partial t} = \beta_\ell \sum_g \nu\Sigma_{\text{f}}^g(\vec{r},t)\phi^g(\vec{r},t) - \lambda_\ell c_\ell(\vec{r},t) \;\; ; \quad \ell = 1, N_d \tag{1.20}$$

Using additional approximations, the new condensation relations are rewritten as

$$\nu\Sigma_{\text{f}}(\vec{r},E) = \sum_j \nu\Sigma_{\text{f},j}(\vec{r},E) = \sum_j \nu_j^{\text{ss}}(\vec{r},E)\, \Sigma_{\text{f},j}(\vec{r},E) \tag{1.21}$$

$$\beta_\ell = \frac{\displaystyle\sum_j \beta_{\ell,j} \int_0^\infty dE\, \nu_j^{\text{ss}}(\vec{r},E)\, \Sigma_{\text{f},j}(\vec{r},E)\, \phi(\vec{r},E)}{\displaystyle\sum_j \int_0^\infty dE\, \nu_j^{\text{ss}}(\vec{r},E)\, \Sigma_{\text{f},j}(\vec{r},E)\, \phi(\vec{r},E)} = \frac{\displaystyle\sum_j \beta_{\ell,j} \sum_g \nu\Sigma_{\text{f},j}^g(\vec{r})\, \phi^g(\vec{r})}{\displaystyle\sum_j \sum_g \nu\Sigma_{\text{f},j}^g(\vec{r})\, \phi^g(\vec{r})} \quad , \tag{1.22}$$

$$
\begin{aligned}
\chi^{\text{pr},g} \;=\;& \frac{\displaystyle\sum_j \left[1 - \sum_\ell \beta_{\ell,j}\right]\int_{E_g}^{E_{g-1}} dE\, \chi_j^{\text{pr}}(E) \int_0^\infty dE'\, \nu_j^{\text{ss}}(\vec{r},E')\, \Sigma_{\text{f},j}(\vec{r},E')\, \phi(\vec{r},E')}{\left[1 - \sum_\ell \beta_\ell\right]\displaystyle\sum_j \int_0^\infty dE\, \nu_j^{\text{ss}}(\vec{r},E)\, \Sigma_{\text{f},j}(\vec{r},E)\, \phi(\vec{r},E)} \\[2mm]
=\;& \frac{\displaystyle\sum_j \left[1 - \sum_\ell \beta_{\ell,j}\right]\chi_j^{\text{pr},g} \sum_h \nu\Sigma_{\text{f},j}^h(\vec{r})\, \phi^h(\vec{r})}{\left[1 - \sum_\ell \beta_\ell\right]\displaystyle\sum_j \sum_h \nu\Sigma_{\text{f},j}^h(\vec{r})\, \phi^h(\vec{r})}
\end{aligned} \tag{1.23}
$$

and

$$
\begin{aligned}
\chi_\ell^{\text{D},g} \;=\;& \frac{\displaystyle\sum_j \beta_{\ell,j} \int_{E_g}^{E_{g-1}} dE\, \chi_{\ell,j}^{\text{D}}(E) \int_0^\infty dE'\, \nu_j^{\text{ss}}(\vec{r},E')\, \Sigma_{\text{f},j}(\vec{r},E')\, \phi(\vec{r},E')}{\beta_\ell \displaystyle\sum_j \int_0^\infty dE\, \nu_j^{\text{ss}}(\vec{r},E)\, \Sigma_{\text{f},j}(\vec{r},E)\, \phi(\vec{r},E)} \;\; ; \quad \ell = 1, N_d \\[2mm]
=\;& \frac{\displaystyle\sum_j \beta_{\ell,j}\, \chi_{\ell,j}^{\text{D},g} \sum_h \nu\Sigma_{\text{f},j}^h(\vec{r})\, \phi^h(\vec{r})}{\beta_\ell \displaystyle\sum_j \sum_h \nu\Sigma_{\text{f},j}^h(\vec{r})\, \phi^h(\vec{r})} \;\; ; \quad \ell = 1, N_d \quad .
\end{aligned} \tag{1.24}
$$

The above definitions ensure that the group-integrated steady-state fission spectrum is given as

$$\chi^{\text{ss},g} = \left[1 - \sum_\ell \beta_\ell\right] \chi^{\text{pr},g} + \sum_\ell \beta_\ell \ \chi_\ell^{\text{D},g} \quad . \tag{1.25}$$

A mean neutron generation time can also be written as

$$\Lambda = \frac{\int\limits_0^\infty dE \ \frac{1}{v(E)} \ \phi(\vec{r},E)}{\sum\limits_j \int\limits_0^\infty dE \ \nu_j^{\text{ss}}(\vec{r},E) \ \Sigma_{\text{f},j}(\vec{r},E) \ \phi(\vec{r},E)} = \frac{\sum\limits_g < 1/v >^g \ \phi^g(\vec{r})}{\sum\limits_j \sum\limits_g \nu\Sigma_{\text{f},j}^g(\vec{r}) \ \phi^g(\vec{r})} \quad . \tag{1.26}$$

2 Contents of a /microlib/ directory

A /microlib/ directory contains the set of multigroup microscopic cross sections associated with a set of isotopes. It also includes a /macrolib/ directory where the macroscopic cross sections for the mixtures to which are associated these isotopes are stored (see Section 1). Finally it may contains a /depletion/ directory (see Section 2.4) which is required for burnup calculation and a /selfshield/ directory which is generated by the `SHI:` or `USS:` operator (see Section 2.8). It is therefore multi-level, namely, it contains sub-directories. Note that the contents of such a directory will vary depending on the operator which was used to create or modify it. Here for convenience we will define the variable $\mathcal{M}$ to identify the creation operator:

$$\mathcal{M} = \begin{cases} 1 & \text{if the microlib is created or modified by the } \texttt{LIB:} \text{ or } \texttt{EVO:} \text{ operator} \\ 2 & \text{if the microlib is created or modified by the } \texttt{EDI:} \text{ or } \texttt{C2M:} \text{ operator} \\ 3 & \text{if the microlib is modified by the } \texttt{SHI:} \text{ or } \texttt{USS:} \text{ operator} \\ 4 & \text{if the microlib is part of a COMPO object and is created by the } \texttt{COMPO:} \text{ operator} \end{cases}$$

In the case where the `LIB:` or `C2M:` operator is used to create the microlib, it appears on the root level of the data structure. For the other case it is embedded as a subdirectory of a surrounding data structure.

2.1 State vector content for the /microlib/ data structure

The dimensioning parameters for the /microlib/ data structure, which are stored in the state vector $\mathcal{S}^m$, represent:

- The maximum number of mixtures $M_m = \mathcal{S}_1^m$

- The number of isotopes $N_I = \mathcal{S}_2^m$

- The number of groups $G = \mathcal{S}_3^m$

- The order for the scattering anisotropy $L = \mathcal{S}_4^m$ ($L = 1$ is an isotropic collision; $L = 2$ is a linearly anisotropic collision, etc.)

- The transport correction option $I_{tr} = \mathcal{S}_5^m$

$$I_{tr} = \begin{cases} 0 & \text{do not use a transport correction} \\ 1 & \text{use an APOLLO-type transport correction (micro-reversibility at all energies)} \\ 2 & \text{recover a transport correction from the cross-section library} \\ 3 & \text{use a WIMS-type transport correction (micro-reversibility below 4eV;} \\ & \text{1/E current spectrum elsewhere)} \\ 4 & \text{use a leakage correction based on } \texttt{NTOT1} \text{ data.} \end{cases}$$

- Format of the included /macrolib/ $I_p = \mathcal{S}_6^m$

$$I_p = \begin{cases} 0 & \text{for the direct macroscopic cross sections} \\ 1 & \text{for the adjoint macroscopic cross sections} \end{cases}$$

- Option for removing delayed neutron effects from the /microlib/ $I_t = \mathcal{S}_7^m$

$$I_t = \begin{cases} 1 & \text{include the delayed and prompt neutron effect} \\ 2 & \text{consider only the prompt neutrons. This option is only available with} \\ & \text{MATXS–type libraries.} \end{cases}$$

- The number of independent libraries $N_{\text{lib}} = \mathcal{S}_8^m$

- The number of fast groups without self-shielding $N_{g,f} = \mathcal{S}_9^m$

  Represents the number of fast energy groups to be treated without including resonance effects. It is automatically determined from the cross-section libraries. This value, which is only used by the self-shielding operator, can be modified using the keyword `GRMAX`.

- The maximum index of all groups with self-shielding $N_{g,e} = \mathcal{S}_{10}^m$.

  In the case of a WIMS–type library, it represents the total number of energy groups above 4.0 eV. Otherwise, it is automatically determined from the cross-section libraries. This value, is used by the self-shielding operator and can be modified locally in this operator using the keyword `GRMIN`.

- The number of depleting isotopes $N_d = \mathcal{S}_{11}^m$

- The number of depleting mixtures $N_{d,f} = \mathcal{S}_{12}^m$

- The number of additional ϕ–weighted editing cross sections $N_e = \mathcal{S}_{13}^m$

- The number of mixtures $N_m = \mathcal{S}_{14}^m$

- The number of resonant mixtures $N_r = \mathcal{S}_{15}^m$

- The number of energy-dependent fission spectra $G_{\mathrm{chi}} = \mathcal{S}_{16}^m$. By default ($G_{\mathrm{chi}} = 0$), a unique fission spectrum is used. The theory of multiple fission spectra is presented in Ref. 2.

- Option for processing the cross-section libraries $I_{\mathrm{proc}} = \mathcal{S}_{17}^m$

$$
I_{\mathrm{proc}} =
\begin{cases}
-1 & \text{skip the library processing (i.e., no interpolation).} \\
0 & \text{perform an interpolation in temperature and dilution.} \\
1 & \text{perform an interpolation in temperature and compute probability} \\
  & \text{tables based on the tabulation in dilution.} \\
2 & \text{perform an interpolation in temperature and build a new temperature-} \\
  & \text{independent cross-section library in DRAGON format.} \\
3 & \text{perform an interpolation in temperature and compute CALENDF–type} \\
  & \text{mathematical probability tables based on BIN–type cross sections. Do} \\
  & \text{not compute the slowing-down correlated weight matrices. Option} \\
  & \text{compatible with the subgroup projection method (SPM).} \\
4 & \text{perform an interpolation in temperature and compute CALENDF–type} \\
  & \text{mathematical probability tables and slowing-down correlated weight} \\
  & \text{matrices based on BIN–type cross sections. Option compatible with} \\
  & \text{the Ribon extended method.} \\
5 & \text{perform an interpolation in temperature and compute CALENDF–type} \\
  & \text{mathematical probability tables based on BIN–type cross sections. This} \\
  & \text{option is similar to the } I_{\mathrm{proc}} = 3 \text{ procedure. Here, the base points of the} \\
  & \text{probability tables corresponding to fission and scattering cross sections} \\
  & \text{and to components of the transfer scattering matrix are also obtained} \\
  & \text{using the CALENDF approach.}
\end{cases}
$$

- Option for computing the macrolib $I_{\mathrm{mac}} = \mathcal{S}_{18}^m$

$$
I_{\mathrm{mac}} =
\begin{cases}
0 & \text{do not build an embedded macrolib.} \\
1 & \text{build an embedded macrolib. Mandatory if the microlib is to be used to} \\
  & \text{perform micro-depletion.}
\end{cases}
$$

- The number of precursor groups producing delayed neutrons $N_{\mathrm{del}} = \mathcal{S}_{19}^m$.

- The number of fissile isotopes producing fission products with `PYIELD` data $N_{\mathrm{dfi}} = \mathcal{S}_{20}^m$ (see Table 17).

- Option for completing the depletion chains with the missing isotopes $I_{\text{cmp}} = \mathcal{S}_{21}^m$.

$$I_{\text{cmp}} = \begin{cases} 0 & \text{complete} \\ 1 & \text{do not complete} \end{cases}$$

- The maximum number of isotopes per mixture $M_{\text{I}} = \mathcal{S}_{22}^m$.

- An integer index (1, 2, 3 or 4) used to set the accuracy of the CALENDF probability tables. The highest the value, the more accurate are the tables. $N_{\text{ipreci}} = \mathcal{S}_{23}^m$.

- Discontinuity factor flag $I_{\text{df}} = \mathcal{S}_{24}^m$. This information is available in /macrolib/ directory (see Section 1).

$$I_{\text{df}} = \begin{cases} 0 & \text{no discontinuity factor information} \\ 1 & \text{multigroup boundary current information is available} \\ 2 & \text{discontinuity factor information (see Section 1.4) is available.} \end{cases}$$

- The maximum Legendre order of the weighting functions $I_w = \mathcal{S}_{25}^m$

$$I_w = \begin{cases} 0 & \text{use the flux as weighting function for all cross sections} \\ 1 & \text{use the fundamental current } \mathcal{J} \text{ as weighting function for scattering cross sections} \\ & \text{with order} \geq 1 \text{ and compute both } \phi\text{– and } \mathcal{J}\text{–weighted total cross sections.} \end{cases}$$

- Number of companion particles in coupled sets $I_{\text{part}} = \mathcal{S}_{26}^M$:

$$I_{\text{part}} = \begin{cases} 0 & \text{the microlib doesn't include coupled sets} \\ > 0 & \text{number of companion particles.} \end{cases}$$

2.2 The main /microlib/ directory

The following records and sub-directories will be found on the first level of a /microlib/ directory:

Table 9: Main records and sub-directories in /microlib/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			Signature of the /microlib/ data structure (SIGNA =L␣LIBRARY␣␣␣).
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^m$, as defined in Section 2.1.
ENERGY␣␣␣␣␣␣	R(G + 1)		eV	Energy groups limits E_g
DELTAU␣␣␣␣␣␣	R(G)			Lethargy width of each group U_g
CHI-ENERGY␣␣	R($G_{\rm chi}$ + 1)	$G_{\rm chi} \neq 0$	eV	$E_{\rm chi}(g)$: Group energy limits defining the energy-dependent fission spectra. By default, a unique fission spectra is used.
CHI-LIMITS␣␣	I($G_{\rm chi}$ + 1)	$G_{\rm chi} \neq 0$		$N_{\rm chi}(g)$: Group limit indices defining the energy-dependent fission spectra. By default, a unique fission spectra is used.
ISOTOPESLIST	Dir(N_I)			List of ISOTOPE directories. Each component of this list follows the /isotope/ specification presented in Tables 14 to 20 and is containing the cross section information associated with a specific isotope. The name of these isotopes is specified by NALIAS$_i$ as given in record ISOTOPESUSED.
ISOTOPESUSED	C(N_I) ∗ 12			Alias name associated with each isotope NALIAS$_i$. The first eight characters of the name of a macroscopic residual are set to '∗MAC∗RES'.
ISOTOPERNAME	C(N_I) ∗ 12	$\mathcal{M} = 1, 3$		Reference name associated with each isotope NISO$_i$
ISOTOPESMIX␣	I(N_I)	$\mathcal{M} \neq 4$		Mixture number associated with each isotope N_I
ISOTOPESDENS	R(N_I)		(cm b)$^{-1}$	Isotopic density ρ_i
ISOTOPESTEMP	R(N_I)		K	Isotope temperature T_i
ISOTOPESTODO	I(N_I)	$\mathcal{M} = 1, 3$		=0: automatic detection of depletion for isotope i; =1: isotope i is forced to be non depleting (keeps its capability to produce energy); =2: isotope i is forced to be depleting; =3: isotope i is at saturation.
ISOTOPESTYPE	I(N_I)			Type index associated with each isotope ITYP$_i$. = 1: the isotope is not fissile and not a fission product; = 2: fissile isotope; = 3: fission product.
ISOTOPESVOL␣	R(N_I)	$\mathcal{M} = 2, 4$	cm^3	Volume occupied by isotope V_i
ILIBRARYTYPE	C(N_I) ∗ 8	$N_{\rm lib} \geq 1$		Library type associated with each isotope NLTY$_i$

Main records and sub-directories in /microlib/ continued from last page

Name	Type	Condition	Units	Comment
ILIBRARYNAME	$C(N_{\mathrm{lib}}) * 64$	$N_{\mathrm{lib}} \geq 1$		Name associated with each cross-section library
ILIBRARYINDX	$I(N_I)$	$N_{\mathrm{lib}} \geq 1$		Index of the cross-section library associated with each isotope $1 \leq \mathsf{LLIB}_i \leq N_{\mathrm{lib}}$
ISOTOPESCOH␣	$C(N_I) * 8$	$N_{\mathrm{lib}} \geq 1$		Name of coherent scattering type at thermal energies NCOH_i
ISOTOPESINC␣	$C(N_I) * 8$	$N_{\mathrm{lib}} \geq 1$		Name of incoherent scattering type at thermal energies NINC_i
ISOTOPESRESK	$C(N_I) * 8$	$N_{\mathrm{lib}} \geq 1$		Name of resonance elastic scattering kernel (RESK) type at epithermal energies NRSK_i
ISOTOPESNTFG	$I(N_I)$	$N_{\mathrm{lib}} \geq 1$		Number of thermal groups involved in coherent or incoherent scattering $G_{s,i}$
ISOTOPESHIN␣	$C(N_I) * 12$	$N_{\mathrm{lib}} \geq 1$		Name of resonant isotope associated with each isotope NSHI_i
ISOTOPESSHI␣	$I(N_I)$	$N_{\mathrm{lib}} \geq 1$		Resonant mixture associated with each isotope $I_{R,i}$
ISOTOPESDSN␣	$R(N_I)$	$N_{\mathrm{lib}} \geq 1$ $I_{\mathrm{proc}} = 0$	b	Standard dilution cross section for isotope $\sigma_{\mathrm{dil},i}$
ISOTOPESDSB␣	$R(N_I)$	$N_{\mathrm{lib}} \geq 1$ $I_{\mathrm{proc}} = 0$	b	Livolant-Jeanpierre dilution cross section for isotope $\sigma_{\mathrm{LJ},i}$
ISOTOPESNIR␣	$I(N_I)$	$N_{\mathrm{lib}} \geq 1$		Use Goldstein-Cohen factor λ_i in groups with index $\geq N_i^{\mathrm{ir}}$. Use $\lambda = 1$ in other groups
ISOTOPESGIR␣	$R(N_I)$	$N_{\mathrm{lib}} \geq 1$	1	Goldstein-Cohen parameter in low-energy resonant groups λ_i. Set to -998.0 if $I_{\mathrm{proc}} = 3$, to -999.0 if $I_{\mathrm{proc}} = 4$ and to -1000.0 if $I_{\mathrm{proc}} = 5$.
MIXTURESVOL␣	$R(N_m)$	$\mathcal{M} = 2, 4$	cm^3	Volume occupied by each mixture
ADDXSNAME-P0	$C(N_e) * 8$	$N_e \geq 1$		Names of the additional ϕ–weighted editing cross sections ADDXS_k stored on /macrolib/
PARTICLE␣␣␣␣	$C * 1$	$I_{\mathrm{part}} \geq 1$		Character name of the particle associated to the microlib. Usual names for particles are N (neutrons), G (photons), B (electrons), C (positrons) and P (protons).
PARTICLE-NAM	$C(I_{\mathrm{part}} + 1) * 1$	$I_{\mathrm{part}} \geq 1$		Character name associated to each particle.
PARTICLE-NGR	$I(I_{\mathrm{part}} + 1)$	$I_{\mathrm{part}} \geq 1$		Number of energy groups associated to each particle.
PARTICLE-MC2	$R(I_{\mathrm{part}} + 1)$	$I_{\mathrm{part}} \geq 1$	eV	Rest energy associated to each particle.
{/penergy/}	$R(G_i + 1)$	$I_{\mathrm{part}} \geq 1$	eV	Set of arrays containing energy groups limits for a companion particle. The character name of each sub-directory is the concatenation of the character*1 name of the particle with "ENERGY". For example, GENERGY contains the energy mesh of secondary photons ($G_i + 1$ values).

Main records and sub-directories in /microlib/

Name	Type	Condition	Units	Comment
TIMESPER␣␣␣␣	$R(2 \times 3)$	$\mathcal{M} = 2$		Array $T_{j,i}$ that contains $T_{j,1} = t$, $T_{j,2} = B$ and $T_{j,3} = w$, the lower ($j = 1$) and upper bounds ($j = 2$) for the reference time in days, burnup in MW day T^{-1} and irradiation in Kb^{-1} respectively for which the perturbative expansion is valid
K-EFFECTIVE␣	$R(1)$	*		Effective multiplication constant k_{eff}
K-INFINITY␣␣	$R(1)$	*		Infinite multiplication constant k_{inf}
B2␣␣B1HOM␣␣␣	$R(1)$	*	cm^{-2}	Homogeneous Buckling B_{hom}
MACROLIB␣␣␣␣	Dir	$I_{\text{mac}} = 1$		directory containing the /macrolib/ associated with this library, following the specification presented in Section 1.2.
DEPL-CHAIN␣␣	Dir	$N_d \geq 1$		Directory containing the /depletion/ associated with this library, following the specification presented in Section 2.4.
SHIBA␣␣␣␣␣␣␣	Dir	$\mathcal{M} = 3$		Directory containing the /selfshield/ associated with this library, following the specification presented in Section 2.7. This data is used by the SHI: operator.
SHIBA_SG␣␣␣␣	Dir	$\mathcal{M} = 3$		Directory containing the /selfshield/ associated with this library, following the specification presented in Section 2.8. This data is used by the USS: operator.
MIXTUREGAS␣␣	$I(N_m)$			State of each mixture (used for stopping power correction).
INDEX␣␣␣␣␣␣␣	Dir	*		Directory containing indexing or table-of-content data for specific library files

One will find in Section 1 the description of a /macrolib/ directory and in Section 2.9 the contents of an /isotope/ directory. Note that if $N_I = 2$ and

$$\text{NALIAS}_i = \begin{cases} \text{U235 0001} & \text{for} \quad i = 1 \\ \text{Pu239 0003} & \text{for} \quad i = 2 \end{cases}$$

then {/isotope/} will correspond to the following two directories:

Table 10: Examples of isotopes directory in a /microlib/

Name	Type	Condition	Units	Comment
U235␣␣␣␣0001	Dir			Directory where the microscopic cross sections of ^{235}U are stored. These are self-shielded cross section already interpolated in temperature. They correspond to the properties of mixture 1
Pu239␣␣␣0003	Dir			Directory where the microscopic cross sections of ^{239}Pu are stored. These are self-shielded cross section already interpolated in temperature. They correspond to the properties of mixture 3

2.3 State vector content for the depletion sub-directory

The dimensioning parameters for the depletion sub-directory, which are stored in the state vector $\mathcal{S}^d$, represent:

- The number of depleting isotopes $N_{\mathrm{depl}} = \mathcal{S}_1^d$

- The number of direct fissile isotopes (i.e., producing fission products) $N_{\mathrm{dfi}} = \mathcal{S}_2^d$

- The number of fission fragments $N_{\mathrm{dfp}} = \mathcal{S}_3^d$. A fission fragment is produced directly by the fission reaction. A fission product is a fission fragment or a daughter isotope produced by decay or neutron-induced reaction.

- The number of heavy isotopes $N_{\mathrm{H}} = \mathcal{S}_4^d$

  This number represents the combination of fissile isotopes and the other isotopes produced from these isotopes by reactions other than fission.

- The number of fission products $N_{\mathrm{fp}} = \mathcal{S}_5^d$

  This number represents the combination of fission fragments and the other daughter isotopes produced by any reaction (decay or neutron induced).

- The number of other isotopes $N_{\mathrm{O}} = \mathcal{S}_6^d$

  This number represents the other depleting isotopes which are not produced by fission or by reaction with fission isotopes or fission products but have a depletion chain.

- The number of stable isotopes $N_{\mathrm{H}} = \mathcal{S}_7^d$

  This number represents the non-depleting isotopes producing energy (mainly by radiative capture). An isotope is considered to be stable if:

  – its radioactive decay constant is zero

  – the isotope has no father and no daughter

  – energy is produced by the isotope.

- The maximum number of depleting reactions, including radioactive decay and neutron-induced reactions $M_{\mathrm{R}} = \mathcal{S}_8^d$

- The maximum number of parent isotopes leading to the production of an isotope in the depletion chain $M_{\mathrm{S}} = \mathcal{S}_9^d$

2.4 The depletion sub-directory /depletion/ in /microlib/

The following records and sub-directories will be found on the first level of a /depletion/ directory:

Table 11: Main records and sub-directories in /depletion/

Name	Type	Condition	Units	Comment
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^d$, as defined in Section 2.3.
ISOTOPESDEPL	C(N_{depl}) $*$ 12			Reference name of the isotopes NISOD_i present in the depletion chain
CHARGEWEIGHT	I(N_{depl})			6-digit (integer number) nuclide identifier with atomic number Z (2 digits), mass number A (3 digits) and energy state E (0 for ground state, 1 for first excited level, etc.). This identifier is not defined for pseudo fission products.
DEPLETE-IDEN	C(M_{R}) $*$ 8			Reference name of the depletion reactions
DEPLETE-REAC	I($M_{\text{R}} \times N_{\text{depl}}$)			List of identifier for the depletion of an isotope $K_{r,i}^{\text{d}}$
DEPLETE-ENER	R($M_{\text{R}} \times N_{\text{depl}}$)		Mev	Energy per reaction associated with each depletion reaction $R_{r,i}^{\text{d}}$
DEPLETE-DECA	R(N_{depl})		10^{-8} s^{-1}	Radioactive decay constants
PRODUCE-REAC	I($M_{\text{S}} \times N_{\text{depl}}$)			List of identifier for the production of an isotope $K_{s,i}^{\text{p}}$
PRODUCE-RATE	R($M_{\text{S}} \times N_{\text{depl}}$)		1	Branching ratio associated with each production reaction $R_{s,i}^{\text{p}}$
FISSIONYIELD	R($N_{\text{dfi}} \times N_{\text{dfp}}$)		1	Fission yield for each direct fissile isotope to each fission fragment $Y_{i \to j}$

An isotope NISO_i defined in Section 2.2 is considered to be part of the depletion chain only if one can find a value of $1 \leq j \leq N_{\text{depl}}$ such that $\mathsf{NISO}_i = \mathsf{NISOD}_j$. Some depleting isotopes may be automatically added to the /microlib/ directory. In this case, the reference name in record ISOTOPERNAME is taken equal to its reference name in ISOTOPESDEPL and the alias name in record ISOTOPESUSED is taken equal to the first 8 characters of its reference name in ISOTOPESDEPL, completed by a 4-digit mixture identifier. If the reference name contains an underscore, the alias name is truncated at the first underscore. For example, an isotope present in mixture 2 with a reference name equal to D2O_3_P5 is translated into an alias name equal to D2O␣␣␣␣␣0002.

The contents of the variables $K_{r,i}^{\text{d}}$ is used to identify the type of isotope under consideration. For each isotope i, r will take successively the values 1 to M_{D} depending on the type of reaction NREAD_r one wishes to analyze, namely

$\mathrm{NREAD}_1 =$`DECAY`␣␣␣	isotope may undergo radioactive decay
$\mathrm{NREAD}_2 =$`NFTOT`␣␣␣	isotope may undergo fission or is a fission fragment
	$^1_0 n + ^A_Z X \rightarrow\ ^{A+1-\nu-B}_{Z-Y} U + ^B_Y V + \nu\ ^1_0 n + \gamma$
$\mathrm{NREAD}_3 =$`NG`␣␣␣␣␣␣	isotope may undergo neutron capture (mt=102)
	$^1_0 n + ^A_Z X \rightarrow\ ^{A+1}_Z X + \gamma$
$\mathrm{NREAD}_4 =$`N2N`␣␣␣␣␣	isotope may undergo (n,2n) reaction (mt=16)
	$^1_0 n + ^A_Z X \rightarrow\ ^{A-1}_Z X + 2\ ^1_0 n + \gamma$
$\mathrm{NREAD}_5 =$`N3N`␣␣␣␣␣	isotope may undergo (n,3n) reaction (mt=17)
$\mathrm{NREAD}_6 =$`N4N`␣␣␣␣␣	isotope may undergo (n,4n) reaction (mt=37)
$\mathrm{NREAD}_7 =$`NA`␣␣␣␣␣␣	isotope may undergo (n,α) reaction (mt=107)
$\mathrm{NREAD}_8 =$`NP`␣␣␣␣␣␣	isotope may undergo (n,p) reaction (mt=103)
$\mathrm{NREAD}_9 =$`N2A`␣␣␣␣␣	isotope may undergo (n,2α) reaction (mt=108)
$\mathrm{NREAD}_{10} =$`NNP`␣␣␣␣␣	isotope may undergo (n,np) reaction (mt=28)
$\mathrm{NREAD}_{11} =$`ND`␣␣␣␣␣␣	isotope may undergo (n,d) reaction (mt=104)
$\mathrm{NREAD}_{12} =$`NT`␣␣␣␣␣␣	isotope may undergo (n,t) reaction (mt=105)

where symbols n, α, p, d and t represent neutron, alpha particle, proton, deuteron and triton, respectively.

The contents of the variable $K^{\mathrm{d}}_{r,i}$ is used to specify the properties of reaction r for each isotope i under consideration. Here $K^{\mathrm{d}}_{r,i}$ contains two different types of informations, namely $d(r)$ and $i(r)$ which are defined as follows:

$$d(r) = K^{\mathrm{d}}_{r,i} \ \mathrm{mod}\ \ 100 \quad \mathrm{and} \quad i(r) = \frac{K^{\mathrm{d}}_{r,i}}{100} \tag{2.1}$$

where

$$d(r) = \begin{cases} 0 & \text{isotope } i \text{ does not deplete by reaction } \mathsf{NREAD}_r \\ 1 & \text{isotope } i \text{ will deplete by reaction } \mathsf{NREAD}_r \\ 2 & \text{isotope } i \text{ does not deplete by reaction } \mathsf{NREAD}_r \text{ but yields energy production} \\ 3 & \text{isotope } i \text{ is fissile without fission yield. Valid only for } r \text{ such that } \mathsf{NREAD}_r = \mathsf{NFTOT} \\ 4 & \text{isotope } i \text{ is fissile with fission yield. Valid only for } r \text{ such that } \mathsf{NREAD}_r = \mathsf{NFTOT} \\ 5 & \text{isotope } i \text{ is a fission fragment. Valid only for } r \text{ such that } \mathsf{NREAD}_r = \mathsf{NFTOT} \end{cases}$$

and $i(r) = 0$ unless $4 \le d(r) \le 5$. When $d(r) = 4$, $i(r)$ represents the fissile isotope index while for $d(r) = 5$, $i(r)$ represents the fission fragment index. The fractional yield for the production of the fission fragment $i(r')$ from the fissile isotope $i(r)$ is stored in matrix $Y_{i(r) \rightarrow i(r')}$. The contents of the vector $R^{\mathrm{d}}_{r,i}$ is the energy in MeV emitted per decay or reaction.

The contents of the variables $K^{\mathrm{p}}_{s,i}$ is used to identify explicitly the parent isotope which can generate the current isotope i. The maximum number of parent reaction for this depletion chain is M_{S}. $K^{\mathrm{p}}_{s,i}$ contains two different types of information, namely $r(s)$ and $i(s)$ which are defined as follows:

$$r(s) = K^{\mathrm{p}}_{s,i} \ \mathrm{mod}\ 100 \quad \mathrm{and} \quad i(s) = \frac{K^{\mathrm{p}}_{s,i}}{100} \tag{2.2}$$

where $r(s) = 0$ indicates that the list of parent isotopes is complete while $r(s) > 0$ refers to the reaction type $\mathsf{NREAD}_{r(s)}$ and can take the following values:

$$r(s) = \begin{cases} 1 & \text{isotope } i \text{ produced by radioactive decay} \\ 2 & \text{isotope } i \text{ produced by fission (this contribution is kept apart from record} \\ & \text{'FISSIONYIELD')} \\ 3 & \text{isotope } i \text{ produced by neutron capture} \\ \ge 4 & \text{isotope } i \text{ produced by } \mathsf{NREAD}_{r(s)} \text{ reaction} \end{cases}$$

In the case where $r(s) > 0$, $i(s)$ represents the isotope index associated with the parent isotope and $R^{\mathrm{p}}_{s,i}$ represents the branching ratio in fraction for the production of isotope NISOD_i from a neutron reaction with the parent isotope $\mathsf{NISOD}_{i(s)}$.

2.5   State vector content for the SHIBA self-shielding sub-directory

The dimensioning parameters for the self-shielding sub-directory, which are stored in the state vector $\mathcal{S}^s$, represent:

- The first group for which self-shielding takes place $G_{\min} = \mathcal{S}_1^s$ By default $G_{\min} = N_{g,f} + 1$

- The last group for which self-shielding takes place $G_{\max} = \mathcal{S}_2^s$ By default $G_{\max} = N_{g,e}$

- The maximum number of iterations in the self-shielding calculation $M_r = \mathcal{S}_3^s$

- Enabling flag for the Livolant-Jeanpierre normalization $I_{\mathrm{lj}} = \mathcal{S}_4^s$

- Enabling flag for the use of Goldstein-Cohen parameters $I_{\mathrm{gc}} = \mathcal{S}_5^s$

- The transport correction option used in self-shielding $I_{\mathrm{tc}} = \mathcal{S}_6^s$

$$I_{\mathrm{tc}} = \begin{cases} 0 & \text{no transport correction applied in self-shielding calculation} \\ 1 & \text{use transport corrected cross section in self-shielding calculation} \end{cases}$$

- Type of self-shielding model $I_{\mathrm{level}} = \mathcal{S}_7^s$

$$I_{\mathrm{level}} = \begin{cases} 0 & \text{Stamm'ler model without distributed self-shielding effects} \\ 1 & \text{Stamm'ler model with the Nordheim (PIC) distributed self-shielding model} \\ 2 & \text{Stamm'ler model with both Nordheim (PIC) distributed self-shielding model} \\ & \text{and Riemann integration method.} \end{cases}$$

- The option to indicate whether a specific flux solver or collision probability matrices are used to perform the self-shielding calculation $I_{\mathrm{flux}} = \mathcal{S}_8^s$ (see `PIJ` and `ARM` keyword in `SHI:` operator input option)

$$I_{\mathrm{flux}} = \begin{cases} 1 & \text{use a specific flux solver (the \texttt{ARM} keyword was selected)} \\ 2 & \text{use collision probability matrices (the \texttt{PIJ} keyword was selected)} \end{cases}$$

2.6   State vector content for the subgroup self-shielding sub-directory

The dimensioning parameters for the self-shielding sub-directory, which are stored in the state vector $\mathcal{S}^s$, represent:

- The first group for which self-shielding takes place $G_{\min} = \mathcal{S}_1^s$ By default $G_{\min} = N_{g,f} + 1$

- The last group for which self-shielding takes place $G_{\max} = \mathcal{S}_2^s$ By default $G_{\max} = N_{g,e}$

- SPH enabling flag $I_{\mathrm{sph}} = \mathcal{S}_3^s$

$$I_{\mathrm{sph}} = \begin{cases} 0 & \text{skip the multigroup equivalence procedure} \\ 1 & \text{perform a multigroup equivalence procedure (SPH procedure or} \\ & \text{Livolant-Jeanpierre equivalence)} \end{cases}$$

- The transport correction option used in self-shielding $I_{\mathrm{tc}} = \mathcal{S}_4^s$

$$I_{\mathrm{tc}} = \begin{cases} 0 & \text{no transport correction applied in self-shielding calculation} \\ 1 & \text{use transport corrected cross section in self-shielding calculation} \end{cases}$$

- The number of iterations in the self-shielding calculation $M_r = \mathcal{S}_5^s$

- The option to indicate whether a specific flux solver or collision probability matrices are used to perform the self-shielding calculation $I_{\text{flux}} = \mathcal{S}_6^s$ (see `PIJ` and `ARM` keyword in `USS:` operator input option)

$$I_{\text{flux}} = \left\{ \begin{array}{ll} 1 & \text{use a specific flux solver (the \texttt{ARM} keyword was selected)} \\ 2 & \text{use collision probability matrices (the \texttt{PIJ} keyword was selected)} \end{array} \right.$$

- The γ factor enabling flag $I_\gamma = \mathcal{S}_7^s$. These factors are used to represent the moderator absorption effect in the Sanchez–Coste self-shielding method.

$$I_\gamma = \left\{ \begin{array}{ll} 0 & \text{the } \gamma \text{ factors are set to 1.0} \\ 1 & \text{the } \gamma \text{ factors are computed} \end{array} \right.$$

- The simplified self-shielding enabling flag $I_{\text{calc}} = \mathcal{S}_8^s$

$$I_{\text{calc}} = \left\{ \begin{array}{ll} 0 & \text{perform a delailed self-shielding calculation} \\ 1 & \text{perform a simplified self-shielding calculation using data recovered from the} \\ & \text{$-$\texttt{DATA}$-$\texttt{CALC}$-$ directory} \end{array} \right.$$

- The flag for ignoring the activation of the mutual resonance shielding model $I_{\text{noco}} = \mathcal{S}_9^s$

$$I_{\text{noco}} = \left\{ \begin{array}{ll} 0 & \text{follow the directives set by \texttt{LIB}} \\ 1 & \text{ignore the directives set by \texttt{LIB}} \end{array} \right.$$

- Maximum number of fixed point iterations for the ST scattering source convergence $I_{\text{max}} = \mathcal{S}_{10}^s$

2.7 The SHIBA self-shielding sub-directory /selfshield/ in /microlib/

Table 12: Main records and sub-directories in /selfshield/

Name	Type	Condition	Units	Comment
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^s$, as defined in Section 2.5.
EPS-SHIBA␣␣␣	R(1)		1	Value of the relative convergence criterion for the self-shielding iterations in SHI:

2.8 The subgroup self-shielding sub-directory /selfshield/ in /microlib/

Table 13: Main records and sub-directories in /selfshield/

Name	Type	Condition	Units	Comment
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^s$, as defined in Section 2.6.
-DATA-CALC-␣	Dir	$I_{\mathrm{calc}} = 1$		name of directory containing the data required by a simplified self-shielding calculation. This type of calculation allows the definition of a single self-shielded isotope in several resonant mixtures.

2.9 Contents of an /isotope/ directory

Each isotope directory always contains a cross section identifier record SCAT-SAVED␣␣ which must be used to verify if a given cross section type has been saved for this isotope.

Table 14: Isotopic cross section identifier records

Name	Type	Condition	Units	Comment
ALIAS␣␣␣␣␣␣␣	C*12	$\mathcal{M} \geq 0$		Alias character*12 name of a microlib isotope. This record is not provided in DRAGLIB objects.

Isotopic cross section identifier records   continued from last page

Name	Type	Condition	Units	Comment
SCAT-SAVED␣␣	I(L)			Vector κ_k^{scat} to identify the various type of Legendre-dependent cross sections saved for this isotope
AWR␣␣␣␣␣␣␣␣␣	R(1)		nau	Ratio of the isotope mass divided by the neutron mass
PT-PHYS␣␣␣␣␣	Dir	$I_{\text{proc}} = 1, \geq 3$		Sub-directory containing probability table information, following the specification given in Section 2.9.1. I_{proc} is defined in Section 2.

Delayed neutron data can be present for some fissile isotopes on the /isotope/ directory. If $N_{\text{del}} \geq 1$ precursor groups are used, the following information is available:

Table 15: Delayed neutron reaction records

Name	Type	Condition	Units	Comment
{nusid}	R(G)	$N_{del} \geq 1$	b	$\nu\sigma_{\text{f},\ell}^{\text{D},g}$: The product of σ_{f}^g, the fission cross section with $\nu_\ell^{\text{D},g}$, the averaged number of fission–emitted delayed neutron produced in the precursor group ℓ.
{chid}	R(G)	$N_{del} \geq 1$	1	$\chi_\ell^{\text{D},g}$: Delayed fission spectrum, normalized to one, for the delayed fission neutrons in precursor group ℓ.
LAMBDA-D␣␣␣␣	R(N_{del})	$N_{\text{del}} \geq 1$	s^{-1}	λ_ℓ^{D}: Decay constant associated with the precursor group ℓ. We must have $0 < \lambda_\ell^{\text{D}} < \lambda_{\ell+1}^{\text{D}}$.

The delayed component of the fission yields in each precursor group ℓ is given as $\nu_\ell^{\text{D},g}$. The quantities $\pi^{\text{D},g}$ and $\nu_\ell^{\text{D},g}\,\sigma_{\text{f}}^g$ are defined as

$$\pi^{\text{D},g} = \frac{\nu^{\text{D},g}\,\sigma_{\text{f}}^g}{(\nu^g\sigma_{\text{f}}^g)^{\text{ss}}} \quad .$$

and

$$\nu_\ell^{\text{D},g}\,\sigma_{\text{f}}^g = \omega_\ell\,\pi^{\text{D},g}\,(\nu^g\sigma_{\text{f}}^g)^{\text{ss}}$$

where the superscript ss indicates steady-state values. The delayed neutron records {nusid} and {chid} will be composed, using the following FORTRAN instructions, as NUSIGD and CHID:

WRITE(NUSIGD,$'$(A6,I2.2)$'$) $'$NUSIGF$'$, ell

WRITE(CHID,$'$(A3,I2.2)$'$) $'$CHI$'$, ell

for $1 \le ell \le N_{\mathrm{del}}$. For example, in the case where two group cross sections are considered ($N_{\mathrm{del}} = 2$), the following records would be generated:

Table 16: Example of delayed–neutron records in /isotope/

Name	Type	Condition	Units	Comment
NUSIGF01␣␣␣␣	R(G)	$N_{\mathrm{del}} \ge 1$	b	$\nu\sigma_{\mathrm{f},1}^{\mathrm{D},g}$: The product of σ_{f}^{g}, the fission cross section with $\nu_{1}^{\mathrm{D},g}$, the averaged number of fission–emitted delayed neutron produced in the precursor group 1.
NUSIGF02␣␣␣␣	R(G)	$N_{\mathrm{del}} \ge 2$	b	$\nu\sigma_{\mathrm{f},2}^{\mathrm{D},g}$: The product of σ_{f}^{g}, the fission cross section with $\nu_{2}^{\mathrm{D},g}$, the averaged number of fission–emitted delayed neutron produced in the precursor group 2.
CHI01␣␣␣␣␣␣␣	R(G)	$N_{\mathrm{del}} \ge 1$	1	$\chi_{1}^{\mathrm{D},g}$: Delayed fission spectrum, normalized to one, for the delayed fission neutrons in precursor group 1.
CHI02␣␣␣␣␣␣␣	R(G)	$N_{\mathrm{del}} \ge 2$	1	$\chi_{2}^{\mathrm{D},g}$: Delayed fission spectrum, normalized to one, for the delayed fission neutrons in precursor group 2.

In cases where the /isotope/ directory is produced by the edition module, some depletion-related information may be available in this directory, in order to facilitate subsequent data processing. This information is described in Table 17.

Table 17: Depletion-related information

Name	Type	Condition	Units	Comment
MEVG␣␣␣␣␣␣␣␣␣	R(1)	$N_d \ge 1$	MeV	Energy in MeV produced by radiative capture. N_d is defined in Section 2.
MEVF␣␣␣␣␣␣␣␣␣	R(1)	$N_d \ge 1$	MeV	Energy in MeV produced by fission.
DECAY␣␣␣␣␣␣␣␣	R(1)	$N_d \ge 1$	10^{-8} s^{-1}	Radioactive decay constant
YIELD␣␣␣␣␣␣␣␣	R($G+1$)	$N_d \ge 1$	1	Fission fragment yield per energy group. The first value is the average yield over all the energy spectrum. This record is given only for fission fragments.
PIFI␣␣␣␣␣␣␣␣␣	I(N_{dfi})	$N_{\mathrm{dfi}} \ge 1$		Position in ISOTOPESUSED of the mother fissile isotopes. This record is given only for fission fragments.
PYIELD␣␣␣␣␣␣	R(N_{dfi})	$N_{\mathrm{dfi}} \ge 1$	1	Fission product yield per fissile isotope. This record is given only for fission fragments.

We will first consider the more usual case where constant vector reactions are stored on the isotopic

directory. A typical example of the microscopic cross section directory may be:

Table 18: Example of isotopic vector reaction records

Name	Type	Condition	Units	Comment
NTOTO␣␣␣␣␣␣␣	R(G)		b	The ϕ–weighted multigroup total cross section σ_0^g
TRANC␣␣␣␣␣␣␣	R(G)		b	The multigroup transport correction σ_{tc}^g
NUSIGF␣␣␣␣␣␣	R(G)		b	The product of σ_f^g, the multigroup fission cross section with ν^g, the steady-state number of neutron produced per fission, $\nu\sigma_f^{\mathrm{ss},g}$
NFTOT␣␣␣␣␣␣␣	R(G)		b	The multigroup fission cross section σ_f^g
CHI␣␣␣␣␣␣␣␣␣	R(G)	$G_{\mathrm{chi}} = 0$		The multigroup energy spectrum of the neutron emitted by fission χ^g
CHI--01␣␣␣␣␣	R(G)	$G_{\mathrm{chi}} \geq 1$		The first energy-dependent multigroup energy spectrum of the neutron emitted by fission $\chi^{g,1}$
CHI--02␣␣␣␣␣	R(G)	$G_{\mathrm{chi}} \geq 2$		The second energy-dependent multigroup energy spectrum of the neutron emitted by fission $\chi^{g,2}$
CHI--03␣␣␣␣␣	R(G)	$G_{\mathrm{chi}} \geq 3$		The third energy-dependent multigroup energy spectrum of the neutron emitted by fission $\chi^{g,3}$
CHI--04␣␣␣␣␣	R(G)	$G_{\mathrm{chi}} \geq 4$		The fourth energy-dependent multigroup energy spectrum of the neutron emitted by fission $\chi^{g,4}$
NG␣␣␣␣␣␣␣␣␣␣	R(G)		b	The multigroup neutron capture cross section σ_c^g
H-FACTOR␣␣␣␣	R(G)		J b	Energy production coefficients H^g (product of each microscopic cross section times the energy emitted by this reaction).
C-FACTOR␣␣␣␣	R(G)	*	electron b	Charge deposition coefficients C^g (product of each microscopic cross section times the charge deposed by this reaction). Information provided if PARTICLE=B, C or P.
N2N␣␣␣␣␣␣␣␣␣	R(G)		b	The multigroup cross section $\sigma_{(n,2n)}^g$ for the reaction $_Z^A X + n \to_Z^{A-1} X + 2n$
N3N␣␣␣␣␣␣␣␣␣	R(G)		b	The multigroup cross section $\sigma_{(n,3n)}^g$ for the reaction $_Z^A X + n \to_Z^{A-2} X + 3n$
N4N␣␣␣␣␣␣␣␣␣	R(G)		b	The multigroup cross section $\sigma_{(n,4n)}^g$ for the reaction $_Z^A X + n \to_Z^{A-3} X + 4n$
NP␣␣␣␣␣␣␣␣␣␣	R(G)		b	The multigroup cross section $\sigma_{(n,p)}^g$ for the reaction $_Z^A X + n \to_{Z-1}^A X + p$
NA␣␣␣␣␣␣␣␣␣␣	R(G)		b	The multigroup cross section $\sigma_{(n,\alpha)}^g$ for the reaction $_Z^A X + n \to_{Z-2}^{A-3} X + \alpha$

Example of isotopic vector reaction records

Name	Type	Condition	Units	Comment
`NGOLD⎵⎵⎵⎵⎵⎵⎵`	$R(G)$			The multigroup Goldstein-Cohen parameters as recovered from `GIR` array in main /microlib/ directory λ^g
`NWT0⎵⎵⎵⎵⎵⎵⎵⎵`	$R(G)$		$s^{-1}cm^{-2}$	The multigroup neutron flux spectrum ϕ_w^g
`STRD⎵⎵⎵⎵⎵⎵⎵⎵`	$R(G)$		b	The multigroup transport cross section homogenized over all directions σ_{strd}^g
`STRD-X⎵⎵⎵⎵⎵⎵`	$R(G)$		b	The $x-$directed multigroup transport cross section $\sigma_{\text{strd},x}^g$
`STRD-Y⎵⎵⎵⎵⎵⎵`	$R(G)$		b	The $y-$directed multigroup transport cross section $\sigma_{\text{strd},y}^g$
`STRD-Z⎵⎵⎵⎵⎵⎵`	$R(G)$		b	The $z-$directed multigroup transport cross section $\sigma_{\text{strd},z}^g$
`OVERV⎵⎵⎵⎵⎵⎵⎵`	$R(G)$		$cm^{-1}s$	The average of the inverse neutron velocity $< 1/v >_m^g$
`NTOT1⎵⎵⎵⎵⎵⎵⎵`	$R(G)$		b	The $\mathcal{J}-$weighted multigroup total cross section σ_1^g
`NWT1⎵⎵⎵⎵⎵⎵⎵⎵`	$R(G)$		$s^{-1}cm^{-2}$	The multigroup fundamental current spectrum $\mathcal{J}_w^g$
`NWAT0⎵⎵⎵⎵⎵⎵⎵`	$R(G)$		1	The multigroup neutron adjoint flux spectrum ϕ_w^{*g}
`NWAT1⎵⎵⎵⎵⎵⎵⎵`	$R(G)$		1	The multigroup fundamental adjoint current spectrum $\mathcal{J}_w^{*g}$

We can also use this isotopic directory to store time dependent cross sections in the form of a power series expansion:

$$v_k^g(t) = \sum_{i=0}^{I} v_{k,i}^g t^i \tag{2.3}$$

where the presence of these various terms is specified using κ_k. Note that the last three characters of each of the records in Table 18 correspond to the extension `EXT='⎵⎵⎵'` that is associated with term $i = 0$ in the power series expansion for the cross sections (see Eq. (2.3)). For $i = 1, 2$, the extension takes successively the value `EXT='LIN'` and `EXT='QUA'`. For example, if one considers the total cross section and assumes that $F_i(\kappa_1) = 1$ for $i = 0, 2$, then this implies the presence of the following additional records in the /isotope/:

Table 19: Additional total cross section records for $I = 2$

Name	Type	Condition	Units	Comment
`TOTAL␣␣␣␣LIN`	R(G)		$d^{-1}b$	array $v_{1,1}^g = \Delta\sigma^g$ containing the first order coefficients in the power series expansion for the multigroup total cross section
`TOTAL␣␣␣␣QUA`	R(G)		$d^{-2}b$	array $v_{1,2}^g = \Delta^2\sigma^g$ containing the second order coefficients in the power series expansion for the multigroup total cross section

The multigroup scattering cross section matrix, which gives the probability for a neutron in group h to appear in group g after a collision with this isotope is represented by the form:

$$\sigma_s^{h \to g}(\vec{\Omega} \to \vec{\Omega}') = \sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi} P_\ell(\vec{\Omega} \cdot \vec{\Omega}')\sigma_\ell^{h \to g} = \sum_{\ell=0}^{L} \sum_{m=-\ell}^{\ell} Y_\ell^m(\vec{\Omega})Y_\ell^m(\vec{\Omega}')\sigma_\ell^{h \to g}$$

using a spherical harmonic series expansion to order $L - 1$. Assuming these spherical harmonic are orthonormalized, namely:

$$\int_{4\pi} d^2\Omega \, Y_\ell^m(\vec{\Omega})Y_{l'}^{m'}(\vec{\Omega}) = \delta_{m,m'}\delta_{\ell,\ell'}$$

we can define $\sigma_\ell^{h \to g}$ in terms of $\sigma_s^{h \to g}(\vec{\Omega} \to \vec{\Omega}')$ using the following integral:

$$\sigma_\ell^{h \to g} = \int_{4\pi} d^2\Omega \, \sigma_s^{h \to g}(\vec{\Omega} \to \vec{\Omega}')P_\ell(\vec{\Omega} \cdot \vec{\Omega}')$$

Note that this definition of $\sigma_\ell^{h \to g}$ is not unique and some authors include the factor $2l + 1$ directly in different angular moments of the scattering cross section.

Here instead of storing on these $G \times G$ matrices $\sigma_\ell^{h \to g}$, a vector which contains a compress form for this matrix will be considered. This choice is justified by the fact that the number of energy groups which will lead to scattering in a specific group is generally relatively small compared to the total number of groups in the library and that these groups are clustered around the final energy group. Here we will first define two different integer vectors n_ℓ^g and h_ℓ^g for each order in the scattering cross section and for each final energy group g which will contain respectively the number of successive initial energy groups for which the scattering cross section does not vanish and the maximum energy group number for which scattering to the final group g does not vanishes. Accordingly, for a scattering cross section of the form:

$\sigma_0^{h \to g}$	$g = 1$	$g = 2$	$g = 3$	$g = 4$
$h = 1$	a_1	a_2	0	0
$h = 2$	0	a_3	a_4	a_5
$h = 3$	0	a_6	a_7	0
$h = 4$	0	a_8	0	a_9
h_0^g	1	4	3	4
n_0^g	1	4	2	3

The compress scattering matrix will then contain the following information:

$$\sigma_{\ell,c} = \left(\sigma_{\ell}^{h^1 \to 1}, \sigma_{\ell}^{h^1-1 \to 1}, \ldots, \sigma_{\ell}^{h^1-n_1+1 \to 1}, \sigma_{\ell}^{h^2 \to 2}, \ldots, \sigma_{\ell}^{h^G-n_G+1 \to G} \right)$$

which for the example above leads to

$$\sigma_{\ell,c} = (a_1, a_8, a_6, a_3, a_2, a_7, a_4, a_9, 0, a_5)$$

As a result $\sigma_{\ell}^{h \to g}$ can be reconstructed using

$$\sigma_{\ell}^{h \to g} = \begin{cases} 0 & \text{if} & h > h_{\ell}^g \\ 0 & \text{if} & h < h_{\ell}^g - n_{\ell}^g + 1 \\ \sigma_{\ell,c}^k & \text{otherwise} & k = \sum_{h=1}^{g-1} n_{\ell}^h + h_{\ell}^g - h + 1 \end{cases}$$

Finally, we will also save the total scattering cross section vector of order ℓ which is defined as

$$\sigma_{\ell,s}^h = \sum_{g=1}^{G} \sigma_{\ell}^{h \to g}$$

In the case where only the order $\ell = 0$ moment of scattering cross section is non vanishing (isotropic scattering) the following records can be found on the isotopic directory.

Table 20: Optional scattering records

Name	Type	Condition	Units	Comment
SIGS00␣␣␣␣␣␣	R(G)		b	The isotropic component ($\ell = 0$) of the multi-group total scattering cross section $\sigma_{0,s}^g$
IJJS00␣␣␣␣␣␣	I(G)			Highest energy group number for which the isotropic component of the scattering cross section to group g does not vanish, h_0^g
NJJS00␣␣␣␣␣␣	I(G)			Number of energy groups for which the isotropic component of the scattering cross section to group g does not vanish, n_0^g
SCAT00␣␣␣␣␣␣	R($\sum_{g=1}^{G} n_0^g$)		b	Compressed isotropic component of the scattering matrix $\sigma_{0,c}^k$
{/subiso/}	Dir	$I_{\text{part}} \geq 1$		Set of sub-directories containing scattering information towards a companion particle. {/subiso/} is the name of the companion particle (set to N, G, B, C or P). This information is used to construct coupled sets of cross sections.

If the scattering cross section is expanded to order $L > 1$ in Legendre polynomials, additional set of scattering records similar to those described above will be presentin the cross section directory. The first four characters and last 6 characters in the names of these records will again be identical to those described above while character 5 and 6 will differ from level to level. For example, the order $\ell = 5$ compressed scattering matrix will be identified by SCAT05␣␣␣␣␣␣ while for order $\ell = 50$ we will use SCAT50␣␣␣␣␣␣.

The `STRD` cross sections are normalized in such a way to permit the calculation of a diffusion coefficient using the following formula:

$$D^g = \frac{1}{3 \sum\limits_{i} N_i \, \sigma^g_{\text{strd},i}} \tag{2.4}$$

where N_i is the isotopic density of isotope i and $\sigma^g_{\text{strd},i}$ is the `STRD` cross section of isotope i in energy group g. The sum is performed over *all* isotopes present in the mixture. The `STRD` cross sections for isotope i are defined as

$$\sigma^g_{\text{strd},i} = \frac{1}{(\mu^g)^2} \frac{\langle\phi\rangle_g}{3 \langle(\Sigma_1 - \Sigma_{s1})\mathcal{J}\rangle_g} (\sigma^g_{1,i} - \sigma^g_{s1,i}) \quad \text{if a streaming model is used} \tag{2.5}$$

$$= \frac{1}{(\mu^g)^2} \frac{\langle\phi\rangle^2_g}{3 \langle D\phi\rangle_g \langle(\Sigma_0 - \Sigma_{s1})\phi\rangle_g} (\sigma^g_{0,i} - \sigma^g_{s1,i}) \quad \text{if no streaming model used} \tag{2.6}$$

where

ϕ^g fundamental flux

$\mathcal{J}^g$ fundamental current

μ^g SPH equivalence factor

Σ^g_0 ϕ–weighted macroscopic total cross section of the mixture

Σ^g_1 $\mathcal{J}$–weighted macroscopic total cross section of the mixture

Σ^g_{s1} macroscopic P_1 scattering cross section of the mixture ($\mathcal{J}$–weighted if a streaming model is used; ϕ–weighted if no streaming model used)

D^g diffusion coefficient

$\sigma^g_{0,i}$ ϕ–weighted microscopic total cross section for isotope i

$\sigma^g_{1,i}$ $\mathcal{J}$–weighted microscopic total cross section for isotope i

$\sigma^g_{s1.i}$ microscopic P_1 scattering cross section for isotope i ($\mathcal{J}$–weighted if a streaming model is used; ϕ–weighted if no streaming model used)

On the other hand the so-called directional cross section `STRD⎵X`, `STRD⎵Y` and `STRD⎵Z` are obtained in such a way that

$$D^g_k = \frac{1}{3 \sum\limits_{i} N_i \, \sigma^g_{\text{strd},k,i}} \, ; \quad k = x, \, y \text{ or } z \quad . \tag{2.7}$$

For example, for an isotope with only total and scattering cross sections, we will find the following records on the cross section directory.

Table 21: Example of cross section records

Name	Type	Condition	Units	Comment
NTOTO␣␣␣␣␣␣	$R(G)$		b	The multigroup total cross section σ^g
SIGS00␣␣␣␣␣␣	$R(G)$		b	The isotropic component $(\ell = 1)$ of the multigroup total scattering cross section $\sigma_{0,s}^g$
IJJS00␣␣␣␣␣␣	$I(G)$			Highest energy group number for which the isotropic component of the scattering cross section to group g does not vanishes, h_0^g
IJJS00␣␣␣	$I(G)$			Highest energy group number for which the first order perturbation in the isotropic component of the scattering cross section to group g does not vanishes, $h_{0,1}^g$
NJJS00␣␣␣␣␣␣	$I(G)$			Number of energy groups for which the isotropic component of the scattering cross section to group g does not vanishes, n_0^g
SCAT00␣␣␣␣␣␣	$R(\sum_{g=1}^{G} n_0^g)$		b	Compressed isotropic component of the scattering matrix $\sigma_{0,c}^k$
SIGS01␣␣␣␣␣␣	$R(G)$		b	The linearly anisotropic component $(\ell = 1)$ of the multigroup total scattering cross section $\sigma_{1,s}^g$
IJJS01␣␣␣␣␣␣	$I(G)$			Highest energy group number for which the linearly anisotropic component of the scattering cross section to group g does not vanishes, h_1^g
NJJS01␣␣␣␣␣␣	$I(G)$			Number of energy groups for which the linearly anisotropic component of the scattering cross section to group g does not vanishes, n_1^g
SCAT01␣␣␣␣␣␣	$R(\sum_{g=1}^{G} n_1^g)$		b	Compressed linearly anisotropic component of the scattering matrix $\sigma_{1,c}^k$

Note that most of these cross sections are not required to perform a cell calculation. In fact, in a typical transport calculation, only σ^g, σ_{tc}^g, $\nu\sigma_f^g$, χ^g and the isotropic and linearly anisotropic scattering matrix are used. For burnup calculations, depending on the depletion chain prescribed, the following cross sections may be required: σ_f^g, σ_c^g, $\sigma_{(n,2n)}^g$, $\sigma_{(n,3n)}^g$, $\sigma_{(n,4n)}^g$, $\sigma_{(n,p)}^g$, $\sigma_{(n,\alpha)}^g$. Finally, when editing isotopic cross sections, all the cross sections types in the library will be processed.

A final note on the use of the transport correction and the homogenized and directional transport cross section. In DARGON, the transport correction cross section is used to correct the total and isotropic scattering cross section using the relations

$$\sigma_c^g = \sigma^g - \sigma_{tc}^g$$
$$\sigma_{c,0}^{g\to g} = \sigma_0^{g\to g} - \sigma_{tc}^g$$

2.9.1 The probability table directory `PT-PHYS` in /isotope/

Physical probability tables ($I_{\text{proc}} = 1$) are obtained from a least-square fit of the self-shielded cross sections against dilution. Mathematical probability tables ($I_{\text{proc}} \geq 3$) are obtained from Autolib data using the CALENDF formalism.

Table 22: Physical probability tables

Name	Type	Condition	Units	Comment
GROUP␣␣␣␣␣␣␣	Dir(G)			List of energy-group sub-directories. Each component of the list is a directory containing the probability-table information associated with a specific group.
NOR␣␣␣␣␣␣␣␣␣	I(G)			Order n_G of the probability table in each energy group
NDEL␣␣␣␣␣␣␣␣	I(1)			Number of delayed neutron precursor groups for this resonant isotope

Table 23: Group-dependent probability table directories

Name	Type	Condition	Units	Comment
PROB-TABLE␣␣	R($12, N_{\mathrm{react}}$)			Probability tables. N_{react} is the total number of reactions represented by probability tables. 12 is the maximum allowed order of a probability table.
SIGQT-SIGS␣␣	R(n_g)	$I_{\mathrm{proc}} = 4$	b	Probability table in secondary slowing-down cross section.
SIGQT-SLOW␣␣	R(n_g, n_g)	$I_{\mathrm{proc}} = 4$	b	Slowing-down correlated weight matrix.
{*/isotope/*}	R(n_g, m_g)	*	1	Set of records, each containing the correlated weights between the current total xs and the total xs of *isotope*. m_g is the order of the probability table for *isotope*. (*) This data is optional and is provided only if $I_{\mathrm{proc}} \geq 3$ and if the mutual self-shielding effect is to be taken into account.
ISM-LIMITS␣␣	I($2, L$)			Minimum (index 1) and maximum (index 2) secondary group for each Legendre order of the scattering matrices

3 Contents of a /geometry/ directory

The `L_GEOM` specification is used to store structured geometric data, i.e., data characterized by some regularity in space. Sub-geometries can be embedded at specific node positions to build a more complex geometry. The following regular geometries can be described with the `L_GEOM` specification:

- Cartesian geometries in 1D, 2D and 3D

- Cylindrical geometries in 1D and 2D ($R - Z$ or $R - \theta$)

- Spherical geometries in 1D

- Hexagonal geometries in 2D/3D

- Various types of cells in 2D/3D Cartesian or hexagonal geometry

- Cells with clusters of fuel rods

- Various synthetic geometries (Do-it-yourself Apollo1 assembly and double-heterogeneity).

This directory contains a compact description of a geometry.

3.1 State vector content for the /geometry/ data structure

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}^G$, represent:

- The type of of geometry $F_t = \mathcal{S}_1^G$

$$
F_t = \begin{cases}
0 & \text{Virtual geometry} \\
1 & \text{Homogeneous geometry} \\
2 & \text{Cartesian 1-D geometry} \\
3 & \text{Tube 1-D geometry} \\
4 & \text{Sphere 1-D geometry} \\
5 & \text{Cartesian 2-D geometry} \\
6 & \text{Tube (R-Z) geometry} \\
7 & \text{Cartesian 3-D geometry} \\
8 & \text{Hexagonal 2-D geometry} \\
9 & \text{Hexagonal 3-D geometry} \\
10 & \text{Tube (R-X) geometry} \\
11 & \text{Tube (R-Y) geometry} \\
12 & \text{hexagonal 2–D geometry with triangular mesh} \\
13 & \text{z-directed hexagonal 3–D geometry with triangular mesh} \\
15 & \text{Tube (R-θ) 2-D geometry} \\
16 & \text{Triangular 2-D geometry} \\
17 & \text{Triangular 3-D geometry} \\
20 & \text{Cartesian 2-D geometry with annular sub-mesh} \\
21 & \text{Cartesian 3-D geometry with $x-$directed cylindrical sub-mesh} \\
22 & \text{Cartesian 3-D geometry with $y-$directed cylindrical sub-mesh} \\
23 & \text{Cartesian 3-D geometry with $z-$directed cylindrical sub-mesh} \\
24 & \text{Hexagonal 2-D geometry with annular sub-mesh} \\
25 & \text{Hexagonal 3-D geometry with $z-$directed cylindrical sub-mesh} \\
30 & \text{Do-it-yourself geometry}
\end{cases}
$$

- The number of annular or cylindric mesh intervals in the geometry $N_r = \mathcal{S}_2^G$

- The number of $x-$directed mesh intervals, hexagon or triangles in the geometry $N_x = \mathcal{S}_3^G$

- The number of $y-$directed mesh intervals in the geometry $N_y = \mathcal{S}_4^G$

- The number of $z-$directed mesh intervals in the geometry $N_z = \mathcal{S}_5^G$

- The total number of mesh intervals in the geometry $N_k = \mathcal{S}_6^G$

  - for $F_t =0$ or 1, $N_k = 1$;
  - for $F_t =2$, 5 or 7, $N_k = \max(N_x, 1) \times \max(N_y, 1) \times \max(N_z, 1)$;
  - for $F_t =3$, 6, 10 or 11, $N_k = N_r \times \max(N_x, 1) \times \max(N_y, 1) \times \max(N_z, 1)$
  - for $F_t =4$, $N_k = N_r$;
  - for $F_t =8$ or 9, $N_k = N_x \times \max(N_z, 1)$;
  - for $F_t =12$ or 13, $N_k = 6 \times N_x^2 \times \max(N_z, 1)$;
  - for $F_t =20$, 21, 22 or 23, $N_k = (N_r + 1) \times \max(N_x, 1) \times \max(N_y, 1) \times \max(N_z, 1)$;
  - for $F_t =24$ or 25, $N_k = (N_r + 1) \times \max(N_z, 1)$.

- The maximum number of mixtures used in this geometry $M_m = \mathcal{S}_7^G$

- The cell flag $F_c = \mathcal{S}_8^G$

$$F_c = \left\{ \begin{array}{ll} 0 & \text{Cell option not activated} \\ 1 & \text{Cell option present} \end{array} \right.$$

- The number of sub-geometries defined in this geometry $F_g = \mathcal{S}_9^G$

- The merge flag $F_m = \mathcal{S}_{10}^G$

$$F_m = \left\{ \begin{array}{ll} 0 & \text{Merge option not activated} \\ 1 & \text{Merge option present} \end{array} \right.$$

- The split flag $F_s = \mathcal{S}_{11}^G$

$$F_s = \left\{ \begin{array}{ll} 0 & \text{Split option not activated} \\ 1 & \text{Split option present} \\ 2 & \text{Split option present. The embedded tubes are not splitted.} \end{array} \right.$$

- The double heterogeneity flag $F_{\mathrm{dh}} = \mathcal{S}_{12}^G$

$$F_{\mathrm{dh}} = \left\{ \begin{array}{ll} 0 & \text{Double heterogeneity option not activated} \\ 1 & \text{Double heterogeneity option present} \end{array} \right.$$

- The number of cluster sub-geometry $N_{\mathrm{cl}} = \mathcal{S}_{13}^G$

- The type of sectorizarion $F_{\mathrm{sec}} = \mathcal{S}_{14}^G$. This information may be given only if $F_t \geq 20$.

$$F_{\mathrm{sec}} = \left\{ \begin{array}{rl} -999 & \text{non-sectorized cell processed as a sectorized cell} \\ -1 & \times\text{--type sectorization} \\ 0 & \text{non-sectorized cell} \\ 1 & +\text{--type sectorization} \\ 2 & \text{simultaneous } \times- \text{ and } +\text{--type sectorization} \\ 3 & \text{simultaneous } \times- \text{ and } +\text{--type sectorization shifted by } 22.5° \\ 4 & \text{windmill-type sectorization.} \end{array} \right.$$

- Number of tubes that are *not* splitted by the sectors if $F_{\text{sec}} \neq 0$. This integer is selected in interval $0 \leq F_{\text{sec2}} \leq N_r$. $F_{\text{sec2}} = \mathcal{S}_{15}^G$.

- The pin location option $\mathcal{S}_{18}^G$. When $\mathcal{S}_{18}^G > 0$, the pin are located according to (r, θ) in 2-D and 3-D (center along the cylinder axis in the cell into which they are inserted) while for $\mathcal{S}_{18}^G < 0$, the pin are located according to (x, y) in 2-D and (x, y, z) in 3-D. A value of $\mathcal{S}_{18}^G = 0$, implies that there is no pin in the geometry.

The radii of a `CARCEL`– or `HEXCEL`–type geometry are defined as shown in the following figure:
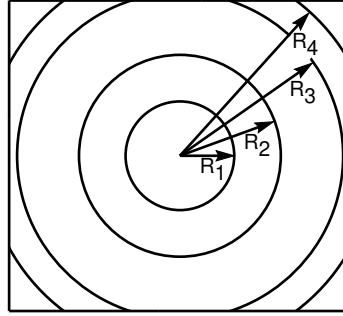
In case where $F_{\text{sec}} \neq 0$, the elementary cell is splitted with sectors. Mixture indices are specific in each splitted region. They are defined as in the following two figures (`isect`$\equiv F_{\text{sec}}$ and `jsect`$\equiv F_{\text{sec2}}$):

isect=-1 jsect=0   isect=-1 jsect=1   isect=-1 jsect=2
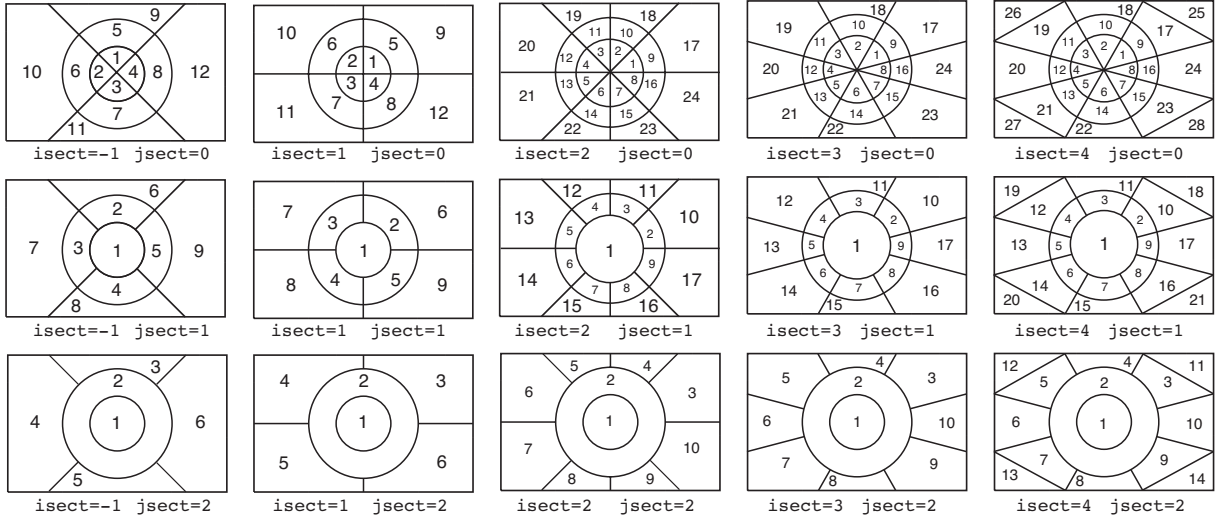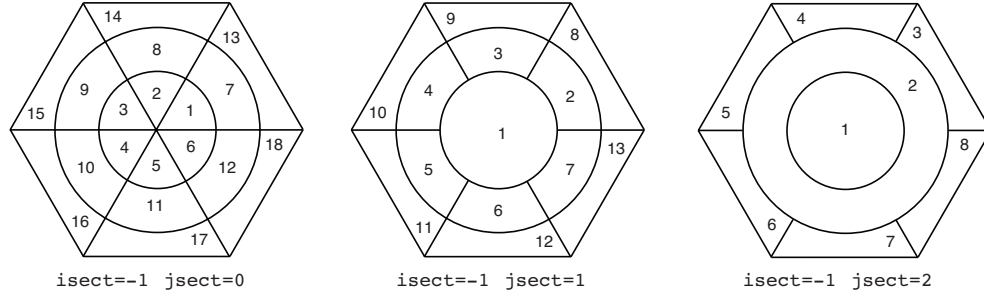
In case of an automatic geometry definition using the `NAP:` module, the number of mixtures corresponding to assembly in the original core definition is named N_{mxa} and the number of assembly along X and Y directions are N_{ax} and N_{ay} respectively.

3.2 The main /geometry/ directory

On its first level, the following records and sub-directories will be found in the /geometry/ directory:

Table 24: Main records and sub-directories in /geometry/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			Signature of the data structure (SIGNA =L␣GEOM␣␣␣␣␣␣)
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^G$, as defined in Section 3.1.
MIX␣␣␣␣␣␣␣␣␣	I(N_k)			Record containing the material mixture index $1 \leq i \leq M_m$ per region (for positive indices) or the sub-geometry index $1 \leq |i| \leq F_g$ per region (for negative indices). MIX(I) is set to zero in voided regions I or in regions located outside the domain.
HMIX␣␣␣␣␣␣␣␣	I(N_k)	∗		array H_i containing the virtual (homogenization) mixtures associated with different regions of the geometry
RADIUS␣␣␣␣␣␣	R($N_r + 1$)	$N_r \geq 1$	cm	The radial mesh R_i position. The first element of this vector is identical to 0.0
OFFCENTER␣␣␣	R(3)	$N_r \geq 1$	cm	The displacement of the center of the annular mesh from the center of a Cartesian cell
MESHX␣␣␣␣␣␣␣	R($N_x + 1$)	$N_x \geq 1$	cm	The $x-$directed mesh position X_i
MESHY␣␣␣␣␣␣␣	R($N_y + 1$)	$N_y \geq 1$	cm	The $y-$directed mesh position Y_i
MESHZ␣␣␣␣␣␣␣	R($N_z + 1$)	$N_z \geq 1$	cm	The $z-$directed mesh position Z_i
SIDE␣␣␣␣␣␣␣␣	R(1)	$8 \leq F_t \leq 11$ $24 \leq F_t \leq 25$	cm	The width of the side of the hexagon H

Main records and sub-directories in /geometry/

Name	Type	Condition	Units	Comment
SPLITR␣␣␣␣␣␣	$I(N_r + 1)$	$F_s \times N_r \geq 1$		Record containing the radial mesh splitting $S_{r,i}$. A negative value permits a splitting into equal sub-volumes; a positive value permits a splitting into equal sub-radius spacings
SPLITX␣␣␣␣␣␣	$I(N_x)$	$F_s \times N_x \geq 1$		Record containing the $x-$directed mesh splitting $S_{x,i}$
SPLITY␣␣␣␣␣␣	$I(N_y)$	$F_s \times N_y \geq 1$		Record containing the $y-$directed mesh splitting $S_{y,i}$
SPLITZ␣␣␣␣␣␣	$I(N_z)$	$F_s \times N_z \geq 1$		Record containing the $z-$directed mesh splitting $S_{z,i}$
SPLITH␣␣␣␣␣␣	$I(1)$	$F_t = 12, 13$		value S_h of the triangular mesh splitting for triangular hexagons in the geometry. This will lead to a spatial triangular mesh spacing of $H_s = H/N_x$
SPLITL␣␣␣␣␣␣	$I(1)$	$F_t = 8, 9$		value S_h of the lozenge mesh splitting for hexagons in the geometry. This will lead to $3\times$SPLITL^2 lozenges per hexagon. If unset, the default value is SPLITL $= 1$.
IHEX␣␣␣␣␣␣␣␣	$I(1)$	$F_t = 8, 9, 12, 13, 24, 25$		The type of hexagonal symmetry β_h
NCODE␣␣␣␣␣␣	$I(6)$			Record containing the types of boundary conditions on each surface $N_{\beta,j}$. NCODE(1): X- or HBC condition; NCODE(2): X+ or R+ condition; NCODE(3): Y- condition; NCODE(4): Y+ condition; NCODE(5): Z- condition; NCODE(6): Z+ condition
ZCODE␣␣␣␣␣␣	$R(6)$			Record containing the albedo value on each surface β_j
ICODE␣␣␣␣␣␣	$I(6)$			Record containing the albedo index on each surface $I_{\beta,j}$. The vector β_j is used only if $I_{\beta,j} > 0$ and $N_{\beta,j} = 6$. In the case where $I_{\beta,j} < 0$ and $N_{\beta,j} = 6$ the vector $\beta_{p,j}$ in the directory /macrolib/ is used
NPIN␣␣␣␣␣␣␣␣	$I(1)$	$|\mathcal{S}_{18}^G| \neq 0$		Number N_{pin} of identical pins in a cluster. All the pins will see identical flux
DPIN␣␣␣␣␣␣␣	$R(1)$	$|\mathcal{S}_{18}^G| \neq 0$	cm^{-3}	Relative density $d_{p,r}$ of pins in a cluster. In this case $N_{\text{pin}} = -1$
RPIN␣␣␣␣␣␣␣	$R(k)$	$\mathcal{S}_{18}^G = 1$	cm	array $R_{\text{pin},j}$ containing the radial positions at which the center of the pins in the cluster are located with respect to the center of the cell $(k = N_{\text{pin}})$. In the case where $R_{\text{pin},j}$ contains a single element $(k = 1)$, it is assumed that the pins are all located at the same radial position $R_{\text{ref}} = R_{\text{pin},1}$

Main records and sub-directories in /geometry/

Name	Type	Condition	Units	Comment
APIN␣␣␣␣␣␣␣␣	$R(k)$	$\mathcal{S}_{18}^G = 1$	rad	array $\theta_{\mathrm{pin},j}$ containing the angular positions at which the center of the pins in the cluster are located with respect to the x, y or z axis respectively for TUBEX, TUBEY and TUBEZ geometry ($k = N_{\mathrm{pin}}$). In the case where $\theta_{\mathrm{pin},j}$ contains a single element ($k = 1$), it is assumed that the first pin is located at $\theta_{\mathrm{ref}} = \theta_{\mathrm{pin},1}$, the remaining pins being located at $\theta_{\mathrm{pin},j} = \theta_{\mathrm{ref}} + 2(j-1)\pi/N_{\mathrm{pin}}$
CPINX␣␣␣␣␣␣␣	$R(N_{\mathrm{pin}})$	$\mathcal{S}_{18}^G = -1$	cm	array $X_{\mathrm{pin},j}$ containing the x positions at which the pins in the cluster are centered with respect to the center of the cell
CPINY␣␣␣␣␣␣␣	$R(N_{\mathrm{pin}})$	$\mathcal{S}_{18}^G = -1$	cm	array $Y_{\mathrm{pin},j}$ containing the y positions at which the pins in the cluster are centered with respect to the center of the cell
CPINZ␣␣␣␣␣␣␣	$R(N_{\mathrm{pin}})$	$\mathcal{S}_{18}^G = -1$	cm	array $Z_{\mathrm{pin},j}$ containing the z positions at which the pins in the cluster are centered with respect to the center of the cell
BIHET␣␣␣␣␣␣␣	Dir	$F_{dh} = 1$		Directory containing double-heterogeneity related data. This directory can only be present on the root directory.
POURCE␣␣␣␣␣␣	$R(\mathcal{S}_3^G)$	$F_t = 30$		The proportion of each cell type in the lattice P_j
PROCEL␣␣␣␣␣␣	$R(\mathcal{S}_3^G, \mathcal{S}_3^G)$	$F_t = 30$		The pre-calculated probability for a neutron leaving a cell of type i to enter in a cell of type j without crossing any other cell $P_{i,j}$
CELL␣␣␣␣␣␣␣␣	$C(F_g) * 12$	$F_c = 1$		The names of the sub-geometries (CELL$_k$)
MERGE␣␣␣␣␣␣␣	$I(N_k)$	$F_m = 1$		The merging index corresponding to each region $G_{m,i}$
TURN␣␣␣␣␣␣␣␣	$I(N_k)$	$F_c = 1$		The orientation index corresponding to each region $G_{t,i}$. Negative values are used to turn a cell in the Z direction.
CLUSTER␣␣␣␣␣	$C(F_{cl}) * 12$	$F_{cl} \geq 1$		The names of the sub-geometries making up the cluster (CLUSTER$_k$)
{/subgeo/}	Dir	$F_g \geq 1$		Set of sub-directories containing a subgeometry
MIX-NAMES␣␣␣	$C(M_m) * 12$	*		The names of the mixtures
A-NX␣␣␣␣␣␣␣␣	$I(N_{ay})$			Number of assemblies on each row
A-IBX␣␣␣␣␣␣␣	$I(N_{ay})$			Position of the first assembly on each row
A-ZONE␣␣␣␣␣␣	$I(N_{ch})$			Number of the assembly associated with each channel. Each assembly may be represented by several channels if they have been heterogeneously homogenized.
A-NMIXP␣␣␣␣␣	$I(1)$			The number of mixtures in one heterogeneously homogenized assembly. N_{mxp}. Note for homogeneously homogenized assembly $N_{mxp} = 1$.

In the case where a cylindrical correction is applied over a full–core Cartesian calculation, the following additional data is provided. It is provided if and only if type 20 (CYLI) boundary conditions are set in

the X–Y plane (see Figure 2).
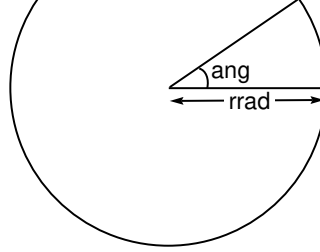
Figure 2: Cylindrical correction in Cartesian geometry

Table 25: Cylindrical correction related records in /geometry/

Name	Type	Condition	Units	Comment
XRO␣␣␣␣␣␣␣␣␣	R(N_{cyl})		cm	Record containing the coordinate of the Z axis from which the cylindrical correction is applied to Cartesian geometries. N_{cyl} is the number of radii.
RRO␣␣␣␣␣␣␣␣␣	R(N_{cyl})		cm	Record containing the radius of the real cylindrical boundary (rrad).
ANG␣␣␣␣␣␣␣␣␣	R(N_{cyl})		1	Record containing the angle (in radian) of the cylindrical notch. ang(ir) $= \frac{\pi}{2}$ by default (i.e. the correction is applied at every angle).

The type of hexagonal symmetry β_h is defined as:

$$\beta_h = \begin{cases} 1 & \text{S30} \\ 2 & \text{SA60} \\ 3 & \text{SB60} \\ 4 & \text{S90} \\ 5 & \text{R120} \\ 6 & \text{R180} \\ 7 & \text{SA180} \\ 8 & \text{SB180} \\ 9 & \text{COMPLETE} \end{cases}$$

S30, SA60 and COMPLETE symmetries are depicted in the following figures. The other types of hexagonal symmetries are defined in the DRAGON users guide.[1]

S30

$\frac{C}{L}$

SA60

$\frac{C}{L}$

$\frac{C}{L}$

$\frac{C}{L}$

$\frac{C}{L}$

COMPLETE
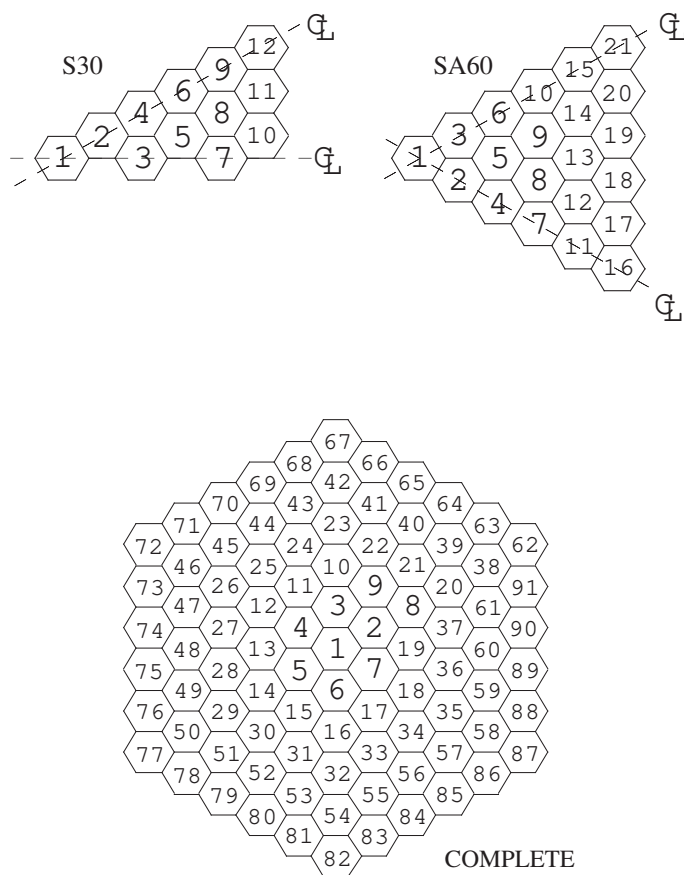
NCODE is a record containing the types of boundary conditions on each surface. In Cartesian geometry, the 6 components of NCODE are related to sides X-, X+, Y-, Y+, Z- and Z+, respectively. The possibilities

are:

$$
N_{\beta,j} = \begin{cases}
\end{cases}
$$

0   side not used

1   `VOID`: zero re-entrant angular flux. This side is an external surface of the domain.

2   `REFL`: reflection boundary condition. In most DRAGON calculations, this implies white boundary conditions. In DRAGON the cell is never unfolded to take into account a REFL boundary condition.

3   `DIAG`: diagonal boundary condition. The side under consideration has the same properties as that associated with a diagonal through the geometry. Note that two and only two `DIAG` sides must be specified. The diagonal symmetry is only permitted for square geometry and in the following combinations: (`X+` and `Y-`) or (`X-` and `Y+`)

4   `TRAN`: translation boundary condition. The side under consideration is connected to the opposite side of a Cartesian domain. This option provides the facility to treat an infinite geometry with translation symmetry. The only combinations of translational symmetry permitted are related to sides (`X-` and `X+`) and/or (`Y-` and `Y+`) and/or (`Z-` and `Z+`).

5   `SYME`: symmetric reflection boundary condition. The side under consideration is located outside the domain and that a reflection symmetry is associated with the adequately directed axis running through the center of the cells closest to this side.

6   `ALBE`: albedo boundary condition. The side under consideration has an arbitrary albedo with a real value given in the record '`ZCODE`' or indexed by the record '`ICODE`'. This side is an external surface of the domain.

7   `ZERO`: zero flux boundary condition. This side is an external surface of the domain.

8   `PI/2`: $\pi/2$ rotation. The side under consideration is characterized by a $\pi/2$ symmetry. The only $\pi/2$ symmetry permitted is related to sides (`X-` and `Y-`). This condition can be combined with a translation boundary condition:(`PI/2 X- TRAN X+`) and/or (`PI/2 Y- TRAN Y+`).

9   `PI`: π rotation

10   `SSYM`: specular relexion boundary condition. Such a condition may be obtained by unfolding the geometry.

20   `CYLI`: use a cylindrical correction in full–core Cartesian geometry

In cylindrical geometry, the 3 components of `NCODE` are related to sides `R+`, `Z-` and `Z+`, respectively. The possibilities are: `VOID`, `REFL`, `ALBE` and/or `ZERO`.

In hexagonal geometry, the 3 components of `NCODE` are related to sides `H+` (the surface surrounding the hexagonal domain in the X–Y plane), `Z-` and `Z+`, respectively. The possibilities are: `VOID`, `REFL`, `SYME`, `ALBE` and/or `ZERO`.

We will now describe the exact meaning of the orientation index $G_{t,i}$. For Cartesian geometries, the eight possible orientations are shown in the following figure:
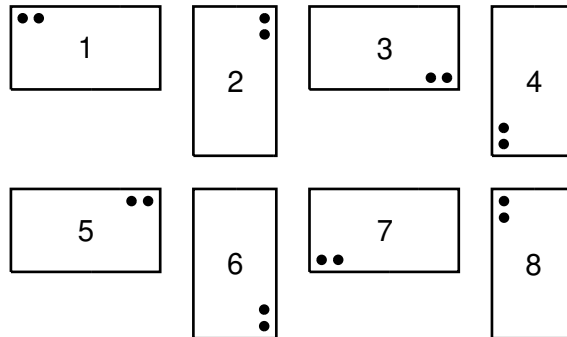
For hexagonal geometries, the twelve possible orientations are shown in the following figure:
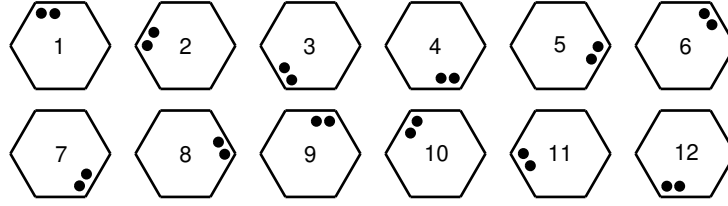
In the case where $F_c = 1$, the set of directory {/subgeo/} will have the same name as the variable CELL$_k$. For example, in the case where $F_g = 2$ and

$$\text{CELL}_k = \begin{cases} \text{GEO1} & \text{for} \quad k = 1 \\ \text{GEO2} & \text{for} \quad k = 2 \end{cases}$$

then the following directories will also be present in the main geometry directory:

Table 26: Cell sub-geometry directory

Name	Type	Condition	Units	Comment
GEO1␣␣␣␣␣␣␣␣	Dir			A first /geometry/ directory
GEO2␣␣␣␣␣␣␣␣	Dir			A second /geometry/ directory

In the case where $F_{cl} \geq 1$, the set of directory {/subgeo/} will have the same name as the variable CLUSTER$_k$. For example, in the case where $F_{cl} = 2$ and

$$\text{CLUSTER}_k = \begin{cases} \text{RODS1} & \text{for} \quad k = 1 \\ \text{RODS2} & \text{for} \quad k = 2 \end{cases}$$

then the following directories will also be present in the main geometry directory:

Table 27: Cluster sub-geometry directory

Name	Type	Condition	Units	Comment
RODS1␣␣␣␣␣␣␣	Dir	$F_g \geq 1$		A first /geometry/ directory
RODS2␣␣␣␣␣␣␣	Dir	$F_g \geq 1$		A second /geometry/ directory

3.3 The /BIHET/ sub-directory in /geometry/

The first level of the geometry directory may contains a double-heterogeneity directory /BIHET/ made of the following records:

Table 28: Records in the `/BIHET/` sub-directory

Name	Type	Condition	Units	Comment
`STATE-VECTOR`	$I(40)$			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^{dh}$
`NS`␣␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_1^{dh})$			The number of sub-regions in the micro-structures $N_{\mathrm{micro},i}$
`RS`␣␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_2^{dh}, \mathcal{S}_1^{dh})$		cm	The radii of the tubes or spherical shells making up the micro-structures $R_{\mathrm{micro},i,j}$
`MILIE`␣␣␣␣␣␣	$I(\mathcal{S}_3^{dh})$			The composite mixture indices used in the definition of the macro-geometry $C_{\mathrm{micro},i,j}$
`MIXDIL`␣␣␣␣␣	$I(\mathcal{S}_3^{dh})$			The mixture indices associated with the diluent in each composite mixtures of the macro-geometry $D_{\mathrm{micro},i,j}$
`MIXGR`␣␣␣␣␣␣	$I(\mathcal{S}_4^{dh}, \mathcal{S}_3^{dh})$			The mixture indices associated with each region of the micro-structures $M_{\mathrm{micro},i,j}$
`FRACT`␣␣␣␣␣␣	$R(\mathcal{S}_1^{dh}, \mathcal{S}_3^{dh})$			The volumetric concentration of each micro-structure $\rho_{\mathrm{micro},i,j}$

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}^{bh}$, represent:

- The number of different kinds of macro-structures $\mathcal{S}_1^{dh}$

- 1 plus the maximum number of annular sub-regions in any micro-structure $\mathcal{S}_2^{dh}$

- The number of composite mixtures to be included the macro-geometry $\mathcal{S}_3^{dh}$

- The maximum number of annular sub-regions in the micro-structure $\mathcal{S}_4^{dh} = (\mathcal{S}_2^{dh} - 1) \times \mathcal{S}_1^{dh}$

- The type of micro-structure $\mathcal{S}_5^{dh}$ where

$$\mathcal{S}_5^{dh} = \left\{ \begin{array}{ll} 3 & \text{Tubular micro-structure} \\ 4 & \text{Spherical micro-structure} \end{array} \right.$$

4 Contents of a /tracking/ directory

This directory contains the information resulting from an analysis of a geometry using a specific calculation operator of DRAGON.

4.1 State vector content for the /tracking/ data structure

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}$, represent:

- The number of regions $N_r = \mathcal{S}_1^t$

- The number of unknown $N_u = \mathcal{S}_2^t$

- The leakage flag $I_L = \mathcal{S}_3^t$

$$I_L = \left\{ \begin{array}{ll} 0 & \text{Leakage is present} \\ 1 & \text{Leakage is absent} \end{array} \right.$$

- The maximum number of mixture used $M_m = \mathcal{S}_4^t$

- The number of outer surfaces $N_s = \mathcal{S}_5^t$

- Flag related to the double-heterogeneity option $\mathcal{S}_{40}^t$ where

$$\mathcal{S}_{40}^t = \left\{ \begin{array}{ll} 0 & \text{the double-heterogeneity option is not used} \\ 1 & \text{the double-heterogeneity option is used.} \end{array} \right.$$

4.2 The main /tracking/ directory

On its first level, the following records and sub-directories will be found in the /tracking/ directory:

Table 29: Main records and sub-directories in /tracking/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			Signature of the data structure (SIGNA =L␣TRACK␣␣␣␣␣).
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^t$, as defined in Section 4.1.
TRACK-TYPE␣␣	C∗12			Type of tracking considered (CDOOR). Allowed values are: 'EXCELL', 'SYBIL', 'MCCG', 'SN', 'BIVAC' and 'TRIVAC'.
LINK.GEOM␣␣␣	C∗12			Name of the GEOMETRY on which the tracking is based.
TITLE␣␣␣␣␣␣␣	C∗72			Identification title (TITLE)
MATCOD␣␣␣␣␣␣	I($\mathcal{S}_1^t$)			Region material M_r
KEYFLX␣␣␣␣␣␣	I($\mathcal{S}_1^t$)			Location in unknown vector of averaged regional flux I_r
VOLUME␣␣␣␣␣␣	R($\mathcal{S}_1^t$)		cm^3	Region volumes V_r

Name	Type	Condition	Units	Comment
`BC-REFL+TRAN`	$I(\mathcal{S}_5^t)$	$\mathcal{S}_5^t \geq 1$		Reflection/transmission matrix localisation operator T_s
`FUNC-TABLES`␣	Dir	*		Directory containing Bickey or/and exponential function tables.
`BIHET`␣␣␣␣␣␣␣␣	Dir	$\mathcal{S}_{40}^t = 1$		Sub-directory containing the data related to a double heterogeneity geometry. The specification of this directory is given in Section 4.9

In addition to the above records, the main /tracking/ directory will also contain information which is specific to each tracking module. This information will be described in the following sub-sections. Also note that the contents of the $\mathcal{S}_i^t$ vector for $i \geq 6$ will depend on the specific tracking module and will be defined in the next sub-sections.

4.3 The `sybilt` dependent records and sub-directories on a /tracking/ directory

When the `SYBILT:` operator is used (`CDOOR='SYBIL'`), the following elements in the vector $\mathcal{S}_i^t$ will also be defined.

- The main SYBIL model $\mathcal{S}_6^t$

$$\mathcal{S}_6^t = \left\{ \begin{array}{ll} 2 & \text{Pure geometry} \\ 3 & \text{Do-it-yourself geometry} \\ 4 & \text{2-D assembly geometry} \end{array} \right.$$

- Minimum space required to store tracks for assembly geometry $\mathcal{S}_7^t$

- Minimum space required to store interface currents for assembly geometry $\mathcal{S}_8^t$

- Number of additional unknowns holding the interface currents $\mathcal{S}_9^t$. These unknowns are used if and only if a current–based inner iterative method is set (with option `ARM`).

The following sub-directories will also be present on the main level of a /tracking/ directory.

Table 30: The `sybilt` records and sub-directories in /tracking/

Name	Type	Condition	Units	Comment
`EPSJ`␣␣␣␣␣␣␣␣	R(1)		1	Stopping criterion for flux-current iterations of the interface current method
`PURE-GEOM`␣␣␣	Dir	$\mathcal{S}_6^t = 2$		Sub-directory containing the data related to a pure geometry
`DOITYOURSELF`	Dir	$\mathcal{S}_6^t = 3$		Sub-directory containing the data related to a do-it-yourself geometry
`EURYDICE`␣␣␣␣	Dir	$\mathcal{S}_6^t = 4$		Sub-directory containing the data related to an assembly geometry

where the sub-directories in Table 30 are described in the following subsections.

4.3.1 The /PURE-GEOM/ sub-directory in `sybilt`

Table 31: The contents of the `sybilt` /PURE-GEOM/ sub-directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣`	I(6)			Record containing the parameters for a SYBIL tracking on a pure geometry $\mathcal{P}_i$
`NCODE␣␣␣␣␣␣␣`	I(6)			Record containing the types of boundary conditions on each surface $N_{\beta,j}$
`ZCODE␣␣␣␣␣␣␣`	R(6)		1	Record containing the albedo value on each surface
`XXX␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_4 + 1$)	$\mathcal{P}_4 \geq 1$	cm	$x-$directed mesh coordinates after mesh-splitting for type 2, 5 and 7 geometries. Region-ordered radius after mesh-splitting for type 3 and 6 geometries
`YYY␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_5 + 1$)	$\mathcal{P}_5 \geq 1$	cm	$y-$directed mesh coordinates after mesh-splitting for type 5, 6 and 7 geometries
`ZZZ␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_6 + 1$)	$\mathcal{P}_6 \geq 1$	cm	$z-$directed mesh coordinates after mesh-splitting for type 7 and 9 geometries
`SIDE␣␣␣␣␣␣␣␣`	R(1)	$\mathcal{P}_1 \geq 8$	cm	Side of a hexagon for type 8 and 9 geometries

with the dimension parameter $\mathcal{P}_i$, representing:

- The type of geometry $\mathcal{P}_1$

$$
\mathcal{P}_1 = \begin{cases}
2 & \text{Cartesian 1-D geometry} \\
3 & \text{Tube 1-D geometry} \\
4 & \text{Spherical 1-D geometry} \\
5 & \text{Cartesian 2-D geometry} \\
6 & \text{Tube 2-D geometry} \\
7 & \text{Cartesian 3-D geometry} \\
8 & \text{Hexagonal 2-D geometry} \\
9 & \text{Hexagonal 3-D geometry}
\end{cases}
$$

- The type of hexagonal symmetry $\beta_h = \mathcal{P}_2$

$$
\beta_h = \begin{cases}
1 & \text{S30} \\
2 & \text{SA60} \\
3 & \text{SB60} \\
4 & \text{S90} \\
5 & \text{R120} \\
6 & \text{R180} \\
7 & \text{SA180} \\
8 & \text{SB180} \\
9 & \text{COMPLETE}
\end{cases}
$$

- The quadrature parameter $\mathcal{P}_3$

- The number of $x-$directed or radial mesh intervals in the geometry $\mathcal{P}_4$

- The number of $y-$directed mesh intervals in the geometry $\mathcal{P}_5$

- The number of $z-$directed mesh intervals in the geometry $\mathcal{P}_6$

The type of boundary conditions used will be defined in the following way

$$N_{\beta,j} = \begin{cases} 0 & \text{Not used} \\ 1 & \text{Void boundary condition} \\ 2 & \text{Reflection boundary condition} \\ 3 & \text{Diagonal reflection boundary condition} \\ 4 & \text{Translation boundary condition condition} \\ 5 & \text{Symmetric reflection boundary condition} \\ 6 & \text{Albedo boundary condition} \end{cases}$$

4.3.2 The `/DOITYOURSELF/` sub-directory in `sybilt`

Table 32: The contents of the `sybilt /DOITYOURSELF/` sub-directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣`	I(3)			Record containing the parameters for a SYBIL tracking on a do-it-yourself geometry $\mathcal{P}_i$
`NMC␣␣␣␣␣␣␣␣␣`	I($M+1$)			Offset of the first region in each cell
`RAYRE␣␣␣␣␣␣␣`	R($N_r + M$)		cm	Radius of the tubes in each cell
`PROCEL␣␣␣␣␣␣`	R(M, M)			Geometric matrix
`POURCE␣␣␣␣␣␣`	R(M)			Weight assigned to each cell
`SURFA␣␣␣␣␣␣␣`	R(M)		cm^2	Surface of each cell

with the dimension parameter $\mathcal{P}_i$, representing:

- The number of cells $\mathcal{P}_1 = M$

- The quadrature parameter $\mathcal{P}_2$

- The statistical option $\mathcal{P}_3$

$$\mathcal{P}_3 = \begin{cases} 0 & \text{the statistical approximation is not used. Record 'PROCEL' is used.} \\ 1 & \text{use the statistical approximation. Record 'PROCEL' is not used.} \end{cases}$$

4.3.3 The /EURYDICE/ sub-directory in `sybilt`

Table 33: The contents of the `sybilt` /EURYDICE/ sub-directory

Name	Type	Condition	Units	Comment
`PARAM`␣␣␣␣␣␣␣	I(16)			Record containing the parameters for a SYBIL tracking on an assembly geometry $\mathcal{P}_i$
`XX`␣␣␣␣␣␣␣␣␣␣␣	R($\mathcal{P}_6$)		cm	$x-$thickness of the generating cells
`YY`␣␣␣␣␣␣␣␣␣␣␣	R($\mathcal{P}_6$)		cm	$y-$thickness of the generating cells
`LSECT`␣␣␣␣␣␣␣	I($\mathcal{P}_6$)			Type of sectorization for each each generating cell. Equal to zero for non-sectorized cells. Allowed values are defined as F_{sec} in Section 3.2
`NMC`␣␣␣␣␣␣␣␣␣␣	I($\mathcal{P}_6 + 1$)			Offset of the first region index in each generating cell
`NMCR`␣␣␣␣␣␣␣␣	I($\mathcal{P}_6 + 1$)			Offset of the first radius index in each generating cell. Equal to `NMC`, unless the cell is sectorized.
`RAYRE`␣␣␣␣␣␣␣	R(M_r)		cm	Radius of the tubes in each generating cell. $M_r =$`NMCR`($\mathcal{P}_6 + 1$)
`MAIL`␣␣␣␣␣␣␣␣	I(2, $\mathcal{P}_6$)			Offsets of the first tracking information in each generating cell. `MAIL(1,:)` contains offsets for the integer array `ZMAILI`; `MAIL(2,:)` contains offsets for the real array `ZMAILR`.
`ZMAILI`␣␣␣␣␣␣	I($\mathcal{P}_{15}$)			The integer tracking information
`ZMAILR`␣␣␣␣␣␣	R($\mathcal{P}_{16}$)		cm	The tracking lengths
`IFR`␣␣␣␣␣␣␣␣␣␣	I($\mathcal{P}_4$, $\mathcal{P}_{14}$)			Index numbers of incoming currents
`ALB`␣␣␣␣␣␣␣␣␣␣	R($\mathcal{P}_4$, $\mathcal{P}_{14}$)			Albedo or transmission factors corresponding to incoming currents
`INUM`␣␣␣␣␣␣␣␣	I($\mathcal{P}_4$)			Index number of the merge cell associated to each cell of the assembly
`MIX`␣␣␣␣␣␣␣␣␣␣	I($\mathcal{P}_5$, $\mathcal{P}_{14}$)			Index numbers of outgoing currents
`DVX`␣␣␣␣␣␣␣␣␣␣	R($\mathcal{P}_5$, $\mathcal{P}_{14}$)			Weights corresponding to outgoing currents
`IGEN`␣␣␣␣␣␣␣␣	I($\mathcal{P}_5$)			Index number of the generating cell associated to each merged cell

with the dimension parameter $\mathcal{P}_i$, representing:

- The type of hexagonal symmetry $\mathcal{P}_1$

$$\mathcal{P}_1 = \begin{cases} 0 & \text{Cartesian assembly} \\ 1 & \text{S30} \\ 2 & \text{SA60} \\ 3 & \text{SB60} \\ 4 & \text{S90} \\ 5 & \text{R120} \\ 6 & \text{R180} \\ 7 & \text{SA180} \\ 8 & \text{SB180} \\ 9 & \text{COMPLETE} \end{cases}$$

- The type of multicell approximation $\mathcal{P}_2$

$$\mathcal{P}_2 = \begin{cases} 1 & \text{Roth approximation} \\ 2 & \text{Roth} \times 4 \text{ or Roth} \times 6 \text{ approximation} \\ 3 & \text{DP-0 approximation} \\ 4 & \text{DP-1 approximation} \end{cases}$$

- The type of cylinderization $\mathcal{P}_3$

$$\mathcal{P}_3 = \begin{cases} 1 & \text{Askew cylinderization} \\ 2 & \text{Wigner cylinderization} \\ 3 & \text{Sanchez cylinderization} \end{cases}$$

- The total number of cells $\mathcal{P}_4$

- The number of merged cells $\mathcal{P}_5$

- The number of generating cells $\mathcal{P}_6$

- The number of distinct interface currents $\mathcal{P}_7$

- The number of angles for 2-D quadrature $\mathcal{P}_8$

- The number of segments for 2-D quadrature $\mathcal{P}_9$

- The number of segments for homogeneous 2-D cells $\mathcal{P}_{10}$

- The number of segments for 1-D cells $\mathcal{P}_{11}$

- The track normalization option $\mathcal{P}_{12}$

$$\mathcal{P}_{12} = \begin{cases} 0 & \text{Normalize the tracks} \\ 1 & \text{Do not normalize the tracks} \end{cases}$$

- The type of quadrature in angle and space $\mathcal{P}_{13}$

$$\mathcal{P}_{13} = \begin{cases} 0 & \text{Gauss quadrature} \\ 1 & \text{Equal weight quadrature} \end{cases}$$

- The number of outgoing interface currents per cell $\mathcal{P}_{14}$

- The number of integer array elements in the tracking arrays $\mathcal{P}_{15}$

- The number of real array elements in the tracking arrays $\mathcal{P}_{16}$

4.4 The `excelt` dependent records on a /tracking/ directory

When the `EXCELT:` modules is used (`CDOOR='EXCELL'`), the following elements in the vector $\mathcal{S}_i^t$ will also be defined.

- $\mathcal{S}_6^t$ is the number of Legendre orders used for the flux expansions, where

$$\mathcal{S}_6^t = \begin{cases} 1 & \text{isotropic} \\ 2 & \text{linearly anisotropic.} \end{cases}$$

- $\mathcal{S}_7^t$ is the specific EXCELL tracking procedure considered where

$$\mathcal{S}_7^t = \begin{cases} 1 & \text{Cartesian 2D/3D assembly using } \texttt{EXCELT:} \\ 2 & \text{hexagonal 2D/3D assembly using } \texttt{EXCELT:} \\ 3 & \text{2D cluster geometry using } \texttt{EXCELT:} \\ 4 & \text{2D and 3D Cartesian assemblies with clusters using } \texttt{NXT:}. \end{cases}$$

- $\mathcal{S}_8^t$ is the track normalization flag where

$$\mathcal{S}_8^t = \begin{cases} -1 & \text{direction dependent track normalization to exact volumes;} \\ 0 & \text{global track normalization to exact volumes;} \\ 1 & \text{no normalization.} \end{cases}$$

- $\mathcal{S}_9^t$ is the tracking type where

$$\mathcal{S}_9^t = \begin{cases} 0 & \text{means that a standard tracking procedure was considered } (\texttt{TISO}); \\ 1 & \text{means that a cyclic tracking procedure was considered } (\texttt{TSPC}). \end{cases}$$

- $\mathcal{S}_{10}^t$ is the type of boundary conditions where

$$\mathcal{S}_{10}^t = \begin{cases} 0 & \text{means that isotropic (white) boundary conditions will be considered } (\texttt{PISO}); \\ 1 & \text{means that mirror-like (specular) boundary conditions will be considered } (\texttt{PSPC}). \end{cases}$$

Note that mirror-like boundary conditions ($\mathcal{S}_{10}^t = 1$) can be used only if a cyclic tracking procedure was considered ($\mathcal{S}_9^t = 1$).

- $\mathcal{S}_{11}^t = N_\Omega$ is the order of the azimuthal (2-D) or solid (3-D) angular quadrature. For 2-D geometry, the order of the azimuthal quadrature represents:

  - the number of equal sectors (trapezoidal quadrature) in the $[0, \pi]$ range when the `EXCELT:` module is used for Cartesian assemblies;

  - the number of equal sectors (trapezoidal quadrature) in the $[0, 2\pi/3]$ range when the `EXCELT:` module is used for hexagonal geometries;

  - the number of equal sectors (trapezoidal quadrature) in the $[0, \max(\mathcal{S}_{12}^t, 2)\,\pi]$ range when the `EXCELT:` module is used for cluster geometries;

  - the number of trapezoidal sectors in the $[0, \pi/2]$ range when the `NXT:` module is used.

  For 3-D geometry, the order of the solid angle quadrature is:

  - the order n of the EQ_n quadrature in a quadrant ($0 \le \varphi \le \pi/2$ and $0 \le \theta \le \pi/2$) when the `EXCELT:` module is used for Cartesian assemblies for $N_{\text{dir}} = n(n+2)/8$ direction in each quadrant;

  - the number of equal sectors (trapezoidal quadrature) in the $[0, 2\pi/3]$ range when the `EXCELT:` module is used for hexagonal geometries;

- not used for the `EXCELT:` module in cluster geometries;

- the order n of the EQ_n , LC_n or LT_n quadrature in a quadrant with $0 \leq \varphi \leq \pi/2$ and $0 \leq \theta \leq \pi/2$. When the `NXT:` modules is used, the number N_{dir} of directions for the azimuthal (2-D) or solid (3-D) angle quadrature results in $N_{\mathrm{dir}} = n(n+2)/8$ directions for the EQ_n quadrature, $N_{\mathrm{dir}} = 3n(n+2)/8$ for the LC_n quadrature and $N_{\mathrm{dir}} = 3n^2/2$ for the LT_n quadrature.

- $\mathcal{S}_{12}^t$ is the angular symmetry factor;

- $\mathcal{S}_{13}^t$ is the polar quadrature type:

$$
\mathcal{S}_{13}^t = \begin{cases}
0 & \text{Gauss-Legendre} \\
1 & \text{CACTUS type 1} \\
2 & \text{CACTUS type 2} \\
3 & \text{McDaniel} \\
4 & \text{McDaniel with } P_1 \text{ constraint} \\
5 & \text{Gauss optimized.}
\end{cases}
$$

- $\mathcal{S}_{14}^t$ is the order of the polar quadrature.

- $\mathcal{S}_{15}^t$ is the azimuthal (2-D) or solid (3-D) angle quadrature type where

$$
\mathcal{S}_{15}^t = \begin{cases}
1 & \text{for a } EQ_n \text{ (3-D) or trapezoidal (2-D) quadrature;} \\
2 & \text{for a Gauss quadrature (2-D hexagonal geometries);} \\
3 & \text{for a median angle quadrature;} \\
4 & \text{for a } LC_n \text{ 3-D quadrature;} \\
5 & \text{for a } LT_n \text{ 3-D quadrature;} \\
6 & \text{for a } \mu_1\text{–optimized level-symmetric 3-D quadrature;} \\
7 & \text{for a quadrupole range (QR) 3-D quadrature.}
\end{cases}
$$

- $\mathcal{S}_{16}^t$ is the number of geometric dimensions (1, 2 or 3).

- $\mathcal{S}_{17}^t$ is the number of tracking points on a line.

- $\mathcal{S}_{18}^t$ is the maximum length of a track.

- $\mathcal{S}_{19}^t$ is the total number of tracks generated.

- $\mathcal{S}_{20}^t$ is the total number of track directions processed.

- $\mathcal{S}_{21}^t$ is the line format option for `TLM:` module, where

$$
\mathcal{S}_{21}^t = \begin{cases}
0 & \text{short format} \\
1 & \text{complete format.}
\end{cases}
$$

- $\mathcal{S}_{22}^t$ is the vectorization option for computing collision probability matrices where

$$
\mathcal{S}_{22}^t = \begin{cases}
0 & \text{scalar algorithm. The tracking is readed for each energy group.} \\
1 & \text{vectorial algorithm. The tracking is readed once and the collision probability} \\
  & \text{matrices are computed in many energy groups.} \\
2 & \text{vectorial algorithm of type } \texttt{EXCELL:}. \text{ The tracking is computed in } \texttt{DOORVP} \\
  & \text{and the collision probability matrices are computed in many energy groups.} \\
3 & \text{vectorial algorithm of type } \texttt{NXT:}. \text{ The tracking is computed in } \texttt{DOORVP} \\
  & \text{and the collision probability matrices are computed in many energy groups.}
\end{cases}
$$

- $\mathcal{S}_{23}^t$ is the tracking flag, where

$$\mathcal{S}_{23}^t = \begin{cases} -1 & \text{the LCM object information is used for Monte-Carlo calculations. No} \\ & \text{tracking file produced.} \\ 0 & \text{this option de-activates the tracking file production if \texttt{TISO} or \texttt{TSPC} are} \\ & \text{specified.} \\ 1 & \text{this option produces the tracking file.} \end{cases}$$

- $\mathcal{S}_{39}^t$ is the prismatic tracking activation flag along z axis for 3D geometry (0/3: off/on-z axis).

The following records will also be present on the main level of a /tracking/ directory.

Table 34: The `EXCELT:` records in /tracking/

Name	Type	Condition	Units	Comment
`EXCELTRACKOP`	R(40)			array $\mathcal{R}_i$ containing additional EXCELL or NXT tracking parameters.
`ICODE␣␣␣␣␣␣␣`	I(6)			array $\mathcal{I}_{\beta,k}$ containing the surface albedo index (geometric surface albedo $\beta_{g,k}$ are used if $\mathcal{I}_{\beta,k} < 0$ while physical surface albedo $\beta_{p,k}$ are used if $\mathcal{I}_{\beta,k} > 0$).
`ALBEDO␣␣␣␣␣␣`	R(6)			array $\beta_{g,k}$ containing the geometric surface albedo (used only if $\mathcal{I}_{\beta,k} \geq 0$).
`EXCELL␣␣␣␣␣␣`	Dir	$\mathcal{S}_7^t < 4$		directory containing additional `EXCELT:` records for the cases where $\mathcal{S}_7^t = 1$ or $\mathcal{S}_7^t = 3$.
`NXTRecords␣␣`	Dir	$\mathcal{S}_7^t = 4$		directory containing additional `NXT:` records.
`PROJECTION␣␣`	Dir	$\mathcal{S}_{39}^t > 0$		directory containing the analysis of the projection of a 3D prismatic geometry.

The record $\mathcal{R}_i$ contains the following information:

- $\mathcal{R}_1$ is the maximum error allowed on the exponential function.

- $\mathcal{R}_2$ is the user requested tracking density in cm^{-1} and in cm^{-2} respectively for 2D and 3D calculations.

- $\mathcal{R}_3$ is the maximum distance in cm between an integration line and a surface.

- $\mathcal{R}_4$ is the computed tracking density in cm^{-1} and in cm^{-2} respectively for 2D and 3D calculations (used only if $\mathcal{S}_7^t = 4$).

- $\mathcal{R}_5$ is the computed line spacing in cm (used only if $\mathcal{S}_7^t = 4$).

- $\mathcal{R}_6$ is the weight of the spatial quadrature (used only if $\mathcal{S}_7^t = 4$).

- $\mathcal{R}_7$ is the minimal radius of the circle (2-D) or sphere (3-D) containing the geometry (used only if $\mathcal{S}_7^t = 4$).

- $\mathcal{R}_8$ is the x position of the center of the minimal circle (2-D) or sphere (3-D) containing the geometry (used only if $\mathcal{S}_7^t = 4$).

- $\mathcal{R}_9$ is the y position of the center of the minimal circle (2-D) or sphere (3-D) containing the geometry (used only if $\mathcal{S}_7^t = 4$).

- $\mathcal{R}_{10}$ is the z position of the center of the minimal circle (2-D) or sphere (3-D) containing the geometry (used only if $\mathcal{S}_7^t = 4$).

- $\mathcal{R}_{40}$ user requested tracking density in cm^{-1} for inline contruction of 3D tracks when a prismatic tracking is considered (only used if $\mathcal{S}_{39}^t > 0$).

The /NXTRecords/ directory contains the information required to track the geometry using the NXT: module module once it has been analyzed. The contents of this directory is presented in Table 35.

Table 35: Global geometry records in /NXTRecords/

Name	Type	Condition	Units	Comment
G00000001DIM	I(40)			array N_i^{GG} containing the dimensioning information required to rebuilt the assembly
G00000001CUF	I$(2, N_5^{\mathrm{GG}})$			array $D_{i,j}^{\mathrm{GG}}$ containing the assembly description of the geometry in terms of cells and rotations. The first element $(i = 1)$ identifies the cell number while the second element identifies the cell rotation
G00000001CIS	I$(4, N_4^{\mathrm{GG}})$			array $S_{i,j}^{\mathrm{GG}}$ containing the cell intrinsic symmetry properties. A value of 1 indicates that a center cell reflexion symmetry is present while a value of 0 indicates that the symmetry is not considered (see below for a more complete description of this array)
G00000001CFE	I$(0:8, N_4^{\mathrm{GG}})$			array $F_{i,j}^{\mathrm{GG}}$ containing the assembly external surface identification index (see below for a more complete description of this array)
G00000001SMX	D$(0 : N_{13}^{\mathrm{GG}})$		cm	array x^{GG} containing the x-directed mesh for the cell assembly in a Cartesian or Cylindrical geometry and the x position of the cell center for an hexagonal assembly (see below for more explanations)
G00000001SMY	D$(0 : N_{14}^{\mathrm{GG}})$		cm	array y^{GG} containing the y-directed mesh for the cell assembly in a Cartesian or Cylindrical geometry and the y position of the cell center for an hexagonal assembly (see below for more explanations)
G00000001SMZ	D$(0 : N_{15}^{\mathrm{GG}})$	$N_1^{\mathrm{GG}} = 3$	cm	array z^{GG} containing the z-directed mesh for the cell assembly (see below for more explanations)
G00000001SMR	D$(0 : 1)$	$N_2^{\mathrm{GG}} = 1$	cm	the radius r^{GG} of the outer assembly boundary (see below for more explanations)
KEYMRG␣␣␣␣␣␣	I$(-N_{23}^{\mathrm{GG}} : N_{22}^{\mathrm{GG}})$			array MRG_i containing the merged surface and region number associated with each individual surfaces and regions in this geometry
MATALB␣␣␣␣␣␣	I$(-N_{23}^{\mathrm{GG}} : N_{22}^{\mathrm{GG}})$			array containing the albedo number associated with each surface and the physical mixture number associated with each region in this geometry

Global geometry records in `/NXTRecords/`

Name	Type	Condition	UnitsComment
`HOMMATALB␣␣␣`	$I(-N_{23}^{\mathrm{GG}} : N_{22}^{\mathrm{GG}})$		array containing the albedo number associated with each surface and the virtual (homogenization) mixture number associated with each region in this geometry
`SAreaRvolume`	$D(-N_{23}^{\mathrm{GG}} : N_{22}^{\mathrm{GG}})$		array containing the area (S_α in cm for 2-D and cm^2 for 3-D problems) and volume (V_i cm^2 for 2-D and cm^3 for 3-D problems) associated with each surface and region in this geometry

The dimensioning vector for the global geometry contains the following information:

- N_1^{GG} number of dimensions for the problem.

- N_2^{GG} type of boundary. A value of 0 indicates a Cartesian geometry, a value of 1 indicates a cylindrical geometry and a value of 2 an hexagonal geometry.

- N_3^{GG} first direction to process in the analysis. For cylinder, this is the direction of the first axis of the plane normal to the cylinder axis. For Cartesian and hexagonal geometries a value of 1 (x-axis) is selected by default.

- N_4^{GG} number of cells in the original geometry (before unfolding).

- N_5^{GG} number of cells in the geometry after the original geometry is unfolded according to the symmetries.

- N_6^{GG} diagonal symmetry flag. A value of 0 indicates that this symmetry is not used. A value of -1 indicates that the symmetry is used for the $x_- = y_+$ plane and a value of 1 that the symmetry is used for the $x_+ = y$ plane.

- N_7^{GG} flag to identify symmetries with respect to the x-axis (x_- or x_+). A value of 0 indicates that no symmetry is present, $N_7^{\mathrm{GG}} = \pm 1$ is for a `SYME` symmetry at the $x_\pm$ plane, $N_7^{\mathrm{GG}} = \pm 2$ represents a `SSYM` symmetry at the $x_\pm$ plane and $N_7^{\mathrm{GG}} = 3$ implies a translation symmetry is the x direction ($x_- = x_+$).

- N_8^{GG} flag to identify symmetries with respect to the y-axis (y_- or y_+). A value of 0 indicates that no symmetry is present, $N_7^{\mathrm{GG}} = \pm 1$ is for a `SYME` symmetry at the $y_\pm$ plane, $N_7^{\mathrm{GG}} = \pm 2$ represents a `SSYM` symmetry at the $y_\pm$ plane and $N_7^{\mathrm{GG}} = 3$ implies a translation symmetry is the y direction ($y_- = y_+$).

- N_9^{GG} flag to identify symmetries with respect to the z-axis (z_- or z_+). A value of 0 indicates that no symmetry is present, $N_7^{\mathrm{GG}} = \pm 1$ is for a `SYME` symmetry at the $z_\pm$ plane, $N_7^{\mathrm{GG}} = \pm 2$ represents a `SSYM` symmetry at the $z_\pm$ plane and $N_7^{\mathrm{GG}} = 3$ implies a translation symmetry is the z direction ($z_- = z_+$).

- N_{10}^{GG} number of x mesh subdivisions or hexagons in the original geometry.

- N_{11}^{GG} number of y mesh subdivisions or hexagons in the original geometry.

- N_{12}^{GG} number of z mesh subdivisions in the original geometry.

- N_{13}^{GG} number of x mesh subdivisions or hexagons in the unfolded geometry.

- N_{14}^{GG} number of y mesh subdivisions or hexagons in the unfolded geometry.

- N_{15}^{GG} number of z mesh subdivisions in the unfolded geometry.

- N_{16}^{GG} maximum number cells required to represent this geometry.

- N_{17}^{GG} maximum number of region for this geometry.

- N_{18}^{GG} total number of clusters in this geometry.

- N_{19}^{GG} maximum number of pins in this geometry.

- N_{20}^{GG} maximum dimensions of any mesh array for a cell in this geometry.

- N_{21}^{GG} maximum dimensions of any mesh array for a pin in this geometry.

- N_{22}^{GG} number of external surfaces for this geometry.

- N_{23}^{GG} number of regions for this geometry.

- N_{24}^{GG} maximum number of external surfaces in a sub-geometry included in this geometry.

- N_{25}^{GG} maximum number of regions in a sub-geometry included in this geometry.

The indexing of array $S_{i,j}^{\mathrm{GG}}$ for the axis of symmetry is as follows

1. Cartesian assemblies:

   - $i = 1$ refers to a reflexion of the geometry on a plane normal the x-axis;
   - $i = 2$ refers to a reflexion of the geometry on a plane normal the y-axis;
   - $i = 3$ refers to a reflexion of the geometry on the plane $x = y$;
   - $i = 4$ refers to a reflexion of the geometry on a plane normal the z-axis.

2. Hexagonal assemblies (symmetries not yet programmed).

   - $i = 1$ refers to a reflexion of the geometry on a plane normal the u-axis;
   - $i = 2$ refers to a reflexion of the geometry on a plane normal the v-axis;
   - $i = 3$ refers to a reflexion of the geometry on the plane w;
   - $i = 4$ refers to a reflexion of the geometry on a plane normal the z axis.

The indexing of array $F_{i,j}^{\mathrm{GG}}$ for external surface identification is as follows. First $F_{0,j}^{\mathrm{GG}}$ represents the number of times the cell appears in the geometry after it has been unfolded. For $i > 0$, $F_{i,j}^{\mathrm{GG}}$ can take the following values

$$F_{i,j}^{\mathrm{GG}} = \begin{cases} 1 & \text{surface associated with direction } i \text{ of cell } j \text{ is an external boundary of the assembly} \\ 0 & \text{surface associated with direction } i \text{ of cell } j \text{ is not an external boundary of the assembly} \end{cases}$$

with the following planes associated with different values of i:

1. Cartesian assemblies:

   - $i = 1$ surfaces on the x_- plane for cell j;
   - $i = 2$ surfaces on the x_+ plane for cell j;
   - $i = 3$ surfaces on the y_- plane for cell j;
   - $i = 4$ surfaces on the y_+ plane for cell j;
   - $i = 5$ surfaces on the z_- plane for cell j;
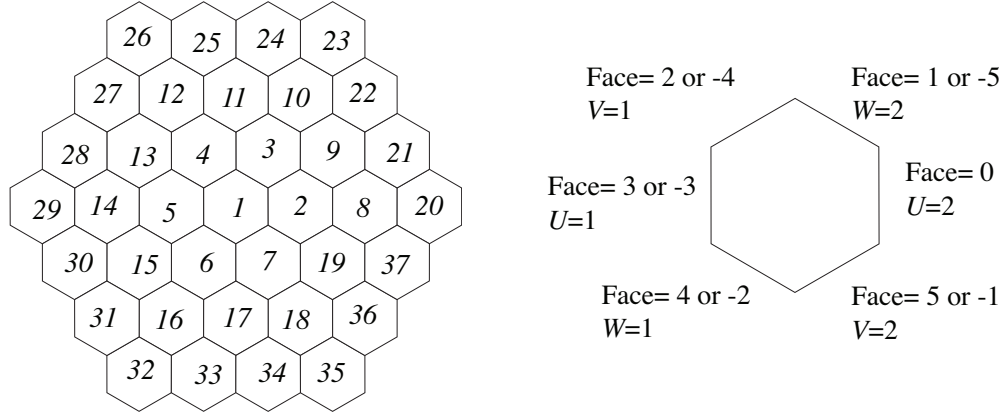
Figure 3: Example of an assembly of hexagons (left) and external faces identification for an hexagon

- $i = 6$ surfaces on the z_+ plane for cell j.

2. Hexagonal assemblies (see Figure 3):

  - $i = 1$ surfaces on the u_- plane for cell j;
  - $i = 2$ surfaces on the u_+ plane for cell j;
  - $i = 3$ surfaces on the v_- plane for cell j;
  - $i = 4$ surfaces on the v_+ plane for cell j;
  - $i = 5$ surfaces on the z_- plane for cell j;
  - $i = 6$ surfaces on the z_+ plane for cell j;
  - $i = 7$ surfaces on the w_- plane for cell j;
  - $i = 8$ surfaces on the w_+ plane for cell j.

The arrays x^{GG}, y^{GG}, z^{GG} and r^{GG} contain the following information:

1. Cartesian assemblies:

  - x_{i-1}^{GG} and x_i^{GG} are the lower and upper x limits of mesh element i $(i = 1, n^x)$;
  - y_{j-1}^{GG} and y_j^{GG} are the lower and upper y limits of mesh element j $(j = 1, n^y)$;
  - z_{k-1}^{GG} and z_k^{GG} are the lower and upper z limits of mesh element k $(k = 1, n^z)$.

2. Hexagonal assemblies (see Figure 3):

  - $x_0^{\mathrm{GG}} = h$ is the width of one face of the hexagon and x_i^{GG} is the position in x of the center of cell i in the assembly;
  - $y_0^{\mathrm{GG}} = h$ is the width of one face of the hexagon and y_j^{GG} is the position in y of the center of cell j in the assembly;
  - z_{k-1}^{GG} and z_k^{GG} are the lower and upper z limits of mesh element k $(k = 1, n^z)$.

As we noted above, the global geometry is always an assembly containing cells. For each cell i in this assembly, several records will be generated in the **/NXTRecords/** directory. These records are identified using a FORTRAN **CHARACTER*12** variable as follows

```
INTEGER     I
CHARACTER*12 NAMREC
CHARACTER*3  NREC
WRITE(NAMREC,'(A1,I8.8,A3)') 'C',I,NREC
```

where the variable `NREC` can take the following values:

- DIM for dimensioning information;

- SMR for the radial mesh description;

- SMX for the x-directed mesh description;

- SMY for the y-directed mesh description;

- SMZ for the z-directed mesh description;

- MIX for physical mixture description;

- HOM for virtual mixture description;

- VSE for areas and volumes results;

- VSI for local surfaces and regions identification;

- RID for final region numbering;

- SID for final surface numbering

- PNT for pin contents description;

- PIN for pins location.

In Table 36, a description of the additional `/NXTRecords/` records associated with cell $i = 1$ can be found.

Table 36: Cell $i = 1$ records in `/NXTRecords/`

Name	Type	Condition	Units	Comment
C00000001DIM	I(40)			array N_j^{GC} containing the dimensioning information required to rebuilt the cell
C00000001SMR	D(N_2^{GC})		cm	array r_j^{GC} containing the cell radial mesh description
C00000001SMX	D(N_3^{GC})		cm	array x_j^{GC} containing the cell x-directed mesh description
C00000001SMY	D(N_4^{GC})		cm	array y_j^{GC} containing the cell y-directed mesh description
C00000001SMZ	D(N_5^{GC})		cm	array z_j^{GC} containing the cell z-directed mesh description
C00000001MIX	I(N_6^{GC})			array M_j^{GC} containing the cell physical mixture for each region
C00000001HOM	I(N_6^{GC})			array H_j^{GC} containing the cell virtual mixture for each region
C00000001VSE	D($-N_9^{\mathrm{GC}} : N_8^{\mathrm{GC}}$)			array $\mathrm{SV}_j^{\mathrm{GC}}$ containing surface area j ($\mathrm{SV}_{-j}^{\mathrm{GC}} = S_j^{\mathrm{GC}}$ in cm for 2-D and cm^2 for 3-D problems) and regional volumes j ($\mathrm{SV}_j^{\mathrm{GC}} = V_j^{\mathrm{GC}}$ in cm^2 for 2-D and cm^3 for 3-D problems)
C00000001VSI	I($4, -N_9^{\mathrm{GC}} : N_8^{\mathrm{GC}}$)			array $\mathrm{VSI}_{k,j}^{\mathrm{GC}}$ containing the location of a surface ($j < 0$) and a region ($j > 0$)

Cell $i = 1$ records in `/NXTRecords/`

Name	Type	Condition	UnitsComment
`C00000001RID`	$I(N_8^{\rm GC})$		index array $\mathrm{RID}_j^{\rm GC}$ associating local and global region numbering
`C00000001SID`	$I(N_9^{\rm GC})$		index array $\mathrm{SID}_{j,i}^{\rm GC}$ associating local and global outer surface numbering
`C00000001PNT`	$I(3, N_{18}^{\rm GC})$		array $\mathrm{PC}_{k,j}^{\rm GC}$ containing the cell pin contents
`C00000001PIN`	$D(-1 : 4, N_{18}^{\rm GC})$		array $p_{k,j}^{\rm GC}$ containing the location of the pins in cell

Note that the record names above are built using the following FORTRAN instructions:

```
WRITE(NAMREC,'(A1,I8.8,A3)') 'C',i,NAMEXT
```

The cell dimensioning array $N_i^{\rm GC}$ for cell i contains the following information:

- $N_1^{\rm GC}$ cell geometry type (see the definition of $\mathcal{S}_1^G$ in Section 3.2);

- $N_2^{\rm GC}$ dimensions of the radial mesh array;

- $N_3^{\rm GC}$ dimensions of the x-directed mesh array;

- $N_4^{\rm GC}$ dimensions of the y-directed mesh array;

- $N_5^{\rm GC}$ dimensions of the z-directed mesh array;

- $N_6^{\rm GC}$ dimensions of the mixture record;

- $N_7^{\rm GC}$ geometry level (1 for cell);

- $N_8^{\rm GC}$ number of regions in the cell before symmetry considerations;

- $N_9^{\rm GC}$ number of surfaces in the cell before symmetry considerations;

- $N_{10}^{\rm GC}$ number of regions in the cell after symmetry considerations;

- $N_{11}^{\rm GC}$ number of surfaces in the cell after symmetry considerations;

- $N_{12}^{\rm GC}$ first global region number for cell;

- $N_{13}^{\rm GC}$ last global region number for cell;

- $N_{14}^{\rm GC}$ first global surface number for cell;

- $N_{15}^{\rm GC}$ last global surface number for cell;

- $N_{16}^{\rm GC}$ number of pin cluster geometries in cell;

- $N_{17}^{\rm GC}$ first pin cluster geometry associated with cell;

- $N_{18}^{\rm GC}$ total number of pins in cell;

- $N_{19}^{\rm GC}$ number of times this cell is used in the global cell.

while the remaining elements are not used.

The array $x_j^{\rm GC}$ contains the following information:

- x_{-1}^{GC} contains the displacement of the center of the cylindrical region with respect to the center of the Cartesian mesh in direction x. This center is located at:

$$x_c = \frac{x_{n^x}^{\mathrm{Gc}} + x_0^{\mathrm{GC}}}{2}$$

  where we have used $n^x = N_3^{\mathrm{GC}}$.

- x_{j-1}^{GC} and x_j^{GC} are the lower and upper x limits of mesh element j $(j = 1, n^x)$.

The array y_j^{GC} contains the following information:

- y_{-1}^{GC} contains the displacement of the center of the cylindrical region with respect to the center of the Cartesian mesh in direction y. This center is located at:

$$y_c = \frac{y_{n^y}^{\mathrm{GC}} + y_0^{\mathrm{GC}}}{2}$$

  where we have used $n^y = N_4^{\mathrm{GC}}$.

- y_{j-1}^{GC} and y_j^{GC} are the lower and upper y limits of mesh element j $(j = 1, n^y)$.

The array z_j^{GC} contains the following information:

- z_{-1}^{GC} contains the displacement of the center of the cylindrical region with respect to the center of the Cartesian mesh in direction z. This center is located at:

$$z_c = \frac{z_{n^z}^{\mathrm{GC}} + z_0^{\mathrm{GC}}}{2}$$

  where we have used $n^z = N_5^{\mathrm{GC}}$.

- z_{j-1}^{GC} and z_j^{GC} are the lower and upper z limits of mesh element j $(j = 1, n^z)$.

The array r_j^{GC} contains the following information:

- $r_{-1}^{\mathrm{GC}} = r_0^{\mathrm{GC}} = 0$.

- $r_{j-1}^{\mathrm{GC}} \le r \le r_j^{\mathrm{GC}}$ describes the position in r of mesh element j $(j = 1, N_2^{\mathrm{GC}})$.

The array p_j^{GC} contains the following information:

- p_{-1}^{GC} is the angular position of z-, x- or y-directed pin with respect to the x, y or z axis.

- p_0^{GC} is the radial position of z-, x- or y-directed pin with respect to the $x - y$, $y - z$ or $z - x$ center of the cell where the pin is located.

- p_1^{GC} is the height of a x-directed pin.

- p_2^{GC} is the height of a y-directed pin.

- p_3^{GC} is the height of a z-directed pin.

- p_4^{GC} is the outer radius of the pin.

In Table 37, a description of the additional `/NXTRecords/` records associated with pin $i = 1$ can be found. These records are identified using a procedure similar to that used for cell records, namely

```
INTEGER      I
CHARACTER*12 NAMREC
CHARACTER*3  NREC
WRITE(NAMREC,'(A1,I8.8,A3)') 'P',I,NREC
```

where the variable `NREC` can take the same values as for cell records, except for `NREC=PNT` and `NREC=PIN` which are now forbidden.

Table 37: Pin $i = 1$ records in `/NXTRecords/`

Name	Type	Condition	Units	Comment
P00000001DIM	I(40)			array N_j^{GP} containing the dimensioning information required to rebuilt the pin
P00000001SMR	D(N_2^{GP})		cm	array r_j^{GP} containing the pin radial mesh description
P00000001SMX	D(N_3^{GP})		cm	array x_j^{GP} containing the pin x-directed mesh description
P00000001SMY	D(N_4^{GP})		cm	array y_j^{GP} containing the pin y-directed mesh description
P00000001SMZ	D(N_5^{GP})		cm	array z_j^{GP} containing the pin z-directed mesh description
P00000001MIX	I(N_6^{GP})			array M_j^{GP} containing the pin physical mixture for each region
P00000001HOM	I(N_6^{GP})			array H_j^{GP} containing the pin virtual mixture for each region
P00000001VSE	D($-N_9^{\mathrm{GP}} : N_8^{\mathrm{GP}}$)			array $\mathrm{SV}_j^{\mathrm{GP}}$ containing surface area j ($\mathrm{SV}_{-j}^{\mathrm{GP}} = S_j^{\mathrm{GP}}$ in cm for 2-D and cm^2 for 3-D problems) and regional volumes j ($\mathrm{SV}_j^{\mathrm{GP}} = V_j^{\mathrm{GP}}$ in cm^2 for 2-D and cm^3 for 3-D problems)
P00000001VSI	I($4, -N_9^{\mathrm{GP}} : N_8^{\mathrm{GP}}$)			array $\mathrm{VSI}_{k,j}^{\mathrm{GP}}$ containing the location of a surface ($j < 0$) and a region ($j > 0$)
P00000001RID	I(N_8^{GP})			index array $\mathrm{RID}_j^{\mathrm{GP}}$ associating local and global region numbering
P00000001SID	I(N_9^{GP})			index array $\mathrm{SID}_{j,i}^{\mathrm{GP}}$ associating local and global outer surface numbering

The pin dimensioning array N^{GP} contains the following information:

- $N_{1,}^{\mathrm{GP}}$ pin geometry type (see the definition of $\mathcal{S}_1^G$ in Section 3.2);

- $N_{2,}^{\mathrm{GP}}$ dimensions of the radial mesh array;

- $N_{3,}^{\mathrm{GP}}$ dimensions of the x-directed mesh array;

- $N_{4,}^{\mathrm{GP}}$ dimensions of the y-directed mesh array;

- $N_{5,}^{\mathrm{GP}}$ dimensions of the z-directed mesh array;

- $N_{6,}^{\mathrm{GP}}$ dimensions of the mixture record;

- $N_{7,}^{\mathrm{GP}}$ geometry level (2 for pins);

- $N_{8,}^{\mathrm{GP}}$ number of regions in the pin before symmetry considerations;

- $N_{9,}^{\mathrm{GP}}$ number of surfaces in the pin before symmetry considerations;

- N_{10}^{GP} number of regions in the pin after symmetry considerations;

- N_{11}^{GP} number of surfaces in the pin after symmetry considerations;

- N_{12}^{GP} first global region number for pins in cluster;

- N_{13}^{GP} last global region number for pins in cluster;

- N_{14}^{GP} first global surface number for pins in cluster;

- N_{15}^{GP} last global surface number for pins in cluster;

- N_{16}^{GP} first pin cluster geometry for pins in cluster.

- N_{17}^{GP} total number of pins in cluster.

while the remaining elements are not used. The array x_j^{GP} contains the following information:

- x_{-1}^{GP} contains the displacement of the center of the cylindrical region with respect to the center of the Cartesian mesh in direction x. This center is located at:

$$x_c = \frac{x_{n^x}^{\mathrm{GP}} + x_0^{\mathrm{GP}}}{2}$$

where we have used $n^x = N_3^{\mathrm{GP}}$.

- x_{j-1}^{GP} and x_j^{GP} re the lower and upper x limits of mesh element j $(j = 1, n^x)$.

The array y_j^{GP} contains the following information:

- y_{-1}^{GP} contains the displacement of the center of the cylindrical region with respect to the center of the Cartesian mesh in direction y. This center is located at:

$$y_c = \frac{y_{n^y}^{\mathrm{GP}} + y_0^{\mathrm{GP}}}{2}$$

where we have used $n^y = N_4^{\mathrm{GP}}$.

- y_{j-1}^{GP} and y_j^{GP} are the lower and upper y limits of mesh element j $(j = 1, n^y)$.

The array z_j^{GP} contains the following information:

- z_{-1}^{GP} contains the displacement of the center of the cylindrical region with respect to the center of the Cartesian mesh in direction z. This center is located at:

$$z_c = \frac{z_{n^z}^{\mathrm{GP}} + z_0^{\mathrm{GP}}}{2}$$

where we have used $n^z = N_5^{\mathrm{GP}}$.

- z_{j-1}^{GP} and z_j^{GP} are the lower and upper z limits of mesh element j $(j = 1, n^z)$.

The array r_j^{GP} contains the following information:

- $r_{-1}^{\mathrm{GP}} = r_0^{\mathrm{GP}} = 0$.

- $r_{j-1}^{\mathrm{GP}} \le r \le r_j^{\mathrm{GP}}$ describes the position in r of mesh element j with $j = 1, N_2^{\mathrm{GP}}$.

Finally the `/NXTRecords/` directory also contains records associated with global identification of the surfaces and volumes as illustrated in Table 38.

Table 38: Global geometry records in /NXTRecords/

Name	Type	Condition	Units	Comment
`TrackingDnsA`	$D(\mathcal{S}_{20}^t)$		cm	array D_i containing the spatial spacing for each track direction
`TrackingDirc`	$D(N_1^{\mathrm{GG}}, \mathcal{S}_{20}^t)$			array $\alpha_{j,i}$ containing the director cosine for axis j for each track direction
`TrackingOrig`	$D(N_1^{\mathrm{GG}}, N_p, \mathcal{S}_{20}^t)$		cm	array $L_{k,j,i}$ containing the origin in space ($k = 1, N_1^{\mathrm{GG}}$) and the direction of the normal plan for each plane j and track direction i
`TrackingWgtD`	$D(\mathcal{S}_{20}^t)$			array W_i containing the integration weight for each track direction
`VTNormalize␣`	$D(N_{22}^{\mathrm{GG}})$			array R_i containing the ratio of the analytical and numerical volume for each region
`VTNormalizeD`	$D(N_{22}^{\mathrm{GG}}, \mathcal{S}_{20}^t)$	$\mathcal{S}_8^t = -1$		array R_i containing the ratio of the analytical and numerical volume for region i for each track direction
`KEYMRG␣␣␣␣␣␣`	$I(-N_{23}^{\mathrm{GG}}, N_{22}^{\mathrm{GG}})$			array MRG_i containing the global merging index
`MATALB␣␣␣␣␣␣`	$I(-N_{23}^{\mathrm{GG}}, N_{22}^{\mathrm{GG}})$			array containing the albedo number associated with each surface and the physical mixture number associated with each region
`HOMMATALB␣␣␣`	$I(-N_{23}^{\mathrm{GG}}, N_{22}^{\mathrm{GG}})$			array containing the albedo number associated with each surface and the virtual mixture number associated with each region
`SAreaRvolume`	$D(-N_{23}^{\mathrm{GG}}, N_{22}^{\mathrm{GG}})$			array containing the area (S_α in cm for 2-D and cm^2 for 3-D problems) and volumes (V_i cm^2 for 2-D and cm^3 for 3-D problems) of each external surface and region in the geometry

4.5 The `mccgt` dependent records on a /tracking/ directory

When the `MCCGT:` module is used (`CDOOR='MCCG'`), an additional state vector named `MCCG-STATE` is set in `EXCELT:` data structure. The components $\mathcal{M}_i^t$ of `MCCG-STATE` are:

- $\mathcal{M}_1^t$: (`LCACT`) The polar quadrature type used with the method of characteristics

$$
\mathcal{M}_1^t = \begin{cases}
0 & \text{Gauss-Legendre} \\
1 & \text{CACTUS type 1} \\
2 & \text{CACTUS type 2} \\
3 & \text{McDaniel} \\
4 & \text{McDaniel with } P_1 \text{ constraint} \\
5 & \text{Gauss optimized.}
\end{cases}
$$

- $\mathcal{M}_2^t$: (`NMU`) The order of the polar quadrature.

- $\mathcal{M}_3^t$: (`KRYL`) GMRES acceleration switch:

$$
\mathcal{M}_3^t = \begin{cases}
0 & \text{free inner iterations} \\
\geq 1 & \text{GMRES}(\mathcal{M}_3^t) \text{ acceleration of inner iterations} \\
\leq 1 & \text{Bi-CGSTAB acceleration of inner iterations}
\end{cases}
$$

- $\mathcal{M}_4^t$: (`IDIFC`) Type of solution operator:

$$
\mathcal{M}_4^t = \begin{cases}
0 & \text{transport flux solution selected} \\
1 & \text{CDD diffusion flux solution selected (no inner iterations are performed} \\
  & \text{in this case, only an ACA resolution is performed)}
\end{cases}
$$

- $\mathcal{M}_5^t$: (`NMAX`) The maximum number of elements in a single track.

- $\mathcal{M}_6^t$: (`LMCU`) The dimension of the connection matrix `MCU`.

- $\mathcal{M}_7^t$: (`IACC`) ACA preconditioning switch:

$$
\mathcal{M}_7^t = \begin{cases}
0 & \text{no ACA preconditioning} \\
\geq 1 & \text{ACA preconditioning of inner/multigroup iterations}
\end{cases}
$$

If the number of inner iterations is set to 1, ACA is used as a rebalancing technique for multigroup iterations and $\mathcal{M}_7^t$ is the maximum number of iterations allowed to solve the ACA system.

- $\mathcal{M}_8^t$: (`ISCR`) SCR preconditioning switch:

$$
\mathcal{M}_8^t = \begin{cases}
0 & \text{no SCR preconditioning} \\
\geq 1 & \text{SCR preconditioning of inner/multigroup iterations}
\end{cases}
$$

If the number of inner iterations is set to 1, SCR is used as a rebalancing technique for multigroup iterations and $\mathcal{M}_8^t$ is the maximum number of iterations allowed to solve the SCR system.

- $\mathcal{M}_9^t$: (`LPS`) The dimension of the surface-to-region collision probabilities array if SCR is used.

- $\mathcal{M}_{10}^t$: (`ILU`) The type of preconditioning for the resolution with BICGSTAB of the ACA corrective system if ACA is used:

$$
\mathcal{M}_{10}^t = \begin{cases}
0 & \text{no preconditioning} \\
1 & \text{diagonal preconditioning} \\
\geq 2 & \text{ILU0 preconditioning}
\end{cases}
$$

- $\mathcal{M}_{11}^t$: (ILEXA) Flag to force the usage of exact exponentials for preconditioner calculation:

$$\mathcal{M}_{11}^t = \begin{cases} 0 & \text{not forced} \\ 1 & \text{forced} \end{cases}$$

- $\mathcal{M}_{12}^t$: (ILEXF) Flag to force the usage of exact exponentials for flux calculation:

$$\mathcal{M}_{12}^t = \begin{cases} 0 & \text{not forced} \\ 1 & \text{forced} \end{cases}$$

- $\mathcal{M}_{13}^t$: (MAXI) Maximum number of inner iterations.

- $\mathcal{M}_{14}^t$: (LTMT) Flag for the usage of a tracking merging technique while building the ACA matrices in order to obtain a two-step ACA acceleration:

$$\mathcal{M}_{14}^t = \begin{cases} 0 & \text{no tracking merging} \\ 1 & \text{tracking merging} \end{cases}$$

- $\mathcal{M}_{15}^t$: (STIS) Flag for the flux integration strategy by the characteristics method:

$$\mathcal{M}_{15}^t = \begin{cases} 0 & \text{direct approach with asymptotical treatment} \\ 1 & \text{``Source term isolation'' approach: optimized strategy with asymptotical treatment} \\ -1 & \text{''MOCC/MCI''-like approach: optimized strategy without asymptotical treatment} \end{cases}$$

- $\mathcal{M}_{16}^t$: (NPJJM) Effective number of angular mode-to-mode self-collision probabilities to be calculated per group and region if $\mathcal{M}_{15}^t = 1$ e.g.

anisotropy	2D	3D
P_0	1	1
P_1	4	7
P_2	13	27
P_3	31	76

- $\mathcal{M}_{17}^t$: (LMCU0) Effective number of non-diagonal elements to store for the ILU0 decomposition for ACA preconditioning.

- $\mathcal{M}_{18}^t$: (IFORW) Flag to set the solution type for the ACA and characteristics system:

$$\mathcal{M}_{18}^t = \begin{cases} 0 & \text{direct solution} \\ 1 & \text{adjoint solution} \end{cases}$$

- $\mathcal{M}_{19}^t$: (NFUNL) Number of spherical harmonics components used to expand the flux and the sources.

- $\mathcal{M}_{20}^t$: (NLIN) Number of polynomial components used to expand the flux and the sources in space.

The following records will also be present on the main level of a /tracking/ directory.

Table 39: The `MCCGT:` records in /tracking/

Name	Type	Condition	UnitsComment
`MCCG-STATE`␣␣	I(40)		Vector describing the various parameters associated with this data structure $\mathcal{M}_i^t$, as defined in Section 4.5.
`REAL-PARAM`␣␣	R(4)		Real parameters $\mathcal{R}_i$ for the MCCG tracking.
`XMU$MCCG`␣␣␣␣	R($\mathcal{M}_2^t$)		Inverse of the polar quadrature sines.
`ZMU$MCCG`␣␣␣␣	R($\mathcal{M}_2^t$)		Cosines of the polar quadrature set.
`WZMU$MCCG`␣␣␣	R($\mathcal{M}_2^t$)		Weights of the polar quadrature set.
`PI$MCCG`␣␣␣␣␣	I($N_{\dim}$)	$\mathcal{S}_{15}^t > 0$	Permutation array for ACA according to $i_{\mathrm{old}} = \Pi(i_{\mathrm{new}})$. The dimension of this array is $$N_{\dim} = \begin{cases} \mathcal{S}_1^t + \mathcal{S}_5^t & \text{if } \mathcal{S}_9^t = 0; \\ \mathcal{S}_1^t & \text{if } \mathcal{S}_9^t = 1. \end{cases}$$
`INVPI$MCCG`␣␣	I($\mathcal{S}_1^t + \mathcal{S}_5^t$)	$\mathcal{S}_{15}^t > 0$	Inverse permutation array for ACA $i_{\mathrm{new}} = \Pi(i_{\mathrm{old}})$
`NZON$MCCG`␣␣␣	I($\mathcal{S}_1^t + \mathcal{S}_5^t$)		Index-number of the mixture type assigned to each volume and the albedo number assigned to each surface.
`NZONA$MCCG`␣␣	I($\mathcal{S}_1^t + \mathcal{S}_5^t$)	$\mathcal{S}_{15}^t > 0$	Index-number of the mixture type assigned to each volume and the albedo number assigned to each surface (-7 for void boundary conditions).
`V$MCCG`␣␣␣␣␣␣	R($\mathcal{S}_1^t + \mathcal{S}_5^t$)		Volumes and numerical surfaces.
`VA$MCCG`␣␣␣␣␣	R($\mathcal{S}_1^t + \mathcal{S}_5^t$)	$\mathcal{S}_{15}^t > 0$	Renumbered Volumes and numerical surfaces.
`KM$MCCG`␣␣␣␣␣	I($N_{\dim}$)	$\mathcal{M}_7^t > 0$	Connection matrix for ACA.
`IM$MCCG`␣␣␣␣␣	I($N_{\dim} + 1$)	$\mathcal{M}_7^t > 0$	Connection matrix for ACA.
`MCU$MCCG`␣␣␣␣	I($\mathcal{M}_6^t$)	$\mathcal{M}_7^t > 0$	Connection matrix for ACA.
`JU$MCCG`␣␣␣␣␣	I($N_{\dim}$)	$\begin{cases} \mathcal{S}_{15}^t > 0 \\ \mathcal{M}_3^t \geq 2 \end{cases}$	Used for ILU0 decomposition in the preconditioning of ACA system.
`IS$MCCG`␣␣␣␣␣	I($\mathcal{S}_5^t$)	$\mathcal{M}_1^t > 0$	Connection matrix for surface-to-volume probability in SCR.
`JS$MCCG`␣␣␣␣␣	I($\mathcal{M}_7^t$)	$\mathcal{M}_1^t > 0$	Connection matrix for surface-to-volume probability in SCR.
`ISGNR$MCCG`␣␣	I($8(\mathcal{S}_6^t)^2$)		Signs for spherical harmonics on the 8 octant angular modes.
`KEYCUR$MCCG`␣	I($\mathcal{S}_5^t$)	$\mathcal{S}_9^t = 1$	Index for outgoing currents at the domain boundaries.
`KEYFLX$ANIS`␣	I($\mathcal{S}_1^t, \mathcal{M}_{20}^t, \mathcal{M}_{19}^t$)		Location in unknown vector of averaged regional flux moments.
`KEYANI$MCCG`␣	I($(\mathcal{S}_6^t)^2$)	$\mathcal{S}_9^t = 1$	Index for currents.
`PJJIND$MCCG`␣	I($2\mathcal{M}_{16}^t$)	$\mathcal{M}_{15}^t = 1$	Index of modes connection for non vanishing angular mode-to-mode self-collision probabilities
`IMO$MCCG`␣␣␣␣	I($N_{\dim} + 1$)	$\begin{cases} \mathcal{M}_7^t > 0 \\ \mathcal{M}_3^t = 3 \end{cases}$	Connection matrix for non-diagonal elements of ILU0-ACA.

Name	Type	Condition	UnitsComment
`MCU0$MCCG`␣␣␣	$I(\mathcal{M}_{17}^t)$	$\begin{cases} \mathcal{M}_7^t > 0 \\ \mathcal{M}_3^t = 3 \end{cases}$	Connection matrix for non-diagonal elements of ILU0-ACA.

with the real parameter $\mathcal{R}_i$, representing:

- $\mathcal{R}_1^t$: Convergence criterion on inner iterations.

- $\mathcal{R}_2^t$: Step characteristics selection criterion:

$$\mathcal{R}_2^t = \begin{cases} 0.0 & \text{step characteristics scheme} \\ > 0.0 & \text{diamond differencing scheme.} \end{cases}$$

- $\mathcal{R}_3^t$: Track spacing in cm for 3D prismatic tracking.

- $\mathcal{R}_4^t$: Tracking symmetry factor for maximum track length calculation during the calculation of a 3D prismatic tracking.

The following records will also be present in the `/PROJECTION/` directory of a /tracking/ directory when a prismatic tracking is considered.

Table 40: The `MCCGT:` records in `/PROJECTION/`

Name	Type	Condition	Units	Comment
`ZCOORD`␣␣␣␣␣␣	$R(\mathcal{M}_{18}^t + 1)$	$\mathcal{S}_{39}^t > 0$	cm	The $z-$directed mesh position
`IND2T3`␣␣␣␣␣␣	$I(N_{ind})$	$\mathcal{S}_{39}^t > 0$		Volume and surfaces index for a 3D prismatic geometry. Its size is $N_{ind} = (N_{2D} + 1)(\mathcal{M}_{18}^t + 2)$ where N_{2D} is the number of volumes and surfaces in the initial 2D tracking
`VNORF`␣␣␣␣␣␣␣	$D(N_{nor})$	$\mathcal{S}_{39}^t > 0$		Angular dependent normalization factors for a 3D prismatic extended tracking. Its size is $N_{nor} = 2\mathcal{S}_1^t \mathcal{M}_2^t N_{\text{angl}}$ where N_{angl} is the number of tracking angles in the initial 2D tracking

4.6   The snt dependent records on a /tracking/ directory

When the SNT: operator is used (CDOOR=’SN’), the following elements in the vector $\mathcal{S}_i^t$ will also be defined.

- $\mathcal{S}_6^t$: (ITYPE) Type of SN geometry:

$$\mathcal{S}_6^t = \begin{cases} 2 & \text{Cartesian 1-D geometry} \\ 3 & \text{Tube 1-D geometry} \\ 4 & \text{Spherical 1-D geometry} \\ 5 & \text{Cartesian 2-D geometry} \\ 6 & \text{Tube 2-D geometry (R-Z geometry)} \\ 7 & \text{Cartesian 3-D geometry} \\ 8 & \text{Hexagonal 2-D geometry} \\ 9 & \text{Hexagonal 3-D geometry} \end{cases}$$

- $\mathcal{S}_7^t$: (NSCT) Number of spherical harmonics components used to expand the flux and the sources.

- $\mathcal{S}_8^t$: (IELEM) Measure of order of the spatial approximation. The Legendre polynomials (for both HODD *and* DG (see $\mathcal{S}_{10}^t$)) used are of order 0 (constant), 1 (linear), 2 (parabolic) or 3 (cubic), corresponding to IELEM values of:

$$\mathcal{S}_8^t = \begin{cases} 1 & \text{Constant (classical diamond scheme) - default for HODD} \\ 2 & \text{Linear - default for DG} \\ 3 & \text{Parabolic} \\ 4 & \text{Cubic (only for DG)} \end{cases}$$

- $\mathcal{S}_9^t$: (NDIM) Number of geometric dimensions (1, 2 or 3).

- $\mathcal{S}_{10}^t$: (ISCHM) Method of spatial discretisation:

$$\mathcal{S}_{10}^t = \begin{cases} 1 & \text{High-Order Diamond Differencing method (HODD) – default option if unspecified} \\ 2 & \text{Discontinuous Galerkin finite element method (DG) – available if } \mathcal{S}_6^t = 2, 5, \text{ or } 8 \end{cases}$$

- $\mathcal{S}_{11}^t$: (LL4) Number of mesh-centered flux components in one energy group. Generally equal to $\mathcal{S}_2^t$ except in cases where surfacic fluxes are appended to the unknown vector. $\mathcal{S}_{11}^t \le \mathcal{S}_2^t$.

- $\mathcal{S}_{12}^t$: (LX) Number of elements along the X axis.

- $\mathcal{S}_{13}^t$: (LY) Number of elements along the Y axis.

- $\mathcal{S}_{14}^t$: (LZ) Number of elements along the Z axis.

- $\mathcal{S}_{15}^t$: (NLF) Order of the S_N approximation (even number ≥ 2).

- $\mathcal{S}_{16}^t$: (ISCAT) Number of terms in the scattering sources:

$$\mathcal{S}_{16}^t = \begin{cases} 1 & \text{Isotropic scattering in the laboratory system} \\ 2 & \text{Linearly anisotropic scattering in the laboratory system} \\ n & \text{order } n-1 \text{ anisotropic scattering in the laboratory system} \end{cases}$$

- $\mathcal{S}_{17}^t$: (IQUAD) Type of angular quadrature:

$$\mathcal{S}_{17}^t = \begin{cases} 1 & \text{Level symmetric, Lathrop and Carlson type} \\ 2 & \text{Level symmetric, optimized } \mu_1 \text{ values} \\ 3 & \text{Level symmetric, compatible with code SNOW} \\ 4 & \text{Legendre-Chebyshev quadrature} \\ 5 & \text{symmetric Legendre-Chebyshev quadrature} \\ 6 & \text{quadrupole range (QR) quadrature} \\ 10 & \text{Gauss-Legendre and Gauss-Chebyshev product quadrature} \end{cases}$$

- $\mathcal{S}_{18}^t$: (IFIX) Flag for negative flux fixup:

$$\mathcal{S}_{18}^t = \begin{cases} 0 & \text{Non enabled} \\ 1 & \text{Enabled} \end{cases}$$

- $\mathcal{S}_{19}^t$: (IDSA) Flag for synthetic diffusion acceleration:

$$\mathcal{S}_{19}^t = \begin{cases} 0 & \text{Non enabled} \\ 1 & \text{Enabled} \end{cases}$$

- $\mathcal{S}_{20}^t$: (NSTART) Type of acceleration for the scattering iterations:

$$\mathcal{S}_{20}^t = \begin{cases} 0 & \text{GMRES non enabled; use a one-parameter Livolant acceleration} \\ > 0 & \text{Restarts the GMRES method every \texttt{NSTART} iterations} \end{cases}$$

- $\mathcal{S}_{21}^t$: (NSDSA) Number if inner flux iterations *without* DSA in 3-D cases if $\mathcal{S}_8^t \geq 2$.

- $\mathcal{S}_{22}^t$: (MAXI) Maximum number of inner iterations (resp. maximum number of GMRES(m) iterations if $\mathcal{S}_{20}^t > 0$).

- $\mathcal{S}_{23}^t$: (ILIVOL) Flag for enabling/disabling Livolant acceleration method.

$$\mathcal{S}_{23}^t = \begin{cases} 0 & \text{Non enabled} \\ 1 & \text{Enabled} \end{cases}$$

- $\mathcal{S}_{24}^t$: (icl1) number of free iterations in the Livolant method.

- $\mathcal{S}_{25}^t$: (icl2) number of accelerated iterations in the Livolant method.

- $\mathcal{S}_{26}^t$: (ISPLH) Type of hexagonal mesh splitting if $\mathcal{S}_6^t \geq 8$:

$$\mathcal{S}_{26}^t = \begin{cases} 1 & \text{3 lozenges per hexagon} \\ K & 3 \times K \times K \text{ lozenges per hexagon} \end{cases}$$

- $\mathcal{S}_{27}^t$: (INSB) Flux vectorization option where

$$\mathcal{S}_{27}^t = \begin{cases} 0 & \text{Scalar algorithm. The multigroup flux is computed as a sequence of one-group} \\ & \text{solutions using Gauss-Seidel iterations.} \\ 1 & \text{Vectorial algorithm. The multigroup flux is computed in parallel for a set of energy} \\ & \text{groups.} \end{cases}$$

- $\mathcal{S}_{28}^t$: (IOMP) Type of OpenMP multithreading strategy in 2D and 3D geometries where

$$\mathcal{S}_{28}^t = \begin{cases} 0 & \text{Standard energy group and discrete angle nested loops} \\ M & \text{Domino type nested loops with } M \times M \text{ or } M \times M \times M \text{ macrocells} \end{cases}$$

- $\mathcal{S}_{29}^t$: (IGAV) Type of condition at axial axis for cylindrical and spherical 1D geometries where

$$\mathcal{S}_{29}^t = \begin{cases} 1 & \text{Specular reflection} \\ 2 & \text{Zero-weight reflection} \\ 3 & \text{Averaged reflection} \end{cases}$$

- $\mathcal{S}_{30}^t$: (LSHOOT) Flag for enabling/disabling the shooting method in 1D.

$$\mathcal{S}_{30}^t = \begin{cases} 0 & \text{Non enabled} \\ 1 & \text{Enabled} \end{cases}$$

- $\mathcal{S}_{31}^t$: (`IBFP`) Type of equation solved by the discrete ordinates method.

$$\mathcal{S}_{31}^t = \begin{cases} 0 & \text{Boltzmann transport equation} \\ 1 & \text{Boltzmann Fokker-Planck equation with Galarkin energy propagation factors} \\ 2 & \text{Boltzmann Fokker-Planck equation with Przybylski and Ligou energy propagation} \\ & \text{factors} \end{cases}$$

The following records will also be present on the main level of a /tracking/ directory.

Table 41: The `snt` records in /tracking/

Name	Type	Condition	UnitsComment
`NCODE`	I(6)		Record containing the types of boundary conditions on each surface. =0 side not used; =1 VOID; =2 REFL; =4 TRAN. `NOODE(5)` and `NOODE(6)` are not used.
`ZCODE`	R(6)		1 Record containing the albedo value (real number) on each surface. `ZOODE(5)` and `ZOODE(6)` are not used.
`KEYFLX$ANIS`	I($\mathcal{S}_1^t, \mathcal{S}_8^t * *\mathcal{S}_9^t, \mathcal{S}_7^t$)		Location in unknown vector of averaged regional flux moments.
`DSA`	Dir	$\mathcal{S}_{19}^t = 1$	Sub-directory containing the data related to the diffusion synthetic acceleration using BIVAC (2D) or TRIVAC (3D). The specification of this directory is given in Section 4.7 or in Section 4.8
`EPSI`	R(1)		1 Record containing the convergence criterion on inner iterations.

If $\mathcal{S}_6^t = 2$ (Cartesian 1-D geometry), the following records will also be present on the main level of a /tracking/ directory.

Table 42: The `snt` records in /tracking/ (Cartesian 1-D geometry)

Name	Type	Condition	UnitsComment
`U`	R($\mathcal{S}_{15}^t$)		1 Base points of the angular Gauss-Legendre quadrature.
`W`	R($\mathcal{S}_{15}^t$)		1 Weights of the angular Gauss-Legendre quadrature.
`PL`	R($\mathcal{S}_{16}^t, \mathcal{S}_{15}^t$)		1 Discrete values of the Legendre polynomials on the quadrature base points.

If $\mathcal{S}_6^t = 3$ (Tube 1-D geometry), the following records will also be present on the main level of a /tracking/ directory. The number of discrete directions in two octants N_{angl} and the number of spherical harmonics components of the flux N_{pn} are given in term of the S_N order $N = \mathcal{S}_{15}^t$ as

$$N_{\mathrm{angl}} = \begin{cases} \frac{1}{2}N\left(1 + \frac{N}{2}\right), & \text{if } \mathcal{S}_{17}^t < 10; \\ \frac{1}{2}N^2, & \text{otherwise.} \end{cases}$$

$$N_{\mathrm{pn}} = \frac{\mathcal{S}_{16}^t}{2}\left(1 + \frac{\mathcal{S}_{16}^t}{2}\right) + \frac{1}{2}(1 + \mathcal{S}_{16}^t)\,(\mathcal{S}_{16}^t\,\mathrm{mod}\,2)$$

Table 43: The `snt` records in /tracking/ (tube 1-D geometry)

Name	Type	Condition	Units	Comment
JOP␣␣␣␣␣␣␣␣␣	I($N/2$)			Number of base points in each ξ level.
U␣␣␣␣␣␣␣␣␣␣␣	R($N/2$)		1	Base points (levels) of the angular quadrature in ξ (positive values).
UPQ␣␣␣␣␣␣␣␣␣	R(N_{angl})		1	Direction cosines of the angular two-octants spherical harmonics quadrature in μ.
WPQ␣␣␣␣␣␣␣␣␣	R(N_{angl})		1	Weights of the angular two-octants spherical harmonics quadrature.
ALPHA␣␣␣␣␣␣␣	R(N_{angl})		1	Angular redistribution parameters.
PLZ␣␣␣␣␣␣␣␣␣	R($N_{\mathrm{pn}}, N/2$)		1	Discrete values of the real spherical harmonics on the zero-weight base points.
PL␣␣␣␣␣␣␣␣␣␣␣	R($N_{\mathrm{pn}}, N_{\mathrm{angl}}$)		1	Discrete values of the real spherical harmonics on the quadrature base points.
SURF␣␣␣␣␣␣␣␣	R($\mathcal{S}_{12}^t + 1$)		1	Surfaces.

If $\mathcal{S}_6^t = 4$ (Spherical 1-D geometry), the following records will also be present on the main level of a /tracking/ directory.

Table 44: The `snt` records in /tracking/ (spherical 1-D geometry)

Name	Type	Condition	Units	Comment
U␣␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_{15}^t$)		1	Base points of the angular Gauss-Legendre quadrature.
W␣␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_{15}^t$)		1	Weights of the angular Gauss-Legendre quadrature.
ALPHA␣␣␣␣␣␣␣	R($\mathcal{S}_{15}^t$)		1	Angular redistribution parameters.
PLZ␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_{16}^t$)		1	Discrete values of the Legendre polynomials on the zero-weight base points at $\mu = -1$.

The `snt` records in /tracking/ (spherical 1-D geometry) continued from last page

Name	Type	Condition	Units	Comment
PL␣␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{16}^t, \mathcal{S}_{15}^t)$		1	Discrete values of the Legendre polynomials on the quadrature base points.
SURF␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{12}^t + 1)$		1	Surfaces.
XXX␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{12}^t + 1)$		1	Mesh-edge radii.

If $\mathcal{S}_6^t = 5$ (Cartesian 2-D geometry) or $\mathcal{S}_6^t = 6$ (R-Z geometry), the following records will also be present on the main level of a /tracking/ directory. The number of discrete directions in four octants (including zero-weight points) N_{angl} and the number of spherical harmonics components of the flux N_{pn} are given in term of the S_N order $N = \mathcal{S}_{15}^t$ as

$$N_{\mathrm{angl}} = \frac{1}{2}(N + 4)N$$

$$N_{\mathrm{pn}} = \frac{\mathcal{S}_{16}^t}{2}\left(1 + \mathcal{S}_{16}^t\right)$$

Table 45: The `snt` records in /tracking/ (Cartesian 2-D and R-Z geometries)

Name	Type	Condition	Units	Comment
DU␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{angl}})$		1	Direction cosines of the angular four-octants spherical harmonics quadrature in μ.
DE␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{angl}})$		1	Direction cosines of the angular four-octants spherical harmonics quadrature in η.
W␣␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{angl}})$		1	Weights of the angular four-octants spherical harmonics quadrature.
MRM␣␣␣␣␣␣␣␣␣	$I(N_{\mathrm{angl}})$			Quadrature offsets.
MRMY␣␣␣␣␣␣␣␣	$I(N_{\mathrm{angl}})$			Quadrature offsets.
DB␣␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{12}^t, N_{\mathrm{angl}})$		1	Diamond-scheme parameter.
DA␣␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{12}^t, \mathcal{S}_{13}^t, N_{\mathrm{angl}})$		1	Diamond-scheme parameter.
DAL␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{12}^t, \mathcal{S}_{13}^t, N_{\mathrm{angl}})$	$\mathcal{S}_6^t = 6$	1	Angular redistribution parameters.
PL␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{pn}}, N_{\mathrm{angl}})$		1	Discrete values of the real spherical harmonics on the quadrature base points.

If $\mathcal{S}_6^t = 7$ (Cartesian 3-D geometry), the following records will also be present on the main level of a /tracking/ directory. The number of discrete directions in height octants N_{angl} and the number of spherical harmonics components of the flux N_{pn} are given in term of the S_N order $N = \mathcal{S}_{15}^t$ as

$$N_{\mathrm{angl}} = (N + 2)N$$

$$N_{\mathrm{pn}} = \left(1 + \mathcal{S}_{16}^t\right)^2$$

Table 46: The `snt` records in /tracking/ (Cartesian 3-D geometry)

Name	Type	Condition	Units	Comment
DU␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{angl}})$		1	Direction cosines of the angular height-octants spherical harmonics quadrature in μ.
DE␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{angl}})$		1	Direction cosines of the angular height-octants spherical harmonics quadrature in η.
DZ␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{angl}})$		1	Direction cosines of the angular height-octants spherical harmonics quadrature in ξ.
W␣␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{angl}})$		1	Weights of the angular height-octants spherical harmonics quadrature.
MRMX␣␣␣␣␣␣␣␣	$I(N_{\mathrm{angl}})$			Quadrature offsets.
MRMY␣␣␣␣␣␣␣␣	$I(N_{\mathrm{angl}})$			Quadrature offsets.
MRMZ␣␣␣␣␣␣␣␣	$I(N_{\mathrm{angl}})$			Quadrature offsets.
DC␣␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}^t_{12}, \mathcal{S}^t_{13}, N_{\mathrm{angl}})$		1	Diamond-scheme parameter.
DB␣␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}^t_{12}, \mathcal{S}^t_{14}, N_{\mathrm{angl}})$		1	Diamond-scheme parameter.
DA␣␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}^t_{13}, \mathcal{S}^t_{14}, N_{\mathrm{angl}})$		1	Diamond-scheme parameter.
PL␣␣␣␣␣␣␣␣␣␣	$R(N_{\mathrm{pn}}, N_{\mathrm{angl}})$		1	Discrete values of the real spherical harmonics on the quadrature base points.

4.7 The `bivact` dependent records on a /tracking/ directory

When the `BIVACT:` operator is used (`CDOOR='BIVAC'`), the following elements in the vector $\mathcal{S}_i^t$ will also be defined.

- $\mathcal{S}_6^t$: (`ITYPE`) Type of BIVAC geometry:

$$\mathcal{S}_6^t = \begin{cases} 2 & \text{Cartesian 1-D geometry} \\ 3 & \text{Tube 1-D geometry} \\ 4 & \text{Spherical 1-D geometry} \\ 5 & \text{Cartesian 2-D geometry} \\ 6 & \text{Tube 2-D geometry} \\ 8 & \text{Hexagonal 2-D geometry} \end{cases}$$

- $\mathcal{S}_7^t$: (`IHEX`) Type of hexagonal symmetry if $\mathcal{S}_6^t = 8$:

$$\mathcal{S}_7^t = \begin{cases} 0 & \text{non-hexagonal geometry} \\ 1 & \text{S30} \\ 2 & \text{SA60} \\ 3 & \text{SB60} \\ 4 & \text{S90} \\ 5 & \text{R120} \\ 6 & \text{R180} \\ 7 & \text{SA180} \\ 8 & \text{SB180} \\ 9 & \text{COMPLETE} \end{cases}$$

- $\mathcal{S}_8^t$: (`IELEM`) Type of finite elements:

$$\mathcal{S}_8^t = \begin{cases} < 0 & \text{Order } -\mathcal{S}_8^t \text{ primal finite elements} \\ > 0 & \text{Order } \mathcal{S}_8^t \text{ dual finite elements. The Thomas-Raviart or Thomas-Raviart-Schneider} \\ & \text{method is used except if } \mathcal{S}_9^t = 4 \text{ in which case a mesh-centered finite difference} \\ & \text{approximation is used} \end{cases}$$

- $\mathcal{S}_9^t$: (`ICOL`) Type of quadrature used to integrate the mass matrix:

$$\mathcal{S}_9^t = \begin{cases} 1 & \text{Analytical integration} \\ 2 & \text{Gauss-Lobatto quadrature (finite difference/collocation method)} \\ 3 & \text{Gauss-Legendre quadrature (superconvergent approximation)} \\ 4 & \text{mesh-centered finite difference approximation in hexagonal geometry} \end{cases}$$

- $\mathcal{S}_{10}^t$: (`ISPLH`) Type of hexagonal mesh splitting:

$$\mathcal{S}_{10}^t = \begin{cases} 1 & \text{No mesh splitting; } or \\ & \text{3 lozenges per hexagon with Thomas-Raviart-Schneider approximation} \\ K & \text{6} \times (K-1) \times (K-1) \text{ triangles per hexagon with finite-difference approximations} \\ & \text{3} \times K \times K \text{ lozenges per hexagon with Thomas-Raviart-Schneider approximation} \end{cases}$$

- $\mathcal{S}_{11}^t$: (`LL4`) Order of the group-wise matrices. Generally equal to $\mathcal{S}_2^t$ except in cases where averaged fluxes are appended to the unknown vector. $\mathcal{S}_{11}^t \leq \mathcal{S}_2^t$.

- $\mathcal{S}_{12}^t$: (`LX`) Number of elements along the X axis in Cartesian geometry or number of hexagons.

- $\mathcal{S}_{13}^t$: (`LY`) Number of elements along the Y axis.

- $\mathcal{S}_{14}^t$: (NLF) Number of components in the angular expansion of the flux. Must be a positive even number. Set to zero for diffusion theory. Set to 2 for P_1 method.

- $\mathcal{S}_{15}^t$: (ISPN) Type of transport approximation if NLF$\neq 0$:

$$\mathcal{S}_{15}^t = \left\{ \begin{array}{ll} 0 & \text{Complete } P_n \text{ approximation of order NLF}-1 \\ 1 & \text{Simplified } P_n \text{ approximation of order NLF}-1 \end{array} \right.$$

- $\mathcal{S}_{16}^t$: (ISCAT) Number of terms in the scattering sources if NLF$\neq 0$:

$$\mathcal{S}_{16}^t = \left\{ \begin{array}{ll} 1 & \text{Isotropic scattering in the laboratory system} \\ 2 & \text{Linearly anisotropic scattering in the laboratory system} \\ \text{n} & \text{order } n-1 \text{ anisotropic scattering in the laboratory system} \end{array} \right.$$

A negative value of $\mathcal{S}_{16}^t$ indicates that $1/3D^g$ values are used as Σ_1^g cross sections.

- $\mathcal{S}_{17}^t$: (NVD) Number of base points in the Gauss-Legendre quadrature used to integrate void boundary conditions if ICOL $= 3$ and NLF$\neq 0$:

$$\mathcal{S}_{17}^t = \left\{ \begin{array}{ll} 0 & \text{Use a (NLF+1)–point quadrature consistent with } P_{\text{NLF}-1} \text{ theory} \\ 1 & \text{Use a NLF–point quadrature consistent with } S_{\text{NLF}} \text{ theory} \\ 2 & \text{Use an analytical integration consistent with diffusion theory} \end{array} \right.$$

The following records will also be present on the main level of a /tracking/ directory.

Table 47: The `bivact` records in /tracking/

Name	Type	Condition	Units	Comment
NCODE␣␣␣␣␣␣␣	I(6)			Record containing the types of boundary conditions on each surface. =0 side not used; =1 VOID; =2 REFL; =4 TRAN; =5 SYME; =7 ZERO. NOODE(5) and NOODE(6) are not used.
ZCODE␣␣␣␣␣␣␣	R(6)		1	Record containing the albedo value (real number) on each surface. ZOODE(5) and ZOODE(6) are not used.
SIDE␣␣␣␣␣␣␣␣	R(1)	$\mathcal{S}_6^t = 8$	cm	Side of a hexagon.
XX␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t$)	$\mathcal{S}_6^t \neq 8$	cm	Element-ordered X-directed mesh spacings after mesh-splitting for type 2 and 5 geometries. Element-ordered radius after mesh-splitting for type 3 and 6 geometries.
YY␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t$)	$\mathcal{S}_6^t = 5$ or 6	cm	Element-ordered Y-directed mesh spacings after mesh-splitting for type 5 and 6 geometries.
DD␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t$)	$\mathcal{S}_6^t = 3$ or 6	cm	Element-ordered position used with type 3 and 6 geometries.
KN␣␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_1^t \times N_{\text{kn}}$)			Element-ordered unknown list. N_{kn} is the number of unknowns per element.
QFR␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t \times N_{\text{surf}}$)			Element-ordered boundary condition. $N_{\text{surf}} = 4$ in Cartesian geometry and $= 6$ in hexagonal geometry.
IQFR␣␣␣␣␣␣␣	I($\mathcal{S}_1^t \times N_{\text{surf}}$)			Element-ordered physical albedo indices. $N_{\text{surf}} = 4$ in Cartesian geometry and $= 6$ in hexagonal geometry.

The `bivact` records in /tracking/

Name	Type	Condition	Units	Comment
BFR␣␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_1^t \times N_{\text{surf}})$			Element-ordered boundary surface fractions.
MU␣␣␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t)$			Indices used with compressed diagonal storage mode matrices.
IPERT␣␣␣␣␣␣	$I(\mathcal{S}_{12}^t \times (\mathcal{S}_{10}^t)^2)$	*		Mixture permutation index. This information is provided if and only if $\mathcal{S}_6^t = 8$, $\mathcal{S}_8^t > 0$ and $\mathcal{S}_9^t \leq 3$.
BIVCOL␣␣␣␣␣	Dir			Sub-directory containing the unit matrices (mass, stiffness, nodal coupling, etc.) for a finite element discretization.

The following records will be present on the /BIVCOL/ sub-directory:

Table 48: Description of the /BIVCOL/ sub-directory

Name	Type	Condition	Units	Comment
T␣␣␣␣␣␣␣␣␣␣␣␣␣	$R(L)$			Cartesian linear product vector. $L = |\mathcal{S}_8^t| + 1$
TS␣␣␣␣␣␣␣␣␣␣␣␣	$R(L)$			Cylindrical linear product vector.
R␣␣␣␣␣␣␣␣␣␣␣␣␣	$R(L \times L)$			Cartesian mass matrix.
RS␣␣␣␣␣␣␣␣␣␣␣␣	$R(L \times L)$			Cylindrical mass matrix.
Q␣␣␣␣␣␣␣␣␣␣␣␣␣	$R(L \times L)$			Cartesian stiffness matrix.
QS␣␣␣␣␣␣␣␣␣␣␣␣	$R(L \times L)$			Cylindrical stiffness matrix.
V␣␣␣␣␣␣␣␣␣␣␣␣␣	$R(L \times (L-1))$			Nodal coupling matrix.
H␣␣␣␣␣␣␣␣␣␣␣␣␣	$R(L \times (L-1))$			Piolat transform coupling matrix (used with Thomas-Raviart-Schneider method).
E␣␣␣␣␣␣␣␣␣␣␣␣␣	$R(L \times L)$			Polynomial coefficients.
RH␣␣␣␣␣␣␣␣␣␣␣␣	$R(6{\times}6)$			Hexagonal mass matrix.
QH␣␣␣␣␣␣␣␣␣␣␣␣	$R(6{\times}6)$			Hexagonal stiffness matrix.
RT␣␣␣␣␣␣␣␣␣␣␣␣	$R(3{\times}3)$			Triangular mass matrix.
QT␣␣␣␣␣␣␣␣␣␣␣␣	$R(3{\times}3)$			Triangular stiffness matrix.

4.8 The `trivat` dependent records on a /tracking/ directory

A TRIVAC–type tracking data structure is holding the information related to the ADI partitionning of the system matrices in 1D, 2D or 3D. A one-speed discretizarion of the diffusion equation leads to a matrix system of the form

$$\mathbf{A} \ \vec{\boldsymbol{\Phi}} = \vec{\mathbf{S}} \tag{4.1}$$

where Φ may contains different types of unknowns: flux values, current values, polynomial coefficients, etc.

The matrix $\mathbf{A}$ can be splitted in different ways. Many TRIVAC discretizations in Cartesian geometry are based on the following ADI splitting:

$$\mathbf{A} = \mathbf{U} + \mathbf{P_x}\mathbf{X}\mathbf{P_x^\top} + \mathbf{P_y}\mathbf{Y}\mathbf{P_y^\top} + \mathbf{P_z}\mathbf{Z}\mathbf{P_z^\top} \tag{4.2}$$

where

$$
\begin{aligned}
\mathbf{U} = & \quad \text{matrix containing the diagonal elements of } \mathbf{A} \\
\mathbf{X}, \mathbf{Y}, \mathbf{Z} = & \quad \text{symetrical matrices containing the nondiagonal elements of } \mathbf{A} \\
\mathbf{P_x}, \mathbf{P_y}, \mathbf{P_z} = & \quad \text{permutation matrices that ensure a minimum bandwidth for matrices } \mathbf{X}, \mathbf{Y} \text{ and } \mathbf{Z}.
\end{aligned}
$$

Similarly, many discretizations in hexagonal geometry are based on the following ADI splitting:

$$\mathbf{A} = \mathbf{U} + \mathbf{P_w}\mathbf{W}\mathbf{P_w^\top} + \mathbf{P_x}\mathbf{X}\mathbf{P_x^\top} + \mathbf{P_y}\mathbf{Y}\mathbf{P_y^\top} + \mathbf{P_z}\mathbf{Z}\mathbf{P_z^\top} \quad . \tag{4.3}$$

The diffusion equation can also be solved using a Thomas-Raviart polynomial basis together with a mixte-dual variational formulation. In this case, the following splitting will be used in Cartesian geometry:

$$\mathbf{A} = \begin{pmatrix}
\mathbf{A_x} & \mathbf{0} & \mathbf{0} & -\mathbf{R_x} \\
\mathbf{0} & \mathbf{A_y} & \mathbf{0} & -\mathbf{R_y} \\
\mathbf{0} & \mathbf{0} & \mathbf{A_z} & -\mathbf{R_z} \\
-\mathbf{R_x^\top} & -\mathbf{R_y^\top} & -\mathbf{R_z^\top} & -\mathbf{T}
\end{pmatrix} \tag{4.4}$$

Similarly, we use the following ADI splitting in hexagonal geometry:

$$\mathbf{A} = \begin{pmatrix}
\mathbf{A_w} & \mathbf{C_{xw}^\top} & \mathbf{C_{wy}} & \mathbf{0} & -\mathbf{R_w} \\
\mathbf{C_{xw}} & \mathbf{A_x} & \mathbf{C_{yx}^\top} & \mathbf{0} & -\mathbf{R_x} \\
\mathbf{C_{wy}^\top} & \mathbf{C_{yx}} & \mathbf{A_y} & \mathbf{0} & -\mathbf{R_y} \\
\mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{A_z} & -\mathbf{R_z} \\
-\mathbf{R_w^\top} & -\mathbf{R_x^\top} & -\mathbf{R_y^\top} & -\mathbf{R_z^\top} & -\mathbf{T}
\end{pmatrix} \tag{4.5}$$

When the `TRIVAT:` operator is used (`CDOOR='TRIVAC'`), the following elements in the vector $\mathcal{S}_i^t$ will also be defined.

- $\mathcal{S}_6^t$: (`ITYPE`) Type of TRIVAC geometry:

$$
\mathcal{S}_6^t = \begin{cases}
2 & \text{Cartesian 1-D geometry} \\
3 & \text{Tube 1-D geometry} \\
5 & \text{Cartesian 2-D geometry} \\
6 & \text{Tube 2-D geometry} \\
7 & \text{Cartesian 3-D geometry} \\
8 & \text{Hexagonal 2-D geometry} \\
9 & \text{Hexagonal 3-D geometry}
\end{cases}
$$

- $\mathcal{S}_7^t$: (IHEX) Type of hexagonal symmetry if $\mathcal{S}_6^t \geq 8$:

$$\mathcal{S}_7^t = \begin{cases} 0 & \text{non-hexagonal geometry} \\ 1 & \text{S30} \\ 2 & \text{SA60} \\ 3 & \text{SB60} \\ 4 & \text{S90} \\ 5 & \text{R120} \\ 6 & \text{R180} \\ 7 & \text{SA180} \\ 8 & \text{SB180} \\ 9 & \text{COMPLETE} \end{cases}$$

- $\mathcal{S}_8^t$: (IDIAG) Diagonal symmetry flag if $\mathcal{S}_6^t = 5$ or $= 7$. $\mathcal{S}_8^t = 1$ if diagonal symmetry is present.

- $\mathcal{S}_9^t$: (IELEM) Type of finite elements:

$$\mathcal{S}_9^t = \begin{cases} < 0 & \text{Order } -\mathcal{S}_9^t \text{ primal finite elements} \\ > 0 & \text{Order } \mathcal{S}_9^t \text{ dual finite elements} \end{cases}$$

- $\mathcal{S}_{10}^t$: (ICOL) Type of quadrature used to integrate the mass matrix:

$$\mathcal{S}_{10}^t = \begin{cases} 1 & \text{Analytical integration} \\ 2 & \text{Gauss-Lobatto quadrature (finite difference/collocation method)} \\ 3 & \text{Gauss-Legendre quadrature (superconvergent approximation)} \end{cases}$$

- $\mathcal{S}_{11}^t$: (LL4) Order of the group-wise matrices. Generally equal to $\mathcal{S}_2^t$ except in cases where averaged fluxes are appended to the unknown vector. $\mathcal{S}_{11}^t \leq \mathcal{S}_2^t$.

- $\mathcal{S}_{12}^t$: (ICHX) Type of discretization algorithm:

$$\mathcal{S}_{12}^t = \begin{cases} 1 & \text{Variational collocation method (mesh-corner finite differences or primal finite} \\ & \text{elements with Gauss-Lobatto quadrature). Eq. (4.2) or Eq. (4.3) is used.} \\ 2 & \text{Dual finite element approximation (Thomas-Raviart or Thomas-Raviart-Schneider} \\ & \text{polynomial basis). Eq. (4.4) or Eq. (4.5) is used.} \\ 3 & \text{Nodal collocation method with full tensorial products (mesh-centered finite} \\ & \text{differences or dual finite elements with Gauss-Lobatto quadrature). Eq. (4.2) or} \\ & \text{Eq. (4.3) is used.} \\ 4 & \text{Nodal expansion method (NEM).} \end{cases}$$

- $\mathcal{S}_{13}^t$: (ISPLH) Type of hexagonal mesh splitting if $\mathcal{S}_6^t \geq 8$:

$$\mathcal{S}_{13}^t = \begin{cases} 1 & \text{No mesh splitting (full hexagons); } or \\ & \text{3 lozenges per hexagon with Thomas-Raviart-Schneider approximation} \\ K & 6 \times (K-1) \times (K-1) \text{ triangles per hexagon with finite-difference approximations} \\ & 3 \times K \times K \text{ lozenges per hexagon with Thomas-Raviart-Schneider approximation} \end{cases}$$

- $\mathcal{S}_{14}^t$: (LX) Number of elements along the X axis in Cartesian geometry or number of hexagons in one axial plane.

- $\mathcal{S}_{15}^t$: (LY) Number of elements along the Y axis.

- $\mathcal{S}_{16}^t$: (LZ) Number of elements along the Z axis.

- $\mathcal{S}_{17}^t$: (ISEG) Number of components in a vector register (used for supervectorial operations). Equal to zero for operations in scalar mode.

- $\mathcal{S}_{18}^t$: (IMPV) Print parameter for supervectorial operations.

- $\mathcal{S}_{19}^t$: (LTSW) Maximum bandwidth for supervectorial operations ($= 2$ for tridiagonal matrices).

- $\mathcal{S}_{20}^t$: (LONW) number of groups of linear systems for matrices $\mathbf{W} + \mathbf{P_w^\top U P_w}$ or $\mathbf{A_w} + \mathbf{R_w T^{-1} R_w^\top}$ (used for supervectorial operations)

- $\mathcal{S}_{21}^t$: (LONX) number of groups of linear systems for matrices $\mathbf{X} + \mathbf{P_x^\top U P_x}$ or $\mathbf{A_x} + \mathbf{R_x T^{-1} R_x^\top}$ (used for supervectorial operations)

- $\mathcal{S}_{22}^t$: (LONY) number of groups of linear systems for matrices $\mathbf{Y} + \mathbf{P_y^\top U P_y}$ or $\mathbf{A_y} + \mathbf{R_y T^{-1} R_y^\top}$ (used for supervectorial operations)

- $\mathcal{S}_{23}^t$: (LONZ) number of groups of linear systems for matrices $\mathbf{Z} + \mathbf{P_z^\top U P_z}$ or $\mathbf{A_z} + \mathbf{R_z T^{-1} R_z^\top}$ (used for supervectorial operations)

- $\mathcal{S}_{24}^t$: (NRO) Number of radii used with the cylindrical correction algorithm for the albedos. Equal to zero if no cylindrical correction is applied.

- $\mathcal{S}_{25}^t$: (LL4F) Order of matrices $\mathbf{T}$ if $\mathcal{S}_{12}^t = 2$

- $\mathcal{S}_{26}^t$: (LL4W) Order of matrices $\mathbf{A_w}$ if $\mathcal{S}_{12}^t = 2$

- $\mathcal{S}_{27}^t$: (LL4X) Order of matrices $\mathbf{A_x}$ if $\mathcal{S}_{12}^t = 2$

- $\mathcal{S}_{28}^t$: (LL4Y) Order of matrices $\mathbf{A_y}$ if $\mathcal{S}_{12}^t = 2$

- $\mathcal{S}_{29}^t$: (LL4Z) Order of matrices $\mathbf{A_z}$ if $\mathcal{S}_{12}^t = 2$

- $\mathcal{S}_{30}^t$: (NLF) Number of components in the angular expansion of the flux. Must be a positive even number. Set to zero for diffusion theory. Set to 2 for P_1 method.

- $\mathcal{S}_{31}^t$: (ISPN) Type of transport approximation if NLF$\neq 0$:

$$\mathcal{S}_{31}^t = \begin{cases} 0 & \text{Complete } P_n \text{ approximation of order NLF}-1 \text{ (currently not available)} \\ 1 & \text{Simplified } P_n \text{ approximation of order NLF}-1 \end{cases}$$

- $\mathcal{S}_{32}^t$: (ISCAT) Number of terms in the scattering sources if NLF$\neq 0$:

$$\mathcal{S}_{32}^t = \begin{cases} 1 & \text{Isotropic scattering in the laboratory system} \\ 2 & \text{Linearly anisotropic scattering in the laboratory system} \\ \text{n} & \text{order } n-1 \text{ anisotropic scattering in the laboratory system} \end{cases}$$

A negative value of $\mathcal{S}_{32}^t$ indicates that $1/3D^g$ values are used as Σ_1^g cross sections.

- $\mathcal{S}_{33}^t$: (NADI) Number of ADI iterations at the inner iterative level.

- $\mathcal{S}_{34}^t$: (NVD) Number of base points in the Gauss-Legendre quadrature used to integrate void boundary conditions if ICOL $= 3$ and NLF$\neq 0$:

$$\mathcal{S}_{34}^t = \begin{cases} 0 & \text{Use a (NLF}+1)\text{–point quadrature consistent with } P_{\text{NLF}-1} \text{ theory} \\ 1 & \text{Use a NLF–point quadrature consistent with } S_{\text{NLF}} \text{ theory} \\ 2 & \text{Use an analytical integration consistent with diffusion theory.} \end{cases}$$

- $\mathcal{S}_{38}^t$: (LUMP) Unknown lumping option with the nodal expansion method (NEM):

$$\mathcal{S}_{38}^t = \begin{cases} 0 & \text{The averaged nodal fluxes and nodal expansion coefficients are saved in the} \\ & \text{flux unknow vector} \\ 1 & \text{Only the averaged nodal fluxes are saved in the flux unknow vector.} \end{cases}$$

- $\mathcal{S}_{39}^t$: (IGMAX) Hyperbolic nodal expansion functions are used in energy groups indices $\geq$ IGMAX.

The following records will also be present on the main level of a /tracking/ directory.

Table 49: The `trivat` records in /tracking/

Name	Type	Condition	Units	Comment
NCODE␣␣␣␣␣␣␣	I(6)			Record containing the types of boundary conditions on each surface. =0 side not used; =1 VOID; =2 REFL; =4 TRAN; =5 SYME; =7 ZERO; =8 CYLI.
ZCODE␣␣␣␣␣␣␣	R(6)		1	Record containing the albedo value (real number) on each surface.
SIDE␣␣␣␣␣␣␣␣	R(1)	$\mathcal{S}_6^t \geq 8$	cm	Side of a hexagon.
XX␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t$)	$\mathcal{S}_6^t < 8$	cm	Element-ordered X-directed mesh spacings after mesh-splitting for type 2, 5 or 7 geometries. Element-ordered radius after mesh-splitting for type 3 or 6 geometries.
YY␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t$)	$\mathcal{S}_6^t = 5$, 6 or 7	cm	Element-ordered Y-directed mesh spacings after mesh-splitting for type 5, 6 or 7 geometries.
ZZ␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t$)	$\mathcal{S}_6^t = 7$ or 9	cm	Element-ordered Y-directed mesh spacings after mesh-splitting for type 7 or 9 geometries.
DD␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t$)	$\mathcal{S}_6^t = 3$ or 6	cm	Element-ordered position used with type 3 and 6 cylindrical geometries.
KN␣␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_1^t \times N_{\mathrm{kn}}$)			Element-ordered unknown list. N_{kn} is the number of unknowns per element.
QFR␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_1^t \times N_{\mathrm{surf}}$)			Element-ordered boundary condition. $N_{\mathrm{surf}} = 6$ in Cartesian geometry and $= 8$ in hexagonal geometry.
IQFR␣␣␣␣␣␣␣␣	I($\mathcal{S}_1^t \times N_{\mathrm{surf}}$)			Element-ordered physical albedo indices. $N_{\mathrm{surf}} = 6$ in Cartesian geometry and $= 8$ in hexagonal geometry.
MUW␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_{11}^t$ or $\mathcal{S}_{26}^t$)	$\mathcal{S}_6^t \geq 8$		Indices used with compressed diagonal storage mode matrices $\mathbf{W} + \mathbf{P_w^\top U P_w}$ or $\mathbf{A_w} + \mathbf{R_w T^{-1} R_w^\top}$.
IPW␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_{11}^t$)	$\mathcal{S}_6^t \geq 8$		Permutation vector ensuring minimum bandwidth for matrices $\mathbf{W} + \mathbf{P_w^\top U P_w}$ or $\mathbf{A_w} + \mathbf{R_w T^{-1} R_w^\top}$.
MUX␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_{11}^t$ or $\mathcal{S}_{27}^t$)	$\mathcal{S}_8^t = 0$		Indices used with compressed diagonal storage mode matrices $\mathbf{X} + \mathbf{P_x^\top U P_x}$ or $\mathbf{A_x} + \mathbf{R_x T^{-1} R_x^\top}$.
IPX␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_{11}^t$)			Permutation vector ensuring minimum bandwidth for matrices $\mathbf{X} + \mathbf{P_x^\top U P_x}$ or $\mathbf{A_x} + \mathbf{R_x T^{-1} R_x^\top}$.
MUY␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_{11}^t$ or $\mathcal{S}_{28}^t$)	$\mathcal{S}_6^t \geq 5$		Indices used with compressed diagonal storage mode matrices $\mathbf{Y} + \mathbf{P_y^\top U P_y}$ or $\mathbf{A_y} + \mathbf{R_y T^{-1} R_y^\top}$.
IPY␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_{11}^t$)	$\mathcal{S}_6^t \geq 5$		Permutation vector ensuring minimum bandwidth for matrices $\mathbf{Y} + \mathbf{P_y^\top U P_y}$ or $\mathbf{A_y} + \mathbf{R_y T^{-1} R_y^\top}$.
MUZ␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_{11}^t$ or $\mathcal{S}_{29}^t$)	$\mathcal{S}_6^t = 7$ or 9		Indices used with compressed diagonal storage mode matrices $\mathbf{Z} + \mathbf{P_z^\top U P_z}$ or $\mathbf{A_z} + \mathbf{R_z T^{-1} R_z^\top}$.
IPZ␣␣␣␣␣␣␣␣␣	I($\mathcal{S}_{11}^t$)	$\mathcal{S}_6^t = 7$ or 9		Permutation vector ensuring minimum bandwidth for matrices $\mathbf{Z} + \mathbf{P_z^\top U P_z}$ or $\mathbf{A_z} + \mathbf{R_z T^{-1} R_z^\top}$.
BIVCOL␣␣␣␣␣␣	Dir			Sub-directory containing the unit matrices (mass, stiffness, nodal coupling, etc.) for a finite element discretization. The specification of this directory is given in Section 4.7

The following records will also be present on the main level of a /tracking/ directory in cases where

a Thomas-Raviart or Thomas-Raviart-Schneider polynomial basis is used ($\mathcal{S}_{12}^t = 2$):

Table 50: The `trivat` records in /tracking/ (contd.)

Name	Type	Condition	UnitsComment
IPF␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{25}^t)$	$\mathcal{S}_{25}^t \neq 0$	Localization vector for flux values in unknown vector.
IPBBW␣␣␣␣␣␣	$I(2\,\mathcal{S}_9^t \times \mathcal{S}_{26}^t)$	$\mathcal{S}_{26}^t \neq 0$	Perdue sparse storage indices for matrices $\mathbf{R_w}$.
IPBBX␣␣␣␣␣␣	$I(2\,\mathcal{S}_9^t \times \mathcal{S}_{27}^t)$	$\mathcal{S}_{27}^t \neq 0$	Perdue sparse storage indices for matrices $\mathbf{R_x}$.
IPBBY␣␣␣␣␣␣	$I(2\,\mathcal{S}_9^t \times \mathcal{S}_{28}^t)$	$\mathcal{S}_{28}^t \neq 0$	Perdue sparse storage indices for matrices $\mathbf{R_y}$.
IPBBZ␣␣␣␣␣␣	$I(2\,\mathcal{S}_9^t \times \mathcal{S}_{29}^t)$	$\mathcal{S}_{29}^t \neq 0$	Perdue sparse storage indices for matrices $\mathbf{R_z}$.
WB␣␣␣␣␣␣␣␣␣␣	$R(2\,\mathcal{S}_9^t \times \mathcal{S}_{26}^t)$	$\mathcal{S}_{26}^t \neq 0$	Matrix component $\mathbf{R_w}$ in Perdue sparse storage mode.
XB␣␣␣␣␣␣␣␣␣␣	$R(2\,\mathcal{S}_9^t \times \mathcal{S}_{27}^t)$	$\mathcal{S}_{27}^t \neq 0$	Matrix component $\mathbf{R_x}$ in Perdue sparse storage mode.
YB␣␣␣␣␣␣␣␣␣␣	$R(2\,\mathcal{S}_9^t \times \mathcal{S}_{28}^t)$	$\mathcal{S}_{28}^t \neq 0$	Matrix component $\mathbf{R_y}$ in Perdue sparse storage mode.
ZB␣␣␣␣␣␣␣␣␣␣	$R(2\,\mathcal{S}_9^t \times \mathcal{S}_{29}^t)$	$\mathcal{S}_{29}^t \neq 0$	Matrix component $\mathbf{R_z}$ in Perdue sparse storage mode.
IPERT␣␣␣␣␣␣	$I(N_{\text{los}})$	$\mathcal{S}_6^t \geq 8$	Mixture permutation index. $N_{\text{los}} = \mathcal{S}_{14}^t \times \mathcal{S}_{15}^t \times (\mathcal{S}_{13}^t)^2$
CTRAN␣␣␣␣␣␣	$D(N_{\text{pio}} \times N_{\text{pio}})$	$\mathcal{S}_6^t \geq 8$	Piolat current coupling matrix. $N_{\text{pio}} = (\mathcal{S}_9^t + 1) \times \mathcal{S}_9^t$
FRZ␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{16}^t)$	$\mathcal{S}_6^t \geq 8$	Volume fractions related to the SYME boundary condition in Z.

The following records will also be present on the main level of a /tracking/ directory in cases where supervectorial operations are used ($\mathcal{S}_{17}^t \neq 0$):

Table 51: The `trivat` records in /tracking/ (contd.)

Name	Type	Condition	UnitsComment
LL4VW␣␣␣␣␣␣	$I(1)$		Order of a reordered $W-$matrix, including supervectorial fill-in. Multiple of $\mathcal{S}_{17}^t$
LL4VX␣␣␣␣␣␣	$I(1)$		Order of a reordered $X-$matrix, including supervectorial fill-in. Multiple of $\mathcal{S}_{17}^t$
LL4VY␣␣␣␣␣␣	$I(1)$		Order of a reordered $Y-$matrix, including supervectorial fill-in. Multiple of $\mathcal{S}_{17}^t$
LL4VZ␣␣␣␣␣␣	$I(1)$		Order of a reordered $Z-$matrix, including supervectorial fill-in. Multiple of $\mathcal{S}_{17}^t$
NBLW␣␣␣␣␣␣␣	$I(\mathcal{S}_{20}^t)$	$\mathcal{S}_{20}^t \neq 0$	Number of linear systems per supervector group for $W-$matrices
NBLX␣␣␣␣␣␣␣	$I(\mathcal{S}_{21}^t)$	$\mathcal{S}_{21}^t \neq 0$	Number of linear systems per supervector group for $X-$matrices

The `trivat` records in /tracking/ (contd.)

Name	Type	Condition	UnitsComment
NBLY␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{22}^t)$	$\mathcal{S}_{22}^t \neq 0$	Number of linear systems per supervector group for $Y-$matrices
NBLZ␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{23}^t)$	$\mathcal{S}_{23}^t \neq 0$	Number of linear systems per supervector group for $Z-$matrices
LBLW␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{20}^t)$	$\mathcal{S}_{20}^t \neq 0$	Number of unknowns per supervector group for $W-$matrices
LBLX␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{21}^t)$	$\mathcal{S}_{21}^t \neq 0$	Number of unknowns per supervector group for $X-$matrices
LBLY␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{22}^t)$	$\mathcal{S}_{22}^t \neq 0$	Number of unknowns per supervector group for $Y-$matrices
LBLZ␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{23}^t)$	$\mathcal{S}_{23}^t \neq 0$	Number of unknowns per supervector group for $Z-$matrices
MUVW␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t$ or $\mathcal{S}_{26}^t)$	$\mathcal{S}_{6}^t \geq 8$	Indices used with $W-$directed compressed diagonal storage mode matrices in supervector mode
MUVX␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t$ or $\mathcal{S}_{27}^t)$	$\mathcal{S}_{8}^t = 0$	Indices used with $X-$directed compressed diagonal storage mode matrices in supervector mode
MUVY␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t$ or $\mathcal{S}_{28}^t)$	$\mathcal{S}_{6}^t \geq 5$	Indices used with $Y-$directed compressed diagonal storage mode matrices in supervector mode
MUVZ␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t$ or $\mathcal{S}_{29}^t)$	$\mathcal{S}_{6}^t = 7$ or 9	Indices used with $Z-$directed compressed diagonal storage mode matrices in supervector mode
IPVW␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t)$	$\mathcal{S}_{6}^t \geq 8$	$W-$directed ADI permutation matrix in supervector mode
IPVX␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t)$		$X-$directed ADI permutation matrix in supervector mode
IPVY␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t)$	$\mathcal{S}_{6}^t \geq 5$	$Y-$directed ADI permutation matrix in supervector mode
IPVZ␣␣␣␣␣␣␣␣␣	$I(\mathcal{S}_{11}^t)$	$\mathcal{S}_{6}^t = 7$ or 9	$Z-$directed ADI permutation matrix in supervector mode

The following records will also be present on the main level of a /tracking/ directory in cases where a cylindrical correction of the albedos is used ($\mathcal{S}_{24}^t \neq 0$):

Table 52: The `trivat` records in /tracking/ (contd.)

Name	Type	Condition	Units	Comment
RRO␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{24}^t)$	$\mathcal{S}_{24}^t \neq 0$	cm	Radii of the cylindrical boundaries in the cylindrical correction
XRO␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{24}^t)$	$\mathcal{S}_{24}^t \neq 0$	cm	Coordinates on principal axis in the cylindrical correction
ANG␣␣␣␣␣␣␣␣␣	$R(\mathcal{S}_{24}^t)$	$\mathcal{S}_{24}^t \neq 0$	1	Angles for applying the cylindrical correction

4.9 The /BIHET/ sub-directory

Table 53: The contents of the /BIHET/ sub-directory

Name	Type	Condition	Units	Comment
PARAM␣␣␣␣␣␣␣	I(8)			Record containing the parameters related to a double-heterogeneity tracking $\mathcal{P}_i$
NS␣␣␣␣␣␣␣␣␣␣	I($\mathcal{P}_4$)			Number of tubes or shells in each kind of micro structure
IBI␣␣␣␣␣␣␣␣␣	I($\mathcal{P}_3$)			Type of mixture in each generating region of the macro geometry
VOLUME␣␣␣␣␣␣	R($\mathcal{P}_3$)		cm^3	Volumes of the macro geometry
RS␣␣␣␣␣␣␣␣␣␣	R($\mathcal{P}_5 + 1, \mathcal{P}_4$)		cm	Radii of the micro regions
FRACT␣␣␣␣␣␣	R($\mathcal{P}_4, \mathcal{P}_2$)			Volume fraction of each type of micro region in each mixture
VOLK␣␣␣␣␣␣␣␣	R($\mathcal{P}_4, \mathcal{P}_5$)			Volume fractions of the tubes or shells in the micro regions
IDIL␣␣␣␣␣␣␣␣	I($\mathcal{P}_2 - \mathcal{P}_1$)			Elementary mixture indices in the diluent of the composite mixtures
MIXGR␣␣␣␣␣␣	I($\mathcal{P}_5, \mathcal{P}_4, \mathcal{P}_2 - \mathcal{P}_1$)			Elementary mixture indices in the micro structures

with the dimension parameter $\mathcal{P}_i$, representing:

- The number of ordinary mixtures pointing to the macrolib. $\mathcal{P}_1$

- The number of mixtures, including the composite mixtures (i.e., containing micro structures) $\mathcal{P}_2$

- The number of regions in the macro geometry $\mathcal{P}_3$

- The number of different kinds of macro structures $\mathcal{P}_4 = \mathcal{S}_1^{dh}$

  A kind of macro structure is characterized by the radii of its tubes or shells. All the micro region of the same kind should own the same nuclear properties in a given macro region.

- The maximum number of regions (tubes or shells) in each kind of macro structure $\mathcal{P}_5 = \mathcal{S}_2^{dh} - 1$

- The type of double-heterogeneity model $\mathcal{P}_6$ where

$$\mathcal{P}_6 = \begin{cases} 1 & \text{Sanchez-Pomraning model} \\ 2 & \text{Hebert model} \\ 3 & \text{She-Liu-Shi model} \end{cases}$$

- The type of micro structures $\mathcal{P}_7 = \mathcal{S}_5^{dh}$ where

$$\mathcal{P}_7 = \begin{cases} 3 & \text{Cylinder} \\ 4 & \text{Sphere} \end{cases}$$

- The quadrature parameter for the 1-D collision probability calculation in the micro structures $\mathcal{P}_8$

5 Contents of a /asminfo/ directory

This directory contains the multigroup collision probabilities and response matrices required in the solution of the transport equation.

5.1 State vector content for the /asminfo/ data structure

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}_i^a$, represent:

- The type of collision probabilities considered $I_T = \mathcal{S}_1^a$ where

$$
I_T = \begin{cases}
1 & \text{Scattering reduced collision probability or response matrix} \\
2 & \text{Direct collision probability or response matrix} \\
3 & \text{Scattering reduced directional collision probability} \\
4 & \text{Direct directional collision probability}
\end{cases}
$$

- The type of collision probability closure relation used $I_C = \mathcal{S}_2^a$ (see `NORM` keyword in `ASM:` operator input option)

$$
I_C = \begin{cases}
0 & \text{No closure relation used} \\
1 & \text{Total reflection closure relation}
\end{cases}
$$

- A parameter related to the albedo leakage model $I_\beta = \mathcal{S}_3^a$ (see `ALSB` keyword in `ASM:` operator input option)

$$
I_\beta = \begin{cases}
0 & \text{No information is stored} \\
1 & \text{Groupwise escape matrices WIS are stored}
\end{cases}
$$

- $\mathcal{S}_4^a$ (not used)

- The option to indicate whether response matrix or collision probability matrices are stored on the structure $I_p = \mathcal{S}_5^a$ (see `PIJ` and `ARM` keyword in `ASM:` operator input option)

$$
I_p = \begin{cases}
1 & \text{Response matrices will be stored (the ARM keyword was selected)} \\
2 & \text{Collision probability matrices will be stored (the PIJ keyword was selected)}
\end{cases}
$$

- The option to indicate the type of streaming model used $I_k = \mathcal{S}_6^a$ (see `PIJK` and `ECCO` keyword in `ASM:` operator input option)

$$
I_k = \begin{cases}
1 & \text{No streaming model used (a leakage model may or may not be used)} \\
2 & \text{Isotropic streaming model used (ECCO model)} \\
3 & \text{Anisotropic streaming model used (TIBÈRE model)}
\end{cases}
$$

- The type of collision probability normalization method used $I_n = \mathcal{S}_7^a$ (see `PNOR` keyword in `ASM:` operator input option)

$$
I_n = \begin{cases}
0 & \text{No normalization} \\
1 & \text{Gelbard normalization algorithm} \\
2 & \text{Diagonal element normalization} \\
3 & \text{Non-linear normalization} \\
4 & \text{Helios type normalization}
\end{cases}
$$

- Number of energy groups $G = \mathcal{S}_8^a$

- Number of unknown in flux system $N_u = \mathcal{S}_9^a$

- Number of mixtures $N_m = \mathcal{S}_{10}^a$

- Number of Legendre orders of the scattering cross sections used in the main transport solution. $N_{\mathrm{ans}} = \mathcal{S}_{11}^a$

- Flag for the availability of diffusion coefficients. $I_{\mathrm{diff}} = \mathcal{S}_{12}^a$

$$I_{\mathrm{diff}} = \begin{cases} 0 & \text{No diffusion coefficients available;} \\ 1 & \text{Diffusion coefficients are available.} \end{cases}$$

- Type of equation solved. $I_{\mathrm{bfp}} = \mathcal{S}_{13}^a$

$$\mathcal{S}_{13}^t = \begin{cases} 0 & \text{Boltzmann transport equation} \\ 1 & \text{Boltzmann Fokker-Planck equation with Galarkin energy propagation factors} \\ 2 & \text{Boltzmann Fokker-Planck equation with Przybylski and Ligou energy propagation} \\ & \text{factors.} \end{cases}$$

5.2 The main /asminfo/ directory

On its first level, the following records and sub-directories will be found in the /asminfo/ directory:

Table 54: Main records and sub-directories in /asminfo/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C*12			Signature of the data structure (SIGNA =L␣PIJ␣␣␣␣␣␣␣).
LINK.MACRO␣␣	C*12			Name of the MACROLIB on which the collision probabilities are based.
LINK.TRACK␣␣	C*12			Name of the TRACKING on which the collision probabilities are based.
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^a$, as defined in Section 5.1.
GROUP␣␣␣␣␣␣␣	Dir($\mathcal{S}_8^a$)			List of energy-group sub-directories. Each component of the list is a directory containing the multi-group collision probabilities and response matrices associated with an energy group. The specification of this directory is given in Sect. 5.3 or 5.4 depending if a double-heterogeneity is present or not. A double-heterogeneity is present if $\mathcal{S}_{40}^t = 1$ in the TRACKING object.

5.3 The `GROUP` double-heterogeneity group sub-directory

This directory is containing the following records, corresponding to a single energy group:

Table 55: Records and sub-directories in `GROUP`

Name	Type	Condition	Units Comment
`DRAGON-TXSC␣`	$R(N_m + 1)$		cm^{-1} where $N_m = \mathcal{P}_1$. The total cross section Σ_m^g for $N_m + 1$ composite mixtures assuming that the first mixture represents void ($\Sigma_m^g = 0$). A transport correction may or may not be included. The first component of this array is always equal to 0.
`DRAGON-SOXSC`	$R(N_m + 1, N_{ans})$		cm^{-1} The within group scattering cross section $\Sigma_{0,m,w}$ (see Section 1.3) for $N_m + 1$ composite mixtures assuming that the first mixture represents void ($\Sigma_{0,m,w}^g = 0$). A transport correction may or may not be included. Many Legendre orders may be given. The first component of this array, for each Legendre order, is always equal to 0.
`NCO␣␣␣␣␣␣␣␣␣`	$I(\mathcal{M})$		where $\mathcal{M} = \mathcal{P}_2 - \mathcal{P}_1$. Number of composite mixtures in each macro-mixture.
`RRRR␣␣␣␣␣␣␣␣`	$R(\mathcal{M})$	$\mathcal{P}_6 = 1, 2$	Group-dependent double-heterogeneity information.
`QKOLD␣␣␣␣␣␣␣`	$R(\mathcal{P}_4, \mathcal{P}_5, \mathcal{M})$	$\mathcal{P}_6 = 1$	Group-dependent double-heterogeneity information related to the escape probabilities in the micro-structures.
`QKDEL␣␣␣␣␣␣␣`	$R(\mathcal{P}_4, \mathcal{P}_5, \mathcal{M})$	$\mathcal{P}_6 = 1, 2$	Group-dependent double-heterogeneity information related to the escape probabilities in the micro-structures.
`PKL␣␣␣␣␣␣␣␣␣`	$R(\mathcal{P}_4, \mathcal{P}_5, \mathcal{P}_5, \mathcal{M})$	$\mathcal{P}_6 = 1, 2$	Group-dependent double-heterogeneity information related to the collision probabilities in the micro-structures.
`COEF␣␣␣␣␣␣␣␣`	$D(\mathcal{F}, \mathcal{F}, \mathcal{M})$	$\mathcal{P}_6 = 1, 2$	where $\mathcal{F} = 1 + \mathcal{P}_4 \times \mathcal{P}_5$. Group-dependent double-heterogeneity information.
`P1I␣␣␣␣␣␣␣␣␣`	$R(\mathcal{P}_4, \mathcal{M})$	$\mathcal{P}_6 = 3$	Group-dependent double-heterogeneity information related to the escape probabilities through the composite.
`P1DI␣␣␣␣␣␣␣␣`	$R(\mathcal{P}_4, \mathcal{M})$	$\mathcal{P}_6 = 3$	Group-dependent double-heterogeneity information related to the escape probabilities from the matrix.
`P1KI␣␣␣␣␣␣␣␣`	$R(\mathcal{P}_4, \mathcal{P}_5, \mathcal{M})$	$\mathcal{P}_6 = 3$	Group-dependent double-heterogeneity information related to the escape probabilities from the micro-structures.
`SIGA1␣␣␣␣␣␣␣`	$R(\mathcal{P}_4, \mathcal{M})$	$\mathcal{P}_6 = 3$	Group-dependent double-heterogeneity information related to the equivalent total cross-section.

Records and sub-directories in `GROUP`   continued from last page

Name	Type	Condition	Units	Comment
`BIHET␣␣␣␣␣␣␣`	Dir			Directory containing collision probability or response matrix information related to the macro-geometry (i.e., the geometry with homogenized micro-structures). The specification of this directory is given in Section 5.4. Note that the value of $N_m = \mathcal{P}_2$ in this object is set to take into account the macro-mixtures. Similarly, the value $N_r = \mathcal{P}_3$ is the number of macro-volumes.

5.4   The `GROUP` or `BIHET` group sub-directory

This directory is containing the following records, corresponding to a single energy group:

Table 56: Records and sub-directories in `GROUP`

Name	Type	Condition	Units	Comment
`ALBEDO␣␣␣␣␣␣`	$R(\mathcal{S}_8^M)$	$\mathcal{S}_8^M > 0$		Surface ordered physical albedos in `GROUP`. The number of physical albedos $\mathcal{S}_8^M$ is defined in Section 1.1.
`ALBEDO-FU␣␣␣`	$R(\mathcal{S}_8^M)$	$\mathcal{S}_8^M > 0$		Surface ordered physical albedo functions in `GROUP`. The number of physical albedos $\mathcal{S}_8^M$ is defined in Section 1.1.
`DRAGON-TXSC␣`	$R(N_m + 1)$		cm^{-1}	The total cross section Σ_m^g for $N_m + 1$ mixtures assuming that the first mixture represents void ($\Sigma_m^g = 0$). A transport correction may or may not be included. The first component of this array is always equal to 0.
`DRAGON-T1XSC`	$R(N_m + 1)$	*	cm^{-1}	where $N_m = \mathcal{P}_1$. The current-weighted total cross section $\Sigma_{1,m}^g$ for $N_m + 1$ composite mixtures assuming that the first mixture represents void ($\Sigma_{1,m}^g = 0$). The first component of this array is always equal to 0.
`DRAGON-T2XSC`	$R(N_m + 1)$	*	cm^{-1}	where $N_m = \mathcal{P}_1$. The second moment-weighted total cross section $\Sigma_{2,m}^g$ for $N_m + 1$ composite mixtures assuming that the first mixture represents void ($\Sigma_{2,m}^g = 0$). The first component of this array is always equal to 0.

Name	Type	Condition	Units	Comment
`DRAGON-SOXSC`	$R(N_m + 1, N_{\mathrm{ans}})$		cm^{-1}	The within group scattering cross section $\Sigma_{0,m,w}$ (see Section 1.3) for $N_m + 1$ mixtures assuming that the first mixture represents void ($\Sigma_{0,m,w}^g = 0$). A transport correction may or may not be included. Many Legendre orders may be given. The first component of this array, for each Legendre order, is always equal to 0.
`DRAGON-DIFF␣`	$R(N_m + 1)$	$I_{\mathrm{diff}} = 1$	cm	Diffusion coefficients D_m^g for $N_m + 1$ mixtures assuming that the first mixture represents void ($D_m^g = 1.0 \times 10^{10}$). The first component of this array is always equal to 1.0×10^{10}.
`STREAMING␣␣␣`	Dir	$I_k = 2$		Directory containing P1 information to be used with the ECCO isotropic streaming model. This directory uses the same specification as `GROUP` where P0 information is replaced with P1 information. Cross sections used in this directory are *not*–transport corrected.

5.4.1 The `trafict` dependent records on a `GROUP` directory

If a collision probability method is used, the following records will also be found on the group subdirectory:

Table 57: Collision probability records in `GROUP`

Name	Type	Condition	Units	Comment
`DRAGON-PCSCT`	$R(N_r, N_r)$	$I_p = 2$		The scattering-reduced ($I_T = 1, 3$) collision probability matrix $\mathbf{W}_g$ or direct ($I_T = 2, 4$) collision probability matrix $\mathbf{p}_g$
`DRAGON1PCSCT`	$R(N_r, N_r)$	$I_k = 3$		The x−directed P1 scattering-reduced ($I_T = 3$) collision probability matrix $\mathbf{Y}_{x,g}$ or direct ($I_T = 4$) collision probability matrix $\mathbf{p}_{x,g}$
`DRAGON2PCSCT`	$R(N_r, N_r)$	$I_k = 3$		The y−directed P1 scattering-reduced ($I_T = 3$) collision probability matrix $\mathbf{Y}_{y,g}$ or direct ($I_T = 4$) collision probability matrix $\mathbf{p}_{y,g}$
`DRAGON3PCSCT`	$R(N_r, N_r)$	$I_k = 3$		The z−directed P1 scattering-reduced ($I_T = 3$) collision probability matrix $\mathbf{Y}_{z,g}$ or direct ($I_T = 4$) collision probability matrix $\mathbf{p}_{z,g}$

Collision probability records in `GROUP`

Name	Type	Condition	Units	Comment
`DRAGON1P*SCT`	$R(N_r, N_r)$	$I_k = 3$		The x−directed matrix $\mathbf{p}_g^{-1}\mathbf{p}_{x,g}^*$
`DRAGON2P*SCT`	$R(N_r, N_r)$	$I_k = 3$		The y−directed matrix $\mathbf{p}_g^{-1}\mathbf{p}_{y,g}^*$
`DRAGON3P*SCT`	$R(N_r, N_r)$	$I_k = 3$		The z−directed matrix $\mathbf{p}_g^{-1}\mathbf{p}_{z,g}^*$
`DRAGON-WIS␣␣`	$R(N_r)$	$I_\beta = 1$		The scattering-reduced leakage matrix W_{is}^g

where

- the reduced collision probability matrix is defined as

$$\mathbf{p}_g = \{p_{ij,g} \, ; \; \forall i \text{ and } j\}$$

- the reduced directional probability matrix, used in the first TIBÈRE equation, is defined as

$$\mathbf{p}_{k,g}^* = \{p_{ij,k,g}^* \, ; \; \forall i \text{ and } j\} \; ; \quad k = x, \; y, \; \text{or } z$$

- the reduced directional probability matrix, used in the second TIBÈRE equation, is defined as

$$\mathbf{p}_{k,g} = \{p_{ij,k,g} \, ; \; \forall i \text{ and } j\} \; ; \quad k = x, \; y, \; \text{or } z \quad .$$

  The total cross sections used to compute this matrix are *not*–transport corrected.

- the P0 scattering reduced collision probability matrix is defined as

$$\mathbf{W}_g = [\mathbf{I} - \mathbf{p}_g \, \mathbf{\Sigma}_{s0,g\leftarrow g}]^{-1}\mathbf{p}_g$$

- the P1 scattering reduced directionnal collision probability matrix is defined as

$$\mathbf{Y}_{k,g} = [\mathbf{I} - \mathbf{p}_{k,g} \, \mathbf{\Sigma}_{s1,g\leftarrow g}]^{-1}\mathbf{p}_{k,g} \; ; \quad k = x, \; y, \; \text{or } z$$

5.4.2 The `sybilt` *dependent records on a* `GROUP` *directory*

This information is provided only if the current iteration method of the interface current method is used in SYBIL. This occurs if the key-word `ARM` is been used in operators `USS:` or `ASM:`. In these cases, the following records will also be found on the `GROUP` directory:

The following dimensions will be used:

Number of generating cells:

$$\mathcal{N}_{\text{gen}} = \begin{cases} \mathcal{P}_1 & \text{if } \mathcal{S}_6^t = 3 \quad \text{(do-it-yourself geometry)} \\ \mathcal{P}_6 & \text{if } \mathcal{S}_6^t = 4 \quad \text{(2D assembly geometry)} \end{cases}$$

Number of entering currents in a cell:

$$N_c = \begin{cases} 4 & \text{if } \mathcal{P}_1^t = 0 \text{ and } 2 \leq \mathcal{P}_2^t \leq 3 \quad (DP_0 \text{ Cartesian cell}) \\ 12 & \text{if } \mathcal{P}_1^t = 0 \text{ and } \mathcal{P}_2^t = 4 \quad (DP_1 \text{ Cartesian cell}) \\ 6 & \text{if } \mathcal{P}_1^t > 0 \text{ and } 2 \leq \mathcal{P}_2^t \leq 3 \quad (DP_0 \text{ hexagonal cell}) \\ 18 & \text{if } \mathcal{P}_1^t > 0 \text{ and } \mathcal{P}_2^t = 4 \quad (DP_1 \text{ hexagonal cell}) \end{cases}$$

Number of transmission probability elements:

$$D_1 = \begin{cases} \mathcal{P}_1 & \text{if } \mathcal{S}_6^t = 3 \quad \text{(do-it-yourself geometry)} \\ \mathcal{P}_6 & \text{if } \mathcal{S}_6^t = 4 \text{ and } \mathcal{P}_2 = 1 \quad \text{(Roth 2D assembly geometry)} \\ N_c \times N_c \times \mathcal{P}_6 & \text{if } \mathcal{S}_6^t = 4 \text{ and } \mathcal{P}_2 \geq 2 \quad \text{(Other 2D assembly geometries)} \end{cases}$$

Number of escape probability elements:

$$D_2 = \begin{cases} \text{NMC}(\mathcal{P}_1 + 1) & \text{if } \mathcal{S}_6^t = 3 \quad \text{(do-it-yourself geometry)} \\ \text{NMC}(\mathcal{P}_6 + 1) & \text{if } \mathcal{S}_6^t = 4 \text{ and } \mathcal{P}_2 = 1 \quad \text{(Roth 2D assembly geometry)} \\ N_c \times \text{NMC}(\mathcal{P}_6 + 1) & \text{if } \mathcal{S}_6^t = 4 \text{ and } \mathcal{P}_2 \geq 2 \quad \text{(Other 2D assembly geometries)} \end{cases}$$

Number of collision probability elements:

$$D_3 = \sum_{i=1}^{\mathcal{N}_{\text{gen}}} [\text{NMC}(i+1) - \text{NMC}(i)]^2$$

Table 58: SYBIL groupwise assembly information in `GROUP`

Name	Type	Condition	Units	Comment
PSSW$SYBIL⊔⊔	R($\mathcal{D}_1$)			Cellwise scattering-reduced transmission probabilities.
PISW$SYBIL⊔⊔	R($\mathcal{D}_2$)			Cellwise scattering-reduced escape probabilities.
PSJW$SYBIL⊔⊔	R($\mathcal{D}_2$)			Cellwise scattering-reduced collision probabilities for incoming neutrons.
PIJW$SYBIL⊔⊔	R($\mathcal{D}_3$)			Cellwise scattering-reduced collision probabilities.

5.4.3 The `mccgt` dependent records on a `GROUP` directory

If the characteristic method (MCCG) is used, the following records will also be found on the `GROUP` directory:

Table 59: MCCG groupwise directories

Name	Type	Condition	Units	Comment
DIAGF\$MCCG␣␣	$R(N_{\dim})$	$\mathcal{S}_{22}^t > 0$		Diagonal elements of the ACA flux matrix.
CF\$MCCG␣␣␣␣␣	$R(\mathcal{S}_{26}^t)$	$\mathcal{S}_{22}^t > 0$		Non-Diagonal elements of the ACA flux matrix.
ILUDF\$MCCG␣␣	$R(N_{\dim})$	$\begin{cases} \mathcal{S}_{22}^t > 0 \\ \mathcal{S}_{23}^t \geq 2 \end{cases}$		Inverse diagonal elements of U from ILU0 decomposition of ACA flux matrix
ILUCF\$MCCG␣␣	$R(\mathcal{S}_{37}^t)$	$\begin{cases} \mathcal{S}_{22}^t > 0 \\ \mathcal{S}_{23}^t \in \{2,3\} \end{cases}$		Non-diagonal elements of U from ILU0 decomposition of ACA flux matrix that differ from CF
DIAGQ\$MCCG␣␣	$R(N_{\dim})$	$\mathcal{S}_{22}^t > 0$		Diagonal elements of the ACA source matrix.
CQ\$MCCG␣␣␣␣␣	$R(\mathcal{S}_{26}^t)$	$\mathcal{S}_{22}^t > 0$		Non-diagonal elements of the ACA source matrix.
PJJ\$MCCG␣␣␣␣	$R(\mathcal{S}_1^t \mathcal{S}_{36}^t)$	$\mathcal{S}_{35}^t = 1$		Mode-to-mode self-collision probabilities for SCR or "STIS=1" integration strategy.
PSJ\$MCCG␣␣␣␣	$R(\mathcal{S}_{22}^t)$	$\mathcal{S}_{21}^t > 0$		Surface-to-volume probabilities for SCR.

6 Contents of a /system/ directory

The L_SYSTEM specification is used to store a set of system matrices (or a set of perturbations on system matrices) obtained after discretization of the algebraic operators contained in the neutron transport or diffusion equation. A complete set of matrices can be written on the root directory. Perturbation matrices corresponding to variations or derivatives of the cross sections can also be found if the STEP directory list is present.

6.1 State vector content for the /system/ data structure

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}_i^s$, represents:

- $\mathcal{S}_1^s$: the number of energy groups

- $\mathcal{S}_2^s$: the order of a system matrix

- $\mathcal{S}_3^s$: the number of delayed neutron precursor groups

- $\mathcal{S}_4^s$: the storage type of system matrices:

$$\mathcal{S}_4^s = \begin{cases} 1 & \text{BIVAC–compatible profile storage matrices for the diffusion theory} \\ 2 & \text{TRIVAC–compatible matrices compatible with the generic ADI splitting in} \\ & \text{Eq. (4.2) or Eq. (4.3)} \\ 3 & \text{TRIVAC–compatible matrices compatible with the Thomas-Raviart ADI} \\ & \text{splitting in Eq. (4.4) or Eq. (4.5) for the diffusion theory} \\ 11 & \text{BIVAC–compatible profile storage matrices for the simplified } P_n \text{ method} \\ 13 & \text{TRIVAC–compatible matrices compatible with the Thomas-Raviart ADI} \\ & \text{splitting in Eq. (4.4) or Eq. (4.5) for the simplified } P_n \text{ method} \end{cases}$$

- $\mathcal{S}_5^s$: set to 1 in case where matrices 'RM' are available

- The number of set of perturbation on system matrices $I_{\text{step}} = \mathcal{S}_6^s$ used for perturbation calculations:

$$I_{\text{step}} = \begin{cases} 0 & \text{no STEP information available} \\ > 0 & \text{number of set of perturbation on system matrices.} \end{cases}$$

- $\mathcal{S}_7^s$: number of material mixtures in the macrolib used to construct the system matrices

- $\mathcal{S}_8^s$: number of Legendre orders used to represent the macroscopic cross sections with the simplified P_n method (maximum integer value of IL). Set to zero with the diffusion theory.

- The type of system matrix assemblies $I_{\text{pert}} = \mathcal{S}_9^s$:

$$I_{\text{pert}} = \begin{cases} 0 & \text{calculation of the system matrices} \\ 1 & \text{calculation of the derivative of these matrices} \\ 2 & \text{calculation of the first variation of these matrices} \\ 3 & \text{identical to } I_{\text{pert}} = 2, \text{ but these variation are added to unperturbed system} \\ & \text{matrices.} \end{cases}$$

6.2 The main /system/ directory

On its first level, the following records and sub-directories will be found in the /system/ directory:

Table 60: Main records and sub-directories in /system/

Name	Type	Condition	UnitsComment
SIGNATURE␣␣␣	C∗12		Signature of the data structure (SIGNA =L_SYSTEM␣␣␣␣).
LINK.MACRO␣␣	C∗12		Name of the MACROLIB on which the system matrices are based.
LINK.TRACK␣␣	C∗12		Name of the TRACKING on which the system matrices are based.
STATE-VECTOR	I(40)		Vector describing the various parameters associated with this data structure $\mathcal{S}_i^s$, as defined in Section 6.1.
ALBEDO_FU//{igr}	R($\mathcal{S}_8^M$)	$\mathcal{S}_8^M > 0$	Surface ordered physical albedo functions in each group. The number of physical albedos $\mathcal{S}_8^M$ is defined in Section 1.1. The character suffix {igr} is the group index defined in format WRITE(TEXT3,'(I3.3)') igr.
{matrix}	R(N_{dim})		Set of system matrices
{removalxs}	R($\mathcal{S}_7^s$)	$\mathcal{S}_4^s > 10$	Set of removal cross section arrays used with the simplified P_n method
RM␣␣␣␣␣␣␣␣␣␣	R($\mathcal{S}_{11}^t$)	$\mathcal{S}_5^s \neq 0$	Unit system matrix, i.e., a system matrix corresponding to cross sections all set to 1.0. This matrix is mandatory in space-time kinetics cases. *This block is always located on the root directory.*
IRM␣␣␣␣␣␣␣␣	R($\mathcal{S}_{11}^t$)	$\mathcal{S}_5^s \neq 0$	Inverse of the unit matrix. This record is available only with BIVAC trackings.
STEP␣␣␣␣␣␣␣	Dir($\mathcal{S}_6^s$)	$\mathcal{S}_6^s \geq 1$	List of perturbation sub-directories. Each component of this list contains a set of perturbation on system matrices corresponding to variations or derivatives of the cross sections. Each STEP component follows the specification presented in the current Section 6.2.

The signature variable for this data structure must be SIGNA=L_SYSTEM␣␣␣␣.

$$
\begin{bmatrix}
\mathbf{A}_{11} & & & & \\
-\mathbf{A}_{21} & \mathbf{A}_{22} & & & \\
& -\mathbf{A}_{32} & \mathbf{A}_{33} & & \\
& -\mathbf{A}_{42} & -\mathbf{A}_{43} & \mathbf{A}_{44} & -\mathbf{A}_{45} \\
& & & -\mathbf{A}_{54} & \mathbf{A}_{55}
\end{bmatrix}
\begin{bmatrix}
\vec{\Phi}_1 \\ \vec{\Phi}_2 \\ \vec{\Phi}_3 \\ \vec{\Phi}_4 \\ \vec{\Phi}_5
\end{bmatrix}
- \frac{1}{K_{\mathrm{eff}}}
\begin{bmatrix}
\mathbf{B}_{11} & \mathbf{B}_{12} & \mathbf{B}_{13} & \mathbf{B}_{14} & \mathbf{B}_{15} \\
\mathbf{B}_{21} & \mathbf{B}_{22} & \mathbf{B}_{23} & \mathbf{B}_{24} & \mathbf{B}_{25} \\
& & & & \\
& & & & \\
& & & &
\end{bmatrix}
\begin{bmatrix}
\vec{\Phi}_1 \\ \vec{\Phi}_2 \\ \vec{\Phi}_3 \\ \vec{\Phi}_4 \\ \vec{\Phi}_5
\end{bmatrix}
=
\begin{bmatrix}
\vec{0} \\ \vec{0} \\ \vec{0} \\ \vec{0} \\ \vec{0}
\end{bmatrix}
$$

Figure 4: Example of a 5 energy group matrix eigenvalue problem

The discretized neutron transport or diffusion equation is assumed to be given in a form similar to

the matrix system represented in Figure 4. Each system matrix {matrix} is stored on a block named `TEXT12`, embodying the primary group index `IGR` and the secondary group index `JGR`.

The first case corresponds to the following situations:

- BIVAC–type discretization ($\mathcal{S}_4^s = 1$). In this case, the dimension of the matrix is equal to $\text{MU}(\mathcal{S}_{11}^t)$

- TRIVAC–type discretization of the out-of-group A matrices ($\text{IGR} \neq \text{JGR}$). In this case, the dimension of the matrix is equal to $\mathcal{S}_{11}^t$

- TRIVAC–type discretization of the B matrices. In this case, the dimension of the matrix is equal to $\mathcal{S}_{11}^t$

The character name of the system matrix is build using

```
WRITE(TEXT12,'(1HA,2I3.3)') JGR,IGR
```

```
WRITE(TEXT12,'(1HB,2I3.3)') JGR,IGR
```

or

```
WRITE(TEXT12,'(1HB,3I3.3)') IDEL,JGR,IGR
```

where `IDEL` is the index of a delayed neutron precursor group (if $\mathcal{S}_3^s \geq 1$).

Otherwise, the TRIVAC–type system matrix is splitted according to Eqs. (4.2) to (4.5). The character name of the system matrix is build using

```
WRITE(TEXT12,'(A2,1HA,2I3.3)') PREFIX,IGR,IGR
```

where `PREFIX` is a character*2 name describing the component of the system matrix under consideration. The following values are available:

PREFIX	type of matrix	dimension N_{dim}
W_	matrix component $\mathbf{W} + \mathbf{P}_{\mathbf{w}}^\top \mathbf{UP}_{\mathbf{w}}$ or $\mathbf{A}_{\mathbf{w}} + \mathbf{R}_{\mathbf{w}}\mathbf{T}^{-1}\mathbf{R}_{\mathbf{w}}^\top$	$\text{MUW}(\mathcal{S}_{11}^t)$ or $\text{MUW}(\mathcal{S}_{26}^t)$
X_	matrix component $\mathbf{X} + \mathbf{P}_{\mathbf{x}}^\top \mathbf{UP}_{\mathbf{x}}$ or $\mathbf{A}_{\mathbf{x}} + \mathbf{R}_{\mathbf{x}}\mathbf{T}^{-1}\mathbf{R}_{\mathbf{x}}^\top$	$\text{MUX}(\mathcal{S}_{11}^t)$ or $\text{MUX}(\mathcal{S}_{27}^t)$
Y_	matrix component $\mathbf{Y} + \mathbf{P}_{\mathbf{y}}^\top \mathbf{UP}_{\mathbf{y}}$ or $\mathbf{A}_{\mathbf{y}} + \mathbf{R}_{\mathbf{y}}\mathbf{T}^{-1}\mathbf{R}_{\mathbf{y}}^\top$	$\text{MUY}(\mathcal{S}_{11}^t)$ or $\text{MUY}(\mathcal{S}_{28}^t)$
Z_	matrix component $\mathbf{Z} + \mathbf{P}_{\mathbf{z}}^\top \mathbf{UP}_{\mathbf{z}}$ or $\mathbf{A}_{\mathbf{z}} + \mathbf{R}_{\mathbf{z}}\mathbf{T}^{-1}\mathbf{R}_{\mathbf{z}}^\top$	$\text{MUZ}(\mathcal{S}_{11}^t)$ or $\text{MUZ}(\mathcal{S}_{29}^t)$
WI	$LDL^\top$ factors of $\mathbf{W} + \mathbf{P}_{\mathbf{w}}^\top \mathbf{UP}_{\mathbf{w}}$ or $\mathbf{A}_{\mathbf{w}} + \mathbf{R}_{\mathbf{w}}\mathbf{T}^{-1}\mathbf{R}_{\mathbf{w}}^\top$	$\text{MUW}(\mathcal{S}_{11}^t)$ or $\text{MUW}(\mathcal{S}_{26}^t)$
XI	$LDL^\top$ factors of $\mathbf{X} + \mathbf{P}_{\mathbf{x}}^\top \mathbf{UP}_{\mathbf{x}}$ or $\mathbf{A}_{\mathbf{x}} + \mathbf{R}_{\mathbf{x}}\mathbf{T}^{-1}\mathbf{R}_{\mathbf{x}}^\top$	$\text{MUX}(\mathcal{S}_{11}^t)$ or $\text{MUX}(\mathcal{S}_{27}^t)$
YI	$LDL^\top$ factors of $\mathbf{Y} + \mathbf{P}_{\mathbf{y}}^\top \mathbf{UP}_{\mathbf{y}}$ or $\mathbf{A}_{\mathbf{y}} + \mathbf{R}_{\mathbf{y}}\mathbf{T}^{-1}\mathbf{R}_{\mathbf{y}}^\top$	$\text{MUY}(\mathcal{S}_{11}^t)$ or $\text{MUY}(\mathcal{S}_{28}^t)$
ZI	$LDL^\top$ factors of $\mathbf{Z} + \mathbf{P}_{\mathbf{z}}^\top \mathbf{UP}_{\mathbf{z}}$ or $\mathbf{A}_{\mathbf{z}} + \mathbf{R}_{\mathbf{z}}\mathbf{T}^{-1}\mathbf{R}_{\mathbf{z}}^\top$	$\text{MUZ}(\mathcal{S}_{11}^t)$ or $\text{MUZ}(\mathcal{S}_{29}^t)$

where all these matrices are stored in diagonal storage mode.

The following values of `PREFIX` will also be used in cases where a Thomas-Raviart or Thomas-Raviart-Schneider polynomial basis is used ($\mathcal{S}_{12}^t = 2$ and $\mathcal{S}_4^s = 3$):

PREFIX	type of matrix	dimension N_{dim}
TF	matrix component $\mathbf{T}$	$\mathcal{S}_{25}^t$
WA	matrix component $\mathbf{A}_{\mathbf{w}}$	$\text{MUW}(\mathcal{S}_{26}^t)$
XA	matrix component $\mathbf{A}_{\mathbf{x}}$	$\text{MUX}(\mathcal{S}_{27}^t)$
YA	matrix component $\mathbf{A}_{\mathbf{y}}$	$\text{MUY}(\mathcal{S}_{28}^t)$
ZA	matrix component $\mathbf{A}_{\mathbf{z}}$	$\text{MUZ}(\mathcal{S}_{29}^t)$
DIFF	diffusion coefficients used with the Thomas-Raviart-Schneider method	N_{los}

where `TF` is a diagonal matrix and where `WA` to `ZA` are stored in diagonal profiled mode. The dimension of `DIFF` is related to the number of lozenges in the domain: $N_{\text{los}} = \mathcal{S}_{14}^t \times \mathcal{S}_{15}^t \times (\mathcal{S}_{13}^t)^2$.

Each removal cross section array {removalxs} is stored on a block named `TEXT12`, embodying the Legendre order `IL`, the primary group index `IGR` and the secondary group index `JGR`. The block name `TEXT12` is build using

```
WRITE(TEXT12,'(4HSCAR,I2.2,2I3.3)') IL-1,JGR,IGR
```

for the mixture-ordered components of the removal cross section, and

```
WRITE(TEXT12,'(4HSCAI,I2.2,2I3.3)') IL-1,JGR,IGR
```

for the mixture-ordered components of the inverse removal cross section matrix at each Legendre order.

7 Contents of a /kinet/ directory

The L_KINET specification is used to store the data related to the space-time neutron kinetics calculations. This directory also contains the main calculations results corresponding to the current time step of a transient.

7.1 State vector content for the /kinet/ data structure

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}_i^k$, represent:

- The current time-step index $N_{tr} = \mathcal{S}_1^k$

- The number of delayed-neutron precursor groups $N_{dg} = \mathcal{S}_2^k$

- The number of energy groups $N_{gr} = \mathcal{S}_3^k$

- The type of geometry $I_{geo} = \mathcal{S}_4^k$

- The total number of finite elements $N_{el} = \mathcal{S}_5^k$

- The total number of unknowns per energy group $N_{un} = \mathcal{S}_6^k$

- The number of flux unknowns per energy group $N_{uf} = \mathcal{S}_7^k$

- The number of precursors unknowns per delayed group $N_{up} = \mathcal{S}_8^k$

- The number of fissile isotopes $N_{fiss} = \mathcal{S}_9^k$

- The type of system matrices $N_{sys} = \mathcal{S}_{10}^k$

- Number of free iteration per variational acceleration cycle $N_f = \mathcal{S}_{11}^k$

- Number of accelerated iteration per variational acceleration cycle $N_a = \mathcal{S}_{12}^k$

- Type of normalization for the flux $I_{\mathrm{norm}} = \mathcal{S}_{13}^k$ where

$$
I_{\mathrm{norm}} = \begin{cases}
0 & \text{No normalization} \\
1 & \text{Imposed factor} \\
2 & \text{Maximum flux normalization} \\
3 & \text{Initial power normalization}
\end{cases}
$$

- Maximum number of thermal (up-scattering) iterations $M_{\mathrm{in}} = \mathcal{S}_{14}^k$

- Maximum number of outer iterations $M_{\mathrm{out}} = \mathcal{S}_{15}^k$

- Initial number of ADI iterations in Trivac $M_{\mathrm{adi}} = \mathcal{S}_{16}^k$

- Temporal integration scheme for fluxes $I_{\mathrm{ifl}} = \mathcal{S}_{17}^k$ where

$$
I_{\mathrm{ifl}} = \begin{cases}
1 & \text{Implicit scheme } (\Theta_{\mathrm{f}} = 1) \\
2 & \text{Crank-Nicholson scheme } (\Theta_{\mathrm{f}} = 0.5) \\
3 & \text{General theta method}
\end{cases}
$$

- Temporal integration scheme for precursors $I_{\mathrm{ipr}} = \mathcal{S}_{18}^k$ where

$$
I_{\mathrm{ipr}} = \begin{cases}
1 & \text{Implicit scheme } (\Theta_{\mathrm{p}} = 1) \\
2 & \text{Crank-Nicholson scheme } (\Theta_{\mathrm{p}} = 0.5) \\
3 & \text{General theta method} \\
4 & \text{Analytical integration method for precursors}
\end{cases}
$$

- Exponential transformation flag $I_{\text{iexp}} = \mathcal{S}_{19}^k$ where

$$I_{\text{iexp}} = \left\{ \begin{array}{ll} 0 & \text{not used} \\ 1 & \text{used} \end{array} \right.$$

- Adjoint kinetics calculation flag $I_{\text{adj}} = \mathcal{S}_{20}^k$ where

$$I_{\text{adj}} = \left\{ \begin{array}{ll} 0 & \text{direct (forward) calculation} \\ 1 & \text{adjoint (backward) calculation} \end{array} \right.$$

7.2 The main /kinet/ directory

The following records and sub-directories will be found in the /kinet/ directory:

Table 61: Main records and sub-directories in /kinet/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C*12			Signature of the data structure (SIGNA =L_KINET␣␣␣␣␣)
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^k$, as defined in Section 7.1.
EPS-CONVERGE	R(4)			Convergence parameters Δ_i^ϵ
TRACK-TYPE␣␣	C*12			Type of tracking considered (CDOOR). Allowed values are: 'BIVAC' and 'TRIVAC'
E-IDLPC␣␣␣␣␣	I(N_{el})			Position of averaged precursor concentrations in vector E-PREC.
DELTA-T␣␣␣␣␣	R(1)		s	Current time increment.
TOTAL-TIME␣␣	R(1)		s	Total elapsed time from the beginning of a transient.
BETA-D␣␣␣␣␣␣	R(N_{dg})			Delayed-neutron fraction for each delayed-neutron precursor group.
LAMBDA-D␣␣␣␣	R(N_{dg})		s^{-1}	Radioactive decay constants of each delayed-neutron precursor group.
CHI-D␣␣␣␣␣␣␣	R(N_{dg}, N_{gr})			Multigroup delayed-neutron fission spectrum in each precursor group.
E-VECTOR␣␣␣␣	R(N_{uf}, N_{gr})			Kinetics solution for fluxes at current time step.
E-PREC␣␣␣␣␣␣	R(N_{up}, N_{dg})			Kinetics solution for precursor concentrations at current time step.
E-KEFF␣␣␣␣␣␣	R(1)			Steady-state value of the initial k_{eff}.
CTRL-FLUX␣␣␣	R(1)			Maximum value of flux used for the controlling purpose.
CTRL-PREC␣␣␣	R($N_{up} \times N_{fiss}$)			Precursor concentrations at location of maximum flux.
CTRL-IDL␣␣␣␣	I(1)			Position of a maximum value within the flux vector.
CTRL-IGR␣␣␣␣	I(1)			Energy group number corresponding to a maximum flux value.
POWER-INI␣␣␣	R(1)	$I_{\text{norm}} = 3$	MW	Initial power.
E-POW␣␣␣␣␣␣␣	R(1)	$I_{\text{norm}} = 3$	MW	Actual power.
OMEGA␣␣␣␣␣␣␣	R(N_{mix}, N_{gr})	$I_{\text{iexp}} = 1$	s^{-1}	Exponential transformation factor. N_{mix} is the number of material mixtures

The convergence parameters Δ_i^ϵ represent:

- Δ_1^ϵ is the thermal (up-scattering) iteration flux convergence parameter

- Δ_2^ϵ is the outer iteration flux convergence parameter

- Θ_f is the value of theta-parameter for fluxes

- Θ_p is the value of theta-parameter for precursors

8 Contents of a /fluxunk/ directory

This directory contains the main flux calculations results, including the multigroup flux, the eigenvalue for the problem and the diffusion coefficients when computed. The following types of equations can be solved:

1. Fixed source problem

$$\mathbf{A}\ \vec{\Phi} = \vec{S} \tag{8.1}$$

   where $\mathbf{A}$ is the coefficient matrix, $\vec{S}$ is the source vector and $\vec{\Phi}$ is the unknown vector.

2. Direct eigenvalue problem

$$\mathbf{A}\ \vec{\Phi}_\alpha + \frac{1}{\mathbf{K}_{\text{eff},\alpha}}\ \mathbf{B}\ \vec{\Phi}_\alpha = \vec{0} \tag{8.2}$$

   where $\mathbf{B}$ is the second coefficient matrix and where $(\frac{1}{K_{\text{eff},\alpha}}, \vec{\Phi}_\alpha)$ is the eigensolution corresponding to the α–th eigenvalue or harmonic mode. Generally, only the eigensolution corresponding to the maximum value of $K_{\text{eff},\alpha}$ is found (the fundamental mode).

3. Adjoint eigenvalue problem

$$\mathbf{A}^\top\ \vec{\Phi}_\alpha^* + \frac{1}{\mathbf{K}_{\text{eff},\alpha}}\ \mathbf{B}^\top\ \vec{\Phi}_\alpha^* = \vec{0} \tag{8.3}$$

   where matrices $\mathbf{A}$ and $\mathbf{B}$ are transposed.

4. Fixed source direct eigenvalue equation (direct GPT)

$$\mathbf{A}\ \vec{\Gamma}_\alpha + \frac{1}{\mathbf{K}_{\text{eff},\alpha}}\ \mathbf{B}\ \vec{\Gamma}_\alpha = \vec{S} \quad \text{where} \quad \left\langle \mathbf{\Phi}_\alpha^*, \vec{S} \right\rangle = \mathbf{0} \tag{8.4}$$

   where the direct source vector $\vec{S}$ is orthogonal to the adjoint flux.

5. Fixed source adjoint eigenvalue equation (adjoint GPT)

$$\mathbf{A}^\top\ \vec{\Gamma}_\alpha^* + \frac{1}{\mathbf{K}_{\text{eff},\alpha}}\ \mathbf{B}^\top\ \vec{\Gamma}_\alpha^* = \vec{S}^* \quad \text{where} \quad \left\langle \mathbf{\Phi}_\alpha, \vec{S}^* \right\rangle = \mathbf{0} \tag{8.5}$$

   where the adjoint source vector $\vec{S}^*$ is orthogonal to the direct flux.

8.1 State vector content for the /fluxunk/ data structure

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}_i^f$, represent:

- The number of energy groups $N_G = \mathcal{S}_1^f$

- The number of unknowns per energy group $N_U = \mathcal{S}_2^f$

- The type of equation considered $I_e = \mathcal{S}_3^f = \alpha_1 + 10\ \alpha_2 + 100\ \alpha_3 + 1000\ \alpha_4$ where

$$\alpha_1 \quad = \quad 0/1: \text{ Fixed source (Eq. (8.1)) or } K_{\text{eff}} \text{ (Eq. (8.2)) direct eigenvalue equation absent/present}$$

$$\alpha_2 \quad = \quad 0/1: \text{ Adjoint eigenvalue equation (Eq. (8.3)) absent/present}$$

$$\alpha_3 \quad = \quad 0/1: \text{ Direct fixed source eigenvalue equation – or GPT equation (Eq. (8.4)) absent/present}$$

$$\alpha_4 \quad = \quad 0/1: \text{ Adjoint fixed source eigenvalue equation – or GPT equation (Eq. (8.5)) absent/present}$$

- The number of harmonics considered $N_h = \mathcal{S}_4^f$ where

$$N_h = \begin{cases} 0 & \text{the harmonic calculation is not enabled} \\ \geq 1 & \text{the harmonic calculation is enabled. } N_h \text{ is the number of harmonics.} \end{cases}$$

- The number of specific GPT equations considered $N_{\text{gpt}} = \mathcal{S}_5^f$ where

$$N_{\text{gpt}} = \begin{cases} 0 & \text{the GPT calculation is not enabled} \\ \geq 1 & \text{the GPT calculation is enabled. } N_{\text{gpt}} \text{ is the number of specific GPT equations.} \end{cases}$$

- The type of B_n solution considered $I_s = \mathcal{S}_6^f$ where

$$I_s = \begin{cases} -1 & \text{No flux calculation, fluxes taken from input file} \\ 0 & \text{Fixed source problem, no eigenvalue} \\ 1 & \text{fixed source eigenvalue problem (GPT type) with fission} \\ 2 & K_{\text{eff}} \text{ eigenvalue problem with fission and without leakage} \\ 3 & K_{\text{eff}} \text{ eigenvalue problem with fission and leakage} \\ 4 & \text{Buckling eigenvalue problem with fission and leakage} \\ 5 & \text{Buckling eigenvalue problem without fission but with leakage} \end{cases}$$

- The type of leakage model $I_l = \mathcal{S}_7^f$ where

$$I_l = \begin{cases} 0 & \text{No leakage model} \\ 1 & \text{Homogeneous } \texttt{PNLR} \text{ calculation} \\ 2 & \text{Homogeneous } \texttt{PNL} \text{ calculation} \\ 3 & \text{Homogeneous } \texttt{SIGS} \text{ calculation} \\ 4 & \text{Homogeneous } \texttt{ALSB} \text{ calculation} \\ 5 & \text{Leakage with isotropic streaming effects} \\ 16 & \text{Leakage with anisotropic streaming effects – imposed buckling} \\ 26 & \text{Leakage with anisotropic streaming effects – X-Buckling search} \\ 36 & \text{Leakage with anisotropic streaming effects – Y-Buckling search} \\ 46 & \text{Leakage with anisotropic streaming effects – Z-Buckling search} \\ 56 & \text{Leakage with anisotropic streaming effects – radial Buckling search} \\ 66 & \text{Leakage with anisotropic streaming effects – total Buckling search} \end{cases}$$

- Number of free iteration per variational acceleration cycle $N_f = \mathcal{S}_8^f$

- Number of accelerated iteration per variational acceleration cycle $N_a = \mathcal{S}_9^f$

- Thermal rebalancing option $I_r = \mathcal{S}_{10}^f$ where

$$I_r = \begin{cases} 0 & \text{No thermal iteration rebalancing} \\ 1 & \text{Thermal iteration rebalancing activated} \end{cases}$$

- Maximum number of thermal (up-scattering) iterations $M_{\mathrm{in}} = \mathcal{S}_{11}^f$

- Maximum number of outer iterations $M_{\mathrm{out}} = \mathcal{S}_{12}^f$

- Initial number of ADI iterations in Trivac $M_{\mathrm{adi}} = \mathcal{S}_{13}^f$

- Block size of the Arnoldi Hessenberg matrix with the implicit restarted Arnoldi method (IRAM) ($= 0$ if the symmetrical variational acceleration technique (SVAT) is used) $N_{\mathrm{blsz}} = \mathcal{S}_{14}^f$

- Number of iterations before restarting with the GMRES(m) acceleration method for solving the ADI-preconditionned linear systems in Trivac ($= 0$ if M_{adi} free iterations are used) $N_{\mathrm{gmr1}} = \mathcal{S}_{15}^f$

- Number of iterations before restarting with the GMRES(m) acceleration method for solving a multigroup fixed-source problem ($= 0$ if the variational acceleration technique is used) $N_{\mathrm{gmr2}} = \mathcal{S}_{16}^f$

8.2 The main /fluxunk/ directory

On its first level, the following records and sub-directories will be found in the /fluxunk/ directory:

Table 62: Main records and sub-directories in /fluxunk/

Name	Type	Condition	UnitsComment
SIGNATURE␣␣␣	C∗12		Signature of the data structure (SIGNA =L_FLUX␣␣␣␣␣␣)
STATE-VECTOR	I(40)		Vector describing the various parameters associated with this data structure $\mathcal{S}_i^f$, as defined in Section 8.1.
OPTION␣␣␣␣␣␣	C∗4		Type of leakage coefficents ('LKRD': recover leakage coefficients in Macrolib; 'RHS': recover leakage coefficients in RHS flux object; 'B0': B_0; 'P0': P_0; 'B1': B_1; 'P1': P_1; 'BOTR': B_0 with transport correction; 'POTR': P_0 with transport correction).
EPS-CONVERGE	R(5)		Convergence parameters Δ_i^ϵ
KEYFLX␣␣␣␣␣␣	I($\mathcal{S}_1^t$)		Location in unknown vector of averaged regional flux I_r
K-EFFECTIVE␣	R(1)	$\mathcal{S}_6^f \geq 1$	Computed or imposed effective multiplication factor for direct eigenvalue problem, corresponding to the fundamental mode
AK-EFFECTIVE	R(1)	$\frac{\mathcal{S}_3^f}{10} \bmod 10 = 1$	Computed effective multiplication factor for adjoint eigenvalue problem, corresponding to the fundamental mode. The theoretical value is equal to 'K-EFFECTIVE' but difference may occurs for numerical reasons.

Main records and sub-directories in /fluxunk/ continued from last page

Name	Type	Condition	Units	Comment
K-INFINITY␣␣	R(1)	$\mathcal{S}_6^f \geq 2$		Computed infinite multiplication constant for eigenvalue problem, corresponding to the fundamental mode
B2␣␣B1HOM␣␣␣	R(1)	$\mathcal{S}_6^f \geq 1$	cm^{-2}	Homogeneous buckling B^2, corresponding to the fundamental mode
DIFFB1HOM␣␣␣	R(G)	$\mathcal{S}_6^f \geq 1$	cm	Multigroup homogeneous leakage coefficients d^g, corresponding to the fundamental mode
B2␣␣HETE␣␣␣␣	R(3)	$\mathcal{S}_7^f \geq 6$	cm^{-2}	Directional buckling components B_i^2, corresponding to the fundamental mode
GAMMA␣␣␣␣␣␣␣	R(G)	$\mathcal{S}_7^f \geq 5$		Gamma factors used with B_n–type streaming models.
FLUX␣␣␣␣␣␣␣␣	Dir($\mathcal{S}_1^f$)			List of real arrays. Each component of this list is a real array of dimension $\mathcal{S}_2^f$ containing the solution of a fixed source (Eq. (8.1)) or of a direct eigenvalue (Eq. (8.2)) equation, corresponding to the fundamental mode.
AFLUX␣␣␣␣␣␣␣	Dir($\mathcal{S}_1^f$)	$\frac{\mathcal{S}_3^f}{10}$ mod 10 = 1		List of real arrays. Each component of this list is a real array of dimension $\mathcal{S}_2^f$ containing the solution of an adjoint eigenvalue (Eq. (8.3)) equation, corresponding to the fundamental mode.
MODE␣␣␣␣␣␣␣␣	Dir($\mathcal{S}_4^f$)	$\mathcal{S}_4^f \geq 1$		List of *harmonic mode* sub-directories. Each component of this list follows the specification presented in Section 8.3.
DFLUX␣␣␣␣␣␣␣	Dir($\mathcal{S}_5^f$)	$\mathcal{S}_3^f = 100$		List of direct (explicit) GPT sub-directories. Each component of this list is a multigroup list of dimension $\mathcal{S}_1^f$. Each component of the multigroup list is a real array of dimension $\mathcal{S}_2^f$ containing the solution of a fixed source direct eigenvalue equation similar to Eq. (8.4).
ADFLUX␣␣␣␣␣␣	Dir($\mathcal{S}_5^f$)	$\mathcal{S}_3^f = 1000$		List of adjoint (implicit) GPT sub-directories. Each component of this list is a multigroup list of dimension $\mathcal{S}_1^f$. Each component of the multigroup list is a real array of dimension $\mathcal{S}_2^f$ containing the solution of a fixed source adjoint eigenvalue equation similar to Eq. (8.5).

The convergence parameters Δ_i^ϵ represent:

- Δ_1^ϵ is the thermal (up-scattering) iteration flux convergence parameter

- Δ_2^ϵ is the outer iteration eigenvalue convergence parameter

- Δ_3^ϵ is the outer iteration flux convergence parameter

- Δ_4^ϵ is the GMRES convergence parameter used at inner iteration

- Δ_5^ξ is the relaxation factor of the flux used in multiphysics applications. $\Delta_5^\xi = 1$ is equivalent to no relaxation.

8.3 The harmonic mode sub-directories in /fluxunk/

Each component of the list named 'MODE' contains the information relative to a specific harmonic mode.

Table 63: Component of the harmonic mode directory

Name	Type	Condition	Units	Comment
K-EFFECTIVE␣	R(1)			Computed effective multiplication factor for eigenvalue problem, corresponding to the α–th mode
FLUX␣␣␣␣␣␣␣␣	$\mathrm{Dir}(\mathcal{S}_1^f)$			List of real arrays. Each component of this list is a real array of dimension $\mathcal{S}_2^f$ containing the solution of the α–th mode of a direct eigenvalue (Eq. (8.2)) equation.
AFLUX␣␣␣␣␣␣␣	$\mathrm{Dir}(\mathcal{S}_1^f)$	$\frac{\mathcal{S}_3^f}{10} \bmod 10 = 1$		List of real arrays. Each component of this list is a real array of dimension $\mathcal{S}_2^f$ containing the solution of the α–th mode of an adjoint eigenvalue (Eq. (8.3)) equation.

9 Contents of a /source/ directory

This directory contains the source components of a fixed source problem. This data structure is also useful for *fixed source eigenvalue problems* as used in the generalized perturbation theory (GPT).

9.1 State vector content for the /source/ data structure

The dimensioning parameters for this data structure, stored in the state vector $\mathcal{S}_i^{sou}$, represent:

- The number of energy groups $N_G = \mathcal{S}_1^{sou}$

- The number of unknowns per energy group $N_U = \mathcal{S}_2^{sou}$

- The number of direct fixed sources $N_D = \mathcal{S}_3^{sou}$

- The number of adjoint fixed sources $N_A = \mathcal{S}_4^{sou}$

9.2 The main /source/ directory

On its first level, the following records and sub-directories will be found in the /source/ directory:

Table 64: Main records and sub-directories in /source/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			Signature of the data structure (SIGNA =L␣SOURCE␣␣␣␣)
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^{sou}$, as defined in Section 9.1.
LINK.FLUX␣␣␣	C∗12			Name of the unperturbed FLUX orthogonal to the fixed sources.
LINK.SYSTEM␣	C∗12			Name of the unperturbed SYSTEM object.
LINK.TRACK␣␣	C∗12			Name of the tracking object used to construct the system matrices.
DSOUR␣␣␣␣␣␣␣	Dir($\mathcal{S}_3^{sou}$)	$\mathcal{S}_3^{sou} \geq 1$		List of direct fixed source sub-directories. Each component of this list is a multigroup list of dimension $\mathcal{S}_1^{sou}$. Each component of the multigroup list is a real array of dimension $\mathcal{S}_2^{sou}$ containing a direct fixed source array.
ASOUR␣␣␣␣␣␣␣	Dir($\mathcal{S}_4^{sou}$)	$\mathcal{S}_4^{sou} \geq 1$		List of adjoint fixed source sub-directories. Each component of this list is a multigroup list of dimension $\mathcal{S}_1^{sou}$. Each component of the multigroup list is a real array of dimension $\mathcal{S}_2^{sou}$ containing an adjoint fixed source array

10 Contents of a /deposition/ directory

This directory accumulates energy and charge deposition information gathered from coupled solutions of the Boltzmann and/or Boltzmann Fokker-Planck transport equations.

10.1 State vector content for the /deposition/ data structure

The dimensioning parameters for this data structure, stored in the state vector $\mathcal{S}_i^{dep}$, represent:

- The number of material mixtures $N_{\mathrm{mix}} = \mathcal{S}_1^{dep}$

- The number of particules contributing to deposition $N_{\mathrm{part}} = \mathcal{S}_2^{dep}$

- Charge deposition index $I_c = \mathcal{S}_3^{dep}$:

$$I_c = \left\{ \begin{array}{ll} 0 & \text{no charge deposition information} \\ 1 & \text{charge deposition information is present.} \end{array} \right.$$

- The number of Boltzmann transport equation iterations $N_{\mathrm{iter}} = \mathcal{S}_4^{dep}$

10.2 The main /deposition/ directory

On its first level, the following records and sub-directories will be found in the /deposition/ directory:

Table 65: Main records and sub-directories in /deposition/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C*12			Signature of the data structure (SIGNA =L␣DEPOSITION)
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^{dep}$, as defined in Section 10.1.
PARTICLE-NAM	C(N_{part})*1			Character name associated to each particle.
VOLUME␣␣␣␣␣␣	R(N_{mix})		cm^3	Volumes.
FLUX-NORM␣␣␣	D(1)		1	Flux normalization factor.
EDEPOS␣␣␣␣␣␣	D($N_{\mathrm{mix}}, N_{\mathrm{part}}$)		MeV·cm^{-3}·s^{-1}	Energy deposition.
CDEPOS␣␣␣␣␣␣	D($N_{\mathrm{mix}}, N_{\mathrm{part}}$)	$I_c = 1$	electron·cm^{-3}·s^{-1}	Charge deposition.
EDEPOS_TOT␣␣	D(N_{mix})		MeV·cm^{-3}·s^{-1}	Volume integrated energy deposition.
CDEPOS_TOT␣␣	D(N_{mix})	$I_c = 1$	electron·cm^{-3}·s^{-1}	Volume integrated charge deposition.

11 Contents of a /edition/ directory

This directory contains the main editing results. For the purpose of illustration we will assume that the `EDI:` module is executed using the following data:

```
EDITING := EDI: FLUX LIBRARY VOLMAT ::
  MERG COMP COND 27 69 ALL SAVE ON EDITCELL2G ;
```

where `EDITING` is the final EDITION data structure. The data structures `FLUX`, `LIBRARY` and `VOLMAT` are respectively of type FLUXUNK, MICROLIB and TRACKING. Assuming that the initial number of regions in `VOLMAT` is N and the number of groups in `LIBRARY` is $G = 69$, then the final information that will be stored in the EDITING data structure will represent a two group ($G_c = 2$) one mixture N_h /microlib/.

11.1 State vector content for the /edition/ data structure

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}_i^{\mathrm{edi}}$, represent:

- The number of homogeneous mixtures saved $N_H = \mathcal{S}_1^{\mathrm{edi}}$ for the last editing step

- The number of condensed groups considered $M_G = \mathcal{S}_2^{\mathrm{edi}}$ for the last editing step

- Editing flag to indicate the presence of 4 factor editing $I_{4f} = \mathcal{S}_3^{\mathrm{edi}}$ for the last editing step

- Editing flag to indicate that the up-scattering contributions have all been transferred to the diagonal part of the scattering matrix $I_U = \mathcal{S}_4^{\mathrm{edi}}$ for the last editing step

- The number of mixture activated $N_A = \mathcal{S}_5^{\mathrm{edi}}$ for the last editing step

- Editing flag to indicate the types of statistics generated by `EDI:` $I_S = \mathcal{S}_6^{\mathrm{edi}}$ for the last editing step

- Editing flag to indicate which boundary flux editions are used in `EDI:`. These editions are required for computing assembly discontinuity factors (ADF) or to perform some types of *superhomogénéisation* (SPH) calculations. $I_{\mathrm{adf}} = \mathcal{S}_7^{\mathrm{edi}}$ for the last editing step

$$
I_{\mathrm{adf}} = \begin{cases} 0 & \text{no boundary flux editions;} \\ 1 & \text{use boundary fluxes obtained using the } \mathtt{ALBS} \text{ keyword in DRAGON;} \\ 2 & \text{use boundary fluxes obtained from informations located in } \mathtt{REF:ADF} \text{ directory;} \\ 3 & \text{use boundary fluxes obtained from the current iteration method in Eurydice;} \\ 4 & \text{use boundary flux information recovered from the } \mathtt{MACROLIB/ADF} \text{ directory.} \end{cases}
$$

- Editing flag to indicate the type of tracking to be performed on a macro-geometry built by module `EDI:`. $I_{\mathrm{cell}} = \mathcal{S}_8^{\mathrm{edi}}$ for the last editing step

$$
I_{\mathrm{cell}} = \begin{cases} 1 & \text{the macro-geometry is tracked by module } \mathtt{SYBILT:} \text{ or } \mathtt{EXCELT:}; \\ 2 & \text{the macro-geometry is tracked by module } \mathtt{NXT:}; \\ 3 & \text{the macro-geometry is tracked by another module.} \end{cases}
$$

- The number of extracted isotopes in the output microlib $I_m = \mathcal{S}_9^{\mathrm{edi}}$ for the last editing step

- The print level considered $I_p = \mathcal{S}_{10}^{\mathrm{edi}}$ for the last editing step

- Editing flag to indicate the types of cross section saved in `EDI:` $I_x = \mathcal{S}_{11}^{\mathrm{edi}}$ for the last editing step

- The type of weighting used for P_1 cross section information $I_{\mathrm{w}} = \mathcal{S}_{12}^{\mathrm{edi}}$ for the last editing step ($= 0$: flux weighting; $= 1$ current weighting)

- The maximum number of isotopes per mixture $M_I = \mathcal{S}_{13}^{\mathrm{edi}}$

- The maximum number of condensed groups in all editing $M_g = \mathcal{S}_{14}^{\mathrm{edi}}$

- The maximum number of homogeneous mixtures in all editing $M_h = \mathcal{S}_{15}^{\mathrm{edi}}$

- The total number of ISOTXS files generated $M_F = \mathcal{S}_{16}^{\mathrm{edi}}$

- The maximum number of regions before homogenization $M_{\max} = \mathcal{S}_{17}^{\mathrm{edi}}$

- Editing flag $= 1$ for H-factor edition; $= 0$ otherwise $I_{H-fac} = \mathcal{S}_{18}^{\mathrm{edi}}$

- Number of delayed neutron precursor groups $N_{\mathrm{del}} = \mathcal{S}_{19}^{\mathrm{edi}}$

- Geometry index $L_{\mathrm{geo}} = \mathcal{S}_{20}^{\mathrm{edi}}$

$$L_{\mathrm{geo}} = \left\{ \begin{array}{ll} 0 & \text{the macro geometry is not available} \\ 1 & \text{the macro-geometry of the last editing is available} \end{array} \right.$$

- Type of weighting for homogenization or/and condensation of cross-section information $I_{\mathrm{adj}} = \mathcal{S}_{21}^{\mathrm{edi}}$

$$I_{\mathrm{adj}} = \left\{ \begin{array}{ll} 0 & \text{use direct flux;} \\ 1 & \text{use adjoint flux.} \end{array} \right.$$

- Type of current used for P_1 weighting if $I_{\mathrm{w}} \neq 0$. $I_{\mathrm{curr}} = \mathcal{S}_{22}^{\mathrm{edi}}$

$$I_{\mathrm{curr}} = \left\{ \begin{array}{ll} 1 & \text{use a current obtained from an heterogeneous leakage model;} \\ 2 & \text{use the Todorova flux;} \\ 4 & \text{use spherical harmonics weighting.} \end{array} \right.$$

- Number of reactions saved on output microlib $N_{\mathrm{reac}} = \mathcal{S}_{23}^{\mathrm{edi}}$

$$N_{\mathrm{reac}} = \left\{ \begin{array}{ll} 0 & \text{all available reactions are saved;} \\ > 0 & \text{only reactions listed in } \texttt{REF:HVOUT} \text{ array are saved.} \end{array} \right.$$

11.2 The main /edition/ directory

On its first level, the following records and sub-directories will be found in the /edition/ directory:

Table 66: Main records and sub-directories in /edition/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C*12			Signature of the data structure (SIGNA =L_EDIT␣␣␣␣␣␣).
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^{\mathrm{edi}}$, as defined in Section 11.1.
TITLE␣␣␣␣␣␣␣	C*72			Title of the last editing performed (TITLE)
LAST-EDIT␣␣␣	C*12	$|\mathcal{S}_{11}^{\mathrm{edi}}| \geq 2$		Name of the last editing sub-directory saved (LAST)

Main records and sub-directories in /edition/ continued from last page

Name	Type	Condition	Units	Comment
LINK.GEOM␣␣␣	C∗12			Name of the GEOMETRY on which the last edition was based.
REF:IMERGE␣␣	$I(\mathcal{S}_{17}^{\mathrm{edi}})$			Merged region number associated with each of the original region number M_r
REF:VOLUME␣␣	$R(\mathcal{S}_{17}^{\mathrm{edi}})$		cm^3	Volume associated with each of the original region number V_r
REF:MATCOD␣␣	$I(\mathcal{S}_{17}^{\mathrm{edi}})$			Mixture number associated with each of the original region number M_{mix}
REF:IGCOND␣␣	$I(\mathcal{S}_{2}^{\mathrm{edi}})$			Reference group limits associated with the merged groups C_g
REF:ADF␣␣␣␣␣	Dir	$\mathcal{S}_7^{\mathrm{edi}} = 2$		ADF–related input data as presented in Section 11.3.
REF:HVOUT␣␣␣	$C(\mathcal{S}_{23}^{\mathrm{edi}}) \ast 8$	$\mathcal{S}_{23}^{\mathrm{edi}} > 0$		Names of the reactions saved in the output microlib.
CARISO␣␣␣␣␣␣	$C(\mathcal{S}_{9}^{\mathrm{edi}}) \ast 12$	$\mathcal{S}_{9}^{\mathrm{edi}} \geq 1$		Name of extracted isotopes saved during the last editing (NAMI)
IACTI␣␣␣␣␣␣␣	$I(\mathcal{S}_{5}^{\mathrm{edi}})$	$\mathcal{S}_{5}^{\mathrm{edi}} \geq 1$		Original mixture numbers for which activation data was generated (A_m)
MACRO-GEOM␣␣	Dir	$\mathcal{S}_{20}^{\mathrm{edi}} = 1$		Macro–*geometry* directory. This geometry may be used to complete the COMPO database, for performing a geometry equivalence (*equigeom*) and/or as the macro–geometry in SPH calculations. This directory follows the specification presented in Section 3.2.
LINK.MACGEOM	C∗12	$\mathcal{S}_{20}^{\mathrm{edi}} = 1$		Name of the macro–*geometry* on which the last edition was based.
{*/micdir/*}	Dir			Set of sub-directories containing the editing information. This directory follows the specification presented in Section 2.2.

The set of directory {/micdir/} names EDIDIR will be composed according to the following rules. In the case where the set of keywords SAVE ON are used followed by a directory name as above, the contents of EDIDIR will be identical the name of the specified directory (e. g., EDITCELL2G␣␣). If the SAVE option is used without specifying a specific directory, then the first eight characters of EDIDIR (EDIDIR(1:8)) will be given as REF-CASE while the last four character (EDIDIR(9:12)) will be a unique character variable representing the successive directory saved. This character variable will be created as follows:

$$\mathrm{WRITE}(\mathrm{EDIDIR}(9:12),'(\mathtt{I4.4})')\ J$$

where $1 \leq J$ represents the Jth execution of the EDI: module. In the case above, we would have a single editing directory of the form:

Table 67: Example of an editing directory

Name	Type	Condition	Units	Comment
`EDITCELL2G`␣␣	Dir			Two groups /microlib/ sub-directory

11.3   The `/REF:ADF/` sub-directory in /edition/

Sub-directory containing input data for ADF-type boundary flux edition.

Table 68: Records in the `/REF:ADF/` sub-directory

Name	Type	Condition	Units	Comment
`NTYPE`␣␣␣␣␣␣␣	I(1)			Number of ADF-type boundary flux edits.
`NADF`␣␣␣␣␣␣␣␣	I(NTYPE)			N_i^{adf}: number of regions included in each ADF-type boundary flux edit.
`HADF`␣␣␣␣␣␣␣␣	C(NTYPE)*4			Name of each ADF-type boundary flux edit. Standard names are: = `FD_C`: corner flux edition; = `FD_B`: surface (assembly gap) flux edition; = `FD_H`: row flux edition. These are the first row of surrounding cells in the assembly.
{*/type/*}	I(N_i^{adf})			Set of integer arrays containing the editing information. Indices of the regions of the reference geometry belonging to the flux edition. Name *type* is a component of `HADF` array.

12 Contents of a /burnup/ directory

This directory contains the main burnup information, namely the multigroup flux and the isotopic concentration at each time or burnup step.

12.1 State vector content for the /burnup/ data structure

The dimensioning parameters for the /burnup/ data structure, which are stored in the state vector $\mathcal{S}^b$, represent:

- The type of solution considered $I_s = \mathcal{S}_1^b$ where

$$
I_s = \left\{ \begin{array}{ll} 1 & \text{Fifth-order Cash-Karp method} \\ 2 & \text{Forth-order Kaps-Rentrop method} \end{array} \right.
$$

- The type of burnup considered $I_t = \mathcal{S}_2^b$ where

$$
I_t = \left\{ \begin{array}{ll} 0 & \text{Out of core or zero flux/power depletion} \\ 1 & \text{Constant flux depletion} \\ 2 & \text{Constant fuel power depletion} \\ 3 & \text{Constant assembly power depletion} \end{array} \right.
$$

- Number of time steps for which burnup properties are present in this directory $N_t = \mathcal{S}_3^b$

- Total number of isotopes $N_I = \mathcal{S}_4^b$

- Number of depleting mixtures $N_M^{\text{depl}} = \mathcal{S}_5^b$

- Number of depleting reactions $N_R^{\text{depl}} = \mathcal{S}_6^b$

- Number of depleting isotopes $N_I^{\text{depl}} = \mathcal{S}_7^b$

- Number of mixtures $N_m = \mathcal{S}_8^b$

- Microscopic reaction rate extrapolation option in solving the burnup equations $I_e = \mathcal{S}_9^b$ where

$$
I_e = \left\{ \begin{array}{ll} 0 & \text{Do not extrapolate} \\ 1 & \text{Perform linear extrapolation} \end{array} \right.
$$

- Constant power normalization option for the burnup calculation $I_g = \mathcal{S}_{10}^b$ where

$$
I_g = \left\{ \begin{array}{ll} 0 & \text{Compute the burnup using the power released in fuel} \\ 1 & \text{Compute the burnup using the power released in the global geometry} \end{array} \right.
$$

This option have an effect only in cases where some non-depleting mixtures are producing energy.

- Saturation of initial number densities $I_s = \mathcal{S}_{11}^b$ where

$$
I_s = \left\{ \begin{array}{ll} 0 & \text{Do not store saturated initial number densities in the BURNUP object} \\ 1 & \text{Store saturated initial number densities} \end{array} \right.
$$

This option have an effect only in cases where some depleting isotopes are at saturation.

- Type of saturation model $I_d = \mathcal{S}_{12}^b$ where

$$I_d = \left\{ \begin{array}{ll} 0 & \text{Do not use Dirac functions in saturated number densities} \\ 1 & \text{Use Dirac functions in saturated number densities} \end{array} \right.$$

This option have an effect only in cases where some depleting isotopes are at saturation.

- Perturbation flag for cross sections $I_p = \mathcal{S}_{13}^b$ where

$$I_p = \left\{ \begin{array}{ll} 0 & \text{Time-dependent cross sections will be used if available} \\ 1 & \text{Time-independent cross sections will be used} \end{array} \right.$$

- Neutron flux recovery flag $I_f = \mathcal{S}_{14}^b$ where

$$I_f = \left\{ \begin{array}{ll} 0 & \text{Neutron flux is recovered from a L\_FLUX object} \\ 1 & \text{Neutron flux is recovered from the embedded macrolib present in a} \\ & \text{L\_LIBRARY object} \end{array} \right.$$

- Fission yield data recovery flag $I_y = \mathcal{S}_{15}^b$ where

$$I_y = \left\{ \begin{array}{ll} 0 & \text{Fission yield data is recovered from } \texttt{DEPL-CHAIN} \text{ directory (see Section 2.4)} \\ 1 & \text{Fission yield data is recovered from } \texttt{PIFI} \text{ and } \texttt{PYIELD} \text{ records in /isotope/} \\ & \text{directory (see Table 17)} \end{array} \right.$$

12.2   The main /burnup/ directory

On its first level, the following records and sub-directories will be found in the /burnup/ directory:

Table 69: Main records and sub-directories in /burnup/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C*12			Signature of the /burnup/ data structure (SIGNA =L␣BURNUP␣␣␣␣).
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^b$, as defined in Section 12.1.
EVOLUTION-R␣	R(5)			Vector describing the various parameters associated with the burnup calculation options R_i
LINK.LIB␣␣␣␣	C*12			Name of the MICROLIB on which the last depletion step was based.
DEPL-TIMES␣␣	R(N_t)		10^8 s	Vector describing the various time steps at which burnup information has been saved T_i
FUELDEN-INIT	R(3)			Vector giving the initial density of heavy element in the fuel ρ_f (g cm^{-3}), the initial mass of heavy element in the fuel m_f (g) and the initial mass of heavy element in the fuel divided by the global geometry volume (g cm^{-3})

Main records and sub-directories in /burnup/ continued from last page

Name	Type	Condition	UnitsComment
VOLUME-MIX␣␣	$R(N_m)$		cm³ Vector giving the mixture volumes
FUELDEN-MIX␣	$R(N_m)$		g Initial mass of heavy element contained in each mixture
WEIGHT-MIX␣␣	$R(N_m)$		g Initial mass of all the isotopes contained in each mixture
DEPLETE-MIX␣	$I(N_m \times N_I^{\text{depl}})$		Matrix giving the index in the ISOTOPESDENS record of each depleting isotope in each mixture.
ISOTOPESUSED	$C(N_I) * 12$		Alias name of the isotopes
ISOTOPESMIX␣	$I(N_I)$		Mixture number associated with each isotope
MIXTURESBurn	$I(N_m)$		Depletion flag array. A component is set to 1 to indicate that a mixture is depleting.
MIXTURESPowr	$I(N_m)$		Power flag array. A component is set to 1 to indicate that a mixture is producing power.
{/depldir/}	Dir		Set of N_t sub-directories containing the properties associated with each burnup step T_i

The set of directory {/depldir/} names DEPLDIR will be composed according to the following laws. The first eight character (DEPLDIR(1:8)) will always be given by DEPL-DAT. The last four characters (DEPLDIR(9:12)) represent the time step saved. For the case where N_t time steps were saved we would use the following FORTRAN instructions to create the last four characters of each of the directory names:

$$\text{WRITE}(\text{DEPLDIR}(9:12),'(\text{I4.4})')\ J$$

for $1 \leq J \leq N_t$ with the time stamp associated with each directory being given by T_J. For the case where ($N_t = 2$), two such directory would be generated, namely

Table 70: Example of depletion directories

Name	Type	Condition	Units	Comment
DEPL-DAT0001	Dir			Sub-directories which contain the information associated with time step 1
DEPL-DAT0002	Dir			Sub-directories which contain the information associated with time step 2

12.3   The depletion sub-directory /depldir/ in /burnup/

Inside each depletion directory the following records and sub-directories will be found:

Table 71: Contents of a depletion sub-directory in /burnup/

Name	Type	Condition	Units	Comment
ISOTOPESDENS	$R(N_I)$		$(\text{cm b})^{-1}$	Isotopic densities ρ_i for each of the isotopes described in the /microlib/ directory where the order of the isotopes is also specified
MICRO-RATES␣	$R(N^{\text{dim}})$		$10^{-8}\ \text{s}^{-1}$	Values of the microscopic reaction rate of the depleting reactions for each depleting isotope and each mixture. The macroscopic reaction rate related to the non-depleting isotopes is stored at location $N_I^{\text{depl}} + 1$. The N_R^{depl} reaction types are stored in the order of the 'DEPLETE-IDEN' array in Table 11, starting with the 'NFTOT' reaction. The flux-induced power factors are stored in location N_R^{depl}. The decay power (delayed) factors are stored in location $N_R^{\text{depl}}+1$ Both flux-induced and decay power are given in units of 10^{-8} MeV/s. $N^{\text{dim}} = (N_I^{\text{depl}} + 1) \times (N_R^{\text{depl}} + 1) \times N_m$
INT-FLUX␣␣␣␣	$R(N_m)$		cm s^{-1}	Integrated flux in each mixture.
FLUX-NORM␣␣␣	$R(1)$		1	Flux normalization constant. It is zero for out of core depletion and represents the normalization of the flux ϕ_r^g that is used to ensure that the cell integrated flux or power is that required when fixed flux or power burnup is requested
ENERG-MIX␣␣␣	$R(N_m)$		Joule	Energy realeased during the time step in each mixture
FORM-POWER␣␣	$R(1)$	$I_t = 3$	1	Ratio of the global power released in the complete geometry divided by the power released in fuel.
BURNUP-IRRAD	$R(2)$			Fuel burnup (MW d T^{-1}) and irradiation (Kb^{-1}) reached at this time step

13 Contents of a /multicompo/ directory

This object, shown in Figure 5, is used to collect information gathered from many DRAGON *elementary calculations* performed under various conditions. Each elementary calculation is characterized by a tuple of *global* and *local parameters*. These parameters are of different types, depending on the nature of the study under consideration: type of assembly, power, temperature in a mixture, concentration of an isotope, time, burnup or exposure rate in a depletion calculation, etc. Each step of a depletion calculation represents an elementay calculation. The MULTICOMPO object is often presented as a *multi-parameter reactor database*.
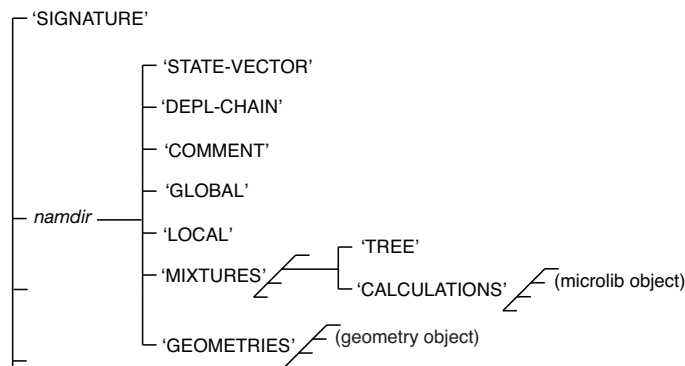

Figure 5: Representation of a MULTICOMPO object.

The MULTICOMPO object contains table-of-content information apart from a list of *homogenized mixture* directories. Each *homogenized mixture* directory contain a list of *elementary calculation* directories whose components are embedded MICROLIB objects containing the useful data. The localization of an elementary calculation is done using a tuple of global and local parameters. The elementary calculation indices are stored in a tree with the number of levels equal to the number of global *and* local parameters. An example of a tree with three parameters is shown in Figure 6. Each node of this tree is associated with the index of the corresponding global parameter (positive index) or local parameter (negative index) and with the reference to the daughter nodes if they exist. The number if leafs is equal to the number of nodes for the last (third) parameter and is equal to the number of elementary calculations stored in the MULTICOMPO object. The index of each elementary calculation is therefore an attribute of each leaf.
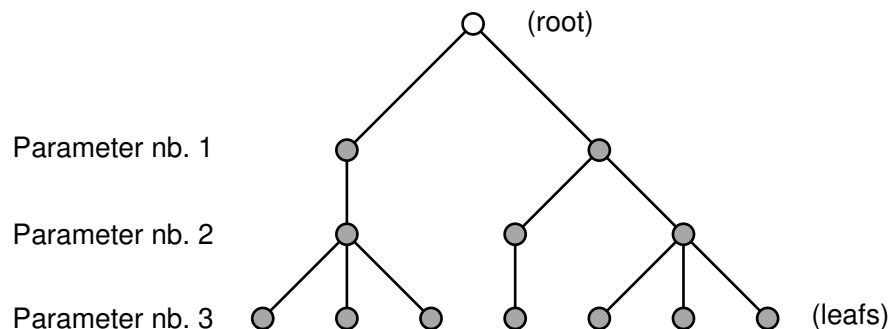

Figure 6: Parameter tree in a MULTICOMPO object

In each embedded MICROLIB directory, the `COMPO:` module recover cross sections for a number of *particularized isotopes* and *macroscopic sets* named `'*MAC*RES'`, a collection of isotopic cross sections

weighted by isotopic number densities. Other information is also recovered: multigroup neutron fluxes, isotopic number densities, fission spectrum and a set of *local parameters*. The local parameters are values that characterize each homogenized mixture: local power, burnup, exposure rate, etc.

13.1   State vector content for the /multicompo/ data structure

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}^{\mathrm{cpo}}$, represent:

- The number of homogenized mixtures $M_m = \mathcal{S}_1^{\mathrm{cpo}}$. $= 0$ for an empty MULTICOMPO object.

- The number of groups $G = \mathcal{S}_2^{\mathrm{cpo}}$

- The exact number of elementary calculations in the MULTICOMPO $N_{\mathrm{cal}} = \mathcal{S}_3^{\mathrm{cpo}}$

- The maximum number of elementary calculations in the MULTICOMPO $N_{\max} = \mathcal{S}_4^{\mathrm{cpo}}$

- The number of global parameters $N_{\mathrm{glob}} = \mathcal{S}_5^{\mathrm{cpo}}$

- The number of local parameters $N_{\mathrm{loc}} = \mathcal{S}_6^{\mathrm{cpo}}$

- The number of global parameters linked with isotopes $N_{\mathrm{gl\_iso}} = \mathcal{S}_7^{\mathrm{cpo}}$

- The number of global parameters linked with MICROLIB objects $N_{\mathrm{gl\_bib}} = \mathcal{S}_8^{\mathrm{cpo}}$

- The number of local parameters linked with isotopes $N_{\mathrm{loc\_iso}} = \mathcal{S}_9^{\mathrm{cpo}}$

- The number of lines of comment $N_{\mathrm{doc}} = \mathcal{S}_{10}^{\mathrm{cpo}}$

- Geometry index $L_{\mathrm{geo}} = \mathcal{S}_{11}^{\mathrm{cpo}}$:

$$L_{\mathrm{geo}} = \begin{cases} 0 & \text{the geometries are not available} \\ 1 & \text{calculation–ordered homogenized geometries are available.} \end{cases}$$

- Version identificator $\mathcal{S}_{12}^{\mathrm{cpo}}$. Currently equal to 2006. This value will change if the MULTICOMPO specification is to be modified in the future.

- The number of user-defined particularized isotopes $\mathcal{S}_{13}^{\mathrm{cpo}}$.

- Group form factor index $N_{\mathrm{gff}} = \mathcal{S}_{14}^{\mathrm{cpo}}$:

$$N_{\mathrm{gff}} = \begin{cases} -1 & \text{the group form factors will be recovered from an EDITION object} \\ 0 & \text{the group form factors are not processed} \\ > 0 & \text{number of group form factors per energy group. The information is stored in} \\ & \text{a MACROLIB subdirectory in the MULTICOMPO.} \end{cases}$$

- Physical albedo index $N_{\mathrm{alb}} = \mathcal{S}_{15}^{\mathrm{cpo}}$:

$$N_{\mathrm{alb}} = \begin{cases} -1 & \text{the physical albedos will be recovered from an EDITION object} \\ 0 & \text{the physical albedos are not processed} \\ > 0 & \text{number of physical albedos per energy group. The information is stored in} \\ & \text{a MACROLIB subdirectory in the MULTICOMPO.} \end{cases}$$

- Discontinuity factor index $I_{\mathrm{df}} = \mathcal{S}_{16}^{\mathrm{cpo}}$:

$$I_{\mathrm{df}} = \begin{cases} -1 & \text{discontinuity factor information will be recovered from an EDITION object} \\ 0 & \text{no discontinuity factor information} \\ 1 & \text{multigroup boundary current information is available} \\ 2 & \text{discontinuity factor information (see Section 1.4) is available.} \end{cases}$$

13.2   The main /multicompo/ directory

On its first level, the following records and sub-directories will be found in the /multicompo/ directory:

Table 72: Main records in /multicompo/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			Signature of the data structure (SIGNA =L␣MULTICOMPO).
{/namdir/}	Dir			Set of sub-directories, each of them containing an independent MULTICOMPO structure

Table 73: Main records and sub-directories in {/namdir/}

Name	Type	Condition	UnitsComment
STATE-VECTOR	I(40)		Vector describing the various parameters associated with this data structure $\mathcal{S}_i^{\mathrm{cpo}}$, as defined in Section 13.1.
DEPL-CHAIN␣␣	Dir	∗	directory containing the /depletion/ associated with directory /namdir/, following the specification presented in Section 2.4.
COMMENT␣␣␣␣␣	C(N_{10}^{cpo}) ∗ 80	$\mathcal{S}_{10}^{\mathrm{cpo}} > 0$	User–defined comments about the data structure
NOMISP␣␣␣␣␣␣	C($\mathcal{S}_{13}^{\mathrm{cpo}}$) ∗ 8	$\mathcal{S}_{13}^{\mathrm{cpo}} \geq 1$	Names of the user-defined particularized isotopes.
GLOBAL␣␣␣␣␣␣	Dir		Table–of–content for global parameter information: definition and tabulated values. The specification is presented in Section 13.3.
LOCAL␣␣␣␣␣␣␣	Dir	$\mathcal{S}_6^{\mathrm{cpo}} \geq 1$	Table–of–content for local parameter information. The specification is presented in Section 13.4.
MIXTURES␣␣␣␣	Dir($\mathcal{S}_1^{\mathrm{cpo}}$)	$\mathcal{S}_1^{\mathrm{cpo}} \geq 1$	List of *homogenized mixture* directories. Each component of this list follows the specification presented in Section 13.5.
GEOMETRIES␣␣	Dir($\mathcal{S}_4^{\mathrm{cpo}}$)	$\mathcal{S}_{11}^{\mathrm{cpo}} = 1$	List of homogenized *geometry* directories. Each component of this list follows the specification presented in Section 3.2.

13.3   The GLOBAL sub-directory in /multicompo/

This directory is a table–of–content for the globals parameters. Its specification follows:

Table 74: Contents of sub-directory `GLOBAL` in /multicompo/

Name	Type	Condition	UnitsComment
PARKEY␣␣␣␣␣␣	$C(\mathcal{S}_5^{\text{cpo}}) * 12$		User–defined key-words for the global parameters.
PARTYP␣␣␣␣␣␣	$C(\mathcal{S}_5^{\text{cpo}}) * 4$		Character identification for the types of global parameters (eg: `TEMP`, `CONC`, `IRRA`, etc.). Temperatures are given in Kelvin.
PARFMT␣␣␣␣␣␣	$C(\mathcal{S}_5^{\text{cpo}}) * 8$		Types for the global parameters (eg: `REAL`, `STRING` or `INTEGER`).
PARCHR␣␣␣␣␣␣	$C(\mathcal{S}_7^{\text{cpo}}) * 8$	$\mathcal{S}_7^{\text{cpo}} \geq 1$	Isotope names linked to type–`CONC` global parameters.
NVALUE␣␣␣␣␣␣	$I(\mathcal{S}_5^{\text{cpo}})$		Number of specific values for a global parameters.
PARCAD␣␣␣␣␣␣	$I(\mathcal{S}_5^{\text{cpo}} + 1)$		Address of the first element in array `PARCHR`.
PARPAD␣␣␣␣␣␣	$I(\mathcal{S}_5^{\text{cpo}} + 1)$		Address of the first element in array `PARBIB`.
PARMIL␣␣␣␣␣␣	$I(\mathcal{S}_8^{\text{cpo}})$	$\mathcal{S}_8^{\text{cpo}} \geq 1$	Mixture indices linked to type–`TEMP` or –`CONC` global parameters.
PARBIB␣␣␣␣␣␣	$C(\mathcal{S}_8^{\text{cpo}}) * 12$	$\mathcal{S}_8^{\text{cpo}} \geq 1$	MICROLIB names linked to type–`TEMP` or –`CONC` global parameters.
{/gvaldir/}	$R(\text{NVALUE(J)})$	*	Set of real global parameter arrays. Each element of {/gvaldir/} contains a real array containing the tabulated values of the J–th global parameter.
{/gvaldir/}	$I(\text{NVALUE(J)})$	*	Set of integer global parameter arrays. Each element of {/gvaldir/} contains an integer array containing the tabulated values of the J–th global parameter.
{/gvaldir/}	$C(\text{NVALUE(J)}) * 12$	*	Set of character∗12 global parameter arrays. Each element of {/gvaldir/} contains a character∗12 array containing the tabulated values of the J–th global parameter.

Item {/gvaldir/} represents a set of $\mathcal{S}_5^{\text{cpo}}$ real, integer or character*12 records. The name of each {/gvaldir/} record is a `character*12` variable (`text12`) composed using the following FORTRAN instruction:

$$\text{WRITE}(\text{text12},'\,(''\text{pval}'',\text{I8.8})')\,J$$

where J is the index of the global parameter with $1 \leq J \leq \mathcal{S}_5^{\text{cpo}}$. The global parameter values of type `REAL` or `INTEGER` are sorted.

13.4   The `LOCAL` sub-directory in /multicompo/

This directory is a table–of–content for the locals parameters. Its specification follows:

Table 75: Contents of sub-directory `LOCAL` in /multicompo/

Name	Type	Condition	Units	Comment
`PARKEY␣␣␣␣␣␣`	$C(\mathcal{S}_6^{\mathrm{cpo}}) * 12$			User–defined key-words for the local parameters.
`PARTYP␣␣␣␣␣␣`	$C(\mathcal{S}_6^{\mathrm{cpo}}) * 4$			Character identification for the types of local parameters (eg: `TEMP`, `IRRA`, `FLUB`, etc.).
`PARCHR␣␣␣␣␣␣`	$C(\mathcal{S}_9^{\mathrm{cpo}}) * 8$	$\mathcal{S}_9^{\mathrm{cpo}} \geq 1$		Isotope names linked to type–`CONC` local parameters.
`PARCAD␣␣␣␣␣␣`	$I(\mathcal{S}_6^{\mathrm{cpo}} + 1)$			Address of the first element in array `PARCHR`.

13.5   The homogenized mixture sub-directory in /multicompo/

Each component of the list named 'MIXTURES' contains the parameter tree and a list of directories:

Table 76: Component of the homogenized mixture directory

Name	Type	Condition	Units	Comment
`TREE␣␣␣␣␣␣␣␣`	Dir			Parameter tree. The specification is presented in Section 13.6.
`CALCULATIONS`	$\mathrm{Dir}(\mathcal{S}_4^{\mathrm{cpo}})$			List of MICROLIB directories. Each component of this list follows the specification presented in Section 2.2 with $M_m = 1$ (1 mixture) and $\mathcal{M} = 4$.

13.6   The `TREE` sub-directory in a `MIXTURES` component

This directory contains local parameter values and the parameter tree. Its specification follows:

Table 77: Contents of sub-directory `TREE` in `MIXTURES`

Name	Type	Condition	Units	Comment
`NCALS␣␣␣␣␣␣`	$I(1)$			Number of elementary calculations.
`NVP␣␣␣␣␣␣␣␣`	$I(2)$			`NVP(1)`: Exact number of nodes in the parameter tree. `NVP(2)`: Maximum number of nodes in the parameter tree.
`NVALUE␣␣␣␣␣␣`	$I(\mathcal{S}_6^{\mathrm{cpo}})$	$\mathcal{S}_6^{\mathrm{cpo}} \geq 1$		Number of specific values for a local parameters.

Contents of sub-directory `TREE` in `MIXTURES`

Name	Type	Condition	Units	Comment
{/*lvaldir*/}	R(NVALUE(J))	$\mathcal{S}_6^{\text{cpo}} \geq 1$		Set of real local parameter arrays. Each element of {/lvaldir/} contains a real array containing the tabulated values of the J–th local parameter.
DEBARB␣␣␣␣␣␣	I(NVP(1)+1)			- If the node does not correspond to the last parameter: index in `DEBARB` of the first daughter of the node. - If the node correspond to the last parameter: index in `DEBARB` where we recover the index of an elementary calculation.
ARBVAL␣␣␣␣␣␣	I(NVP(1))			-For a global parameter: index of the parameter in the {/gvaldir/} record (see Table 74). -For a local parameter: index of the parameter in the {/lvaldir/} record
ORIGIN␣␣␣␣␣␣	I($\mathcal{S}_4^{\text{cpo}}$)			Index of the mother elementary calculation. This information is useful to follow the historical relation between calculations.

Item {/*lvaldir*/} represents a set of $\mathcal{S}_6^{\text{cpo}}$ real records. The name of each {/*lvaldir*/} record is a `character*12` variable (`text12`) composed using the following FORTRAN instruction:

$$\text{WRITE}(\text{text12},' ('' \text{pval}'', \text{I8.8})') \, J$$

where J is the index of the local parameter with $1 \leq J \leq \mathcal{S}_6^{\text{cpo}}$. The local parameter values are sorted.

The parameter tree has the same number of stages as global *and* local parameters. The local parameters always follow the global parameters. For each value of the i–th parameter, the tree indicates the beginning position of the $(i+1)$–th parameter. The arrays `DEBARB` and `ARBVAL` are set to localize the results of an elementary calculation identified by a specific parameter tuple.

An example of a parameter tree is represented here:

```
dn = value in DEBARB,  (m) = value in ARBVAL

Root                          *(0)
                               !
Param. Nb 1                   d2(1)
                  -------------------
                  !                   !
Param. Nb 2      d3(1)               4(2)
                -------          ---------
                !     !          !   !   !
Param. Nb 3   d5(1)  6(3)      d7(1) 8(2) 9(3)   d10

Calculation Nb:  4         5          1   2   3

DEBARB:       2  3  5  7 10  4  5  1  2  3
ARBVAL:       0  1  1  2  1  3  1  2  3
```

The useful dimensions of variables `DEBARB`, `ARBVAL` and `ORIGIN` in Table 77 are respectively equal to `NVP(1)+1`, `NVP(1)` and $\mathcal{S}_3^{\text{cpo}}$. The allocated sizes may be bigger.

Each elementary calculation is fully identified by a parameter tuple (the Fortran array `MUPLET(NPTOT)`), an integer array of dimension `NPTOT=` $\mathcal{S}_5^{\text{cpo}}+\mathcal{S}_6^{\text{cpo}}$. The first $\mathcal{S}_5^{\text{cpo}}$ components correspond to global parameter indices; the following $\mathcal{S}_6^{\text{cpo}}$ components correspond to local parameter indices. Here, `NVP` represents the useful size of the `ARBVAL` array. A recursive procedure is required to search the elementary calculation index `ICAL` corresponding to this parameter tuple `MUPLET`. Note that some components of the tuple can be set to zero in case where the number of global and local parameters is overdetermined. The recursive function is called using

```
ICAL=NICAL(1,NVP,NPTOT,DEBARB,ARBVAL,MUPLET)
```

and is implemented in Fortran-90 as

```
RECURSIVE INTEGER FUNCTION NICAL(II,NVP,NPTOT,DEBARB,ARBVAL,MUPLET) RESULT(ICAL)
   INTEGER II,NVP,NPTOT,DEBARB(NVP+1),ARBVAL(NVP),MUPLET(NPTOT)
   IF(NPTOT==0) THEN
      ICAL=DEBARB(II+1)
      RETURN
   ENDIF
   NBOK=0
   IKEEP=0
   DO I=DEBARB(II),DEBARB(II+1)-1
      IF((MUPLET(1)==0).OR.(MUPLET(1)==ARBVAL(I))) THEN
         JICAL=NICAL(I,NVP,NPTOT-1,DEBARB,ARBVAL,MUPLET(2))
         IF(JICAL > 0) THEN
            IKEEP=JICAL
            NBOK=NBOK+1
         ELSE IF(JICAL==-1) THEN
            NBOK=2
         ENDIF
      ENDIF
   ENDDO
   IF(NBOK > 1) THEN
      ! Many elementary calculation exist for this tuple.
      ICAL=-1
   ELSE IF(NBOK==0) THEN
      ! No elementary calculation exists for this tuple.
      ICAL=0
   ELSE
      ICAL=IKEEP
   ENDIF
END FUNCTION NICAL
```

Similarly, another Fortran program can be used to search the parameter tuple corresponding to the `ICAL`–th elementary calculation:

```
SUBROUTINE COMUPL(NVP,NPTOT,ICAL,NCALS,DEBARB,ARBVAL,MUPLET)
   INTEGER NVP,NPTOT,ICAL,NCALS,DEBARB(NVP+1),ARBVAL(NVP),MUPLET(NPTOT)
   DO I=NVP-NCALS+1,NVP
      IF(DEBARB(I+1)==ICAL) THEN
         IO=I
         EXIT
      ENDIF
```

```
   ENDDO
   MUPLET(NPTOT)=ARBVAL(IO)
   DO IPAR=NPTOT-1,1,-1
      DO I=1,NVP-NCALS
         IF(DEBARB(I+1) > IO) THEN
            IO=I
            EXIT
         ENDIF
      ENDDO
      MUPLET(IPAR)=ARBVAL(IO)
   ENDDO
END SUBROUTINE COMUPL
```

14 Contents of a /CPO/ directory

This directory contains a burnup dependent hierarchical reactor database. For the purpose of illustration we will assume that the `CPO:` module is executed using the following data:

```
CpoResults := CPO: EdiResults EvoResults ::
BURNUP REF-CASE
EXTRACT ALL
NAME MIXTH ;
```

where `EdiResults` is a EDITION data structure that contains 2 homogeneous mixtures, evaluated and saved at 2 time steps, `EvoResults` is a BURNUP data structure containing information for the successive burnup calculations used to generate `EdiResults` and finally `CpoResults` is the final CPO data structure that contains the resulting reactor database.

14.1 The main directory

The following records and sub-directories will be found in the /CPO/ directory:

Table 78: Main records and sub-directories in /CPO/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			parameter SIGNA containing the signature of the data structure
STATE-VECTOR	I(40)			array $\mathcal{S}_i^c$ containing various parameters that are required to describe this data structure
{/MIXDIR/}	Dir			list of sub-directories that contain homogeneous mixture information

The signature for this data structure is SIGNA=L_COMPO␣␣␣␣␣. The array $\mathcal{S}_i^c$ contains the following information:

- $\mathcal{S}_1^c = N_H$ contains the total number of homogeneous mixtures saved.

- $\mathcal{S}_2^c = M_G$ contains the maximum number of groups considered.

- $\mathcal{S}_3^c = M_I$ contains the maximum number of isotopes.

- $\mathcal{S}_4^c = M_L$ contains the maximum order for the scattering anisotropy.

- $\mathcal{S}_5^c = M_B$ contains the maximum number of burnup steps per mixtures.

The list of directory {/MIXDIR/} names MIXDIR will be composed according to the following laws. The first eight character (MIXDIR(1:8)) will be identical to the first 8 character of the user data following the keyword NAME in the CPO: module (here MIXTH␣␣␣. If the keyword NAME is not used then MIXDIR(1:8) takes the value COMPO␣␣␣. The last four characters (MIXDIR(9:12)) represent the various homogeneous mixture number saved on the EDITION data structure. For the case where N_H such mixtures were produces the following FORTRAN instructions are used to create the last four character of each of the directory names:

```
    WRITE(MIXDIR(9:12),'(I4)')  J
```

for $1 \leq J \leq N_H$. For the example given above ($N_H = 2$), two such directories will be generated, namely

Table 79: Example of homogeneous mixture directories

Name	Type	Condition	Units	Comment
MIXTH⎵⎵⎵⎵⎵⎵1	Dir			is the sub-directory that contains the information associated with homogeneous mixture 1
MIXTH⎵⎵⎵⎵⎵⎵2	Dir			is the sub-directory that contains the information associated with homogeneous mixture 2

14.2   The mixture sub-directory

Each mixture directory contains the following records and sub-directories will be found:

Table 80: Contents of a mixture sub-directory in /CPO/

Name	Type	Condition	Units	Comment
TITLE⎵⎵⎵⎵⎵⎵	C*72			parameter T containing the title of the run which produced this mixture
PARAM⎵⎵⎵⎵⎵⎵	I(4)			array $\mathcal{P}_i^{\mathrm{cpo}}$ containing the various parameters associated with this mixture
VOLUME⎵⎵⎵⎵⎵⎵	R(1)		cm^3	parameter V_i containing the volume of the region associated this homogeneous mixture in the EDITION data structure
ENERGY⎵⎵⎵⎵⎵⎵	R(G + 1)		eV	array E_g containing the energy groups limits
BURNUP⎵⎵⎵⎵⎵⎵	R($\mathcal{P}_4^{\mathrm{cpo}}$)		MW d T^{-1}	array B_k containing the burnup steps
N/KB⎵⎵⎵⎵⎵⎵⎵⎵	R($\mathcal{P}_4^{\mathrm{cpo}}$)		Kb^{-1}	array w_k containing the fuel irradiation for the different burnup steps
ISOTOPESNAME	C($\mathcal{P}_2^{\mathrm{cpo}}$) * 12			array ISO_i containing the name of the various isotopes saved for this mixture
{/BRNDIR/}	Dir			list of sub-directories that contain the burnup dependent cross sections associated with this homogeneous mixture

The following information is stored in $\mathcal{P}^{\mathrm{cpo}}$:

- $\mathcal{P}_1^{\mathrm{cpo}} = G$ contains the number of groups for this homogeneous mixture.

- $\mathcal{P}_2^{\mathrm{cpo}} = N_I$ contains the number of isotopes in this mixture.

- $\mathcal{P}_3^{\mathrm{cpo}} = N_L$ contains the order of the scattering anisotropy for this mixture.

- $\mathcal{P}_4^{\text{cpo}} = N_B$ contains the number of burnup steps for this mixture.

The list of directory {/BRNDIR/} names BRNDIR will be composed according to the following FOR-TRAN instructions:

```
WRITE(BRNDIR,'(A8,I4)'), 'BURN    ', J
```

for $1 \le J \le N_B$. For the example given above ($N_B = 2$), two such directories will be generated, namely

Table 81: Example of homogeneous mixture directories

Name	Type	Condition	Units	Comment
BURN␣␣␣␣␣␣␣1	Dir			is the sub-directory that contains the information associated with burnup step 1
BURN␣␣␣␣␣␣␣2	Dir			is the sub-directory associated with burnup step 2

14.3   The burnup sub-directory

A burnup sub-directory contains the following records and sub-directories:

Table 82: Contents of a burnup sub-directory in /CPO/

Name	Type	Condition	Units	Comment
ISOTOPESDENS	$R(N_I)$		$(\text{cm b})^{-1}$	array ρ_i containing the density of each isotopes
ISOTOPES-EFJ	$R(N_I)$		J	array H_i containing the energy produced per fission for each isotope
FLUX-INTG␣␣␣	$R(G)$		cm s^{-1}	array Φ_m^g containing the integrated flux
OVERV␣␣␣␣␣␣␣	$R(G)$		cm^{-1}s	array $1/v_m^g$ containing the inverse of the average neutron velocity
FLUXDISAFACT	$R(G)$			array F_g containing the ratio of the flux in the fuel to the flux in the cell
{/ISOTOPE/}	Dir			list of N_I sub-directories that contain the isotopic microscopic cross section for this burnup step

The list of directory names is specified by ISODIR = ISO$_i$ for $i = 1$ to N_I. The first isotope ISODIR is named MACR␣␣␣␣␣␣␣␣ and represents an equivalent macroscopic isotope with a density of 1.0 $(\text{cm b})^{-1}$. The content of the isotopic multigroup cross section directory is described in Section 2.9.

15 Contents of a /saphyb/ directory

This object is used to collect information gathered from many DRAGON *elementary calculations* performed under various conditions. Each elementary calculation is characterized by a tuple of *global parameters*. These global parameters are of different types, depending on the nature of the study under consideration: type of assembly, power, temperature in a mixture, concentration of an isotope, time, burnup or exposure rate in a depletion calculation, etc. Each step of a depletion calculation represents an elementay calculation. The SAPHYB object is often presented as a *multi-parameter reactor database*. It is used in the SAPHYR code system.

The SAPHYB object contains table-of-content information apart from a set of specific *elementary calculation* directories. These directories are themselve subdivided into *homogenized mixture* directories. The localization of an elementary calculation is done using a tuple of global parameters. The elementary calculation indices are stored in a tree with the number of levels equal to the number of global parameters. An example of a tree with three global parameters is shown in Figure 7. Each node of this tree is associated with the index of the corresponding global parameter and with the reference to the daughter nodes if they exist. The number if leafs is equal to the number of nodes for the last (third) parameter and is equal to the number of elementary calculations stored in the SAPHYB object. The index of each elementary calculation is therefore an attribute of each leaf.
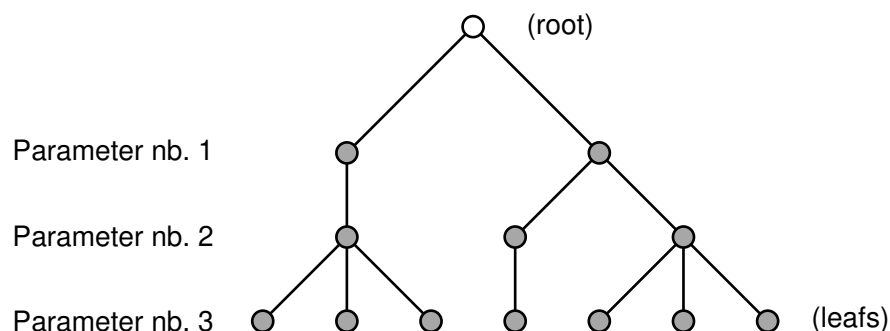

Figure 7: Global parameter tree in a SAPHYB object

In each homogenized mixture directory, the `SAP:` module recovers cross sections for a number of *particularized isotopes* and *macroscopic sets*, a collection of isotopic cross sections weighted by isotopic number densities. Cross sections for particularized isotopes and macroscopic sets are recovered for *selected reactions*. Other information is also recovered: multigroup neutron fluxes, isotopic number densities, fission spectrum and a set of *local variables*. The local variables are values that characterize each homogenized mixture: local power, burnup, exposure rate, etc. Some local variables are arrays of values (eg: SPH equivalence factors). Finally, note that cross section information written on the SAPHYB is *not* transport corrected and *not* SPH corrected.

15.1 The main /saphyb/ directory

On its first level, the following records and sub-directories will be found in the /saphyb/ directory:

Table 83: Main records and sub-directories in /saphyb/

Name	Type	Condition	UnitsComment
SIGNATURE␣␣␣	C$*$12		Signature of the data structure SIGNA
TITLE␣␣␣␣␣␣␣	C$*$80		Signature of the data structure (for this level of specification,$=$'SAPHYB LIBRARY VER, 0.02')
NOMLIB␣␣␣␣␣␣	C$*$80		User–defined name of the data structure
DIMSAP␣␣␣␣␣␣	I(50)		Vector describing the various parameters associated with this data structure $\mathcal{S}_i^{\mathbf{sap}}$
COMMEN␣␣␣␣␣␣	C($N_1^{\mathbf{sap}}$)$*$80	$\mathcal{S}_1^{\mathbf{sap}} > 0$	User–defined comments about the data structure
constphysiq␣	Dir		General physical data
contenu␣␣␣␣␣	Dir		Content description
geom␣␣␣␣␣␣␣␣	Dir		Geometric data
adresses␣␣␣␣	Dir		General localization data for the cross sections
paramdescrip	Dir		General localization data for the global parameters
paramarbre␣␣	Dir		Global parameter tree
paramvaleurs	Dir		Global parameter values
varlocdescri	Dir		General localization data for the local variables
{*/caldir/*}	Dir		Set of $\mathcal{S}_{19}^{\mathbf{sap}}$ sub-directories containing the cross section information associated with a specific elementary calculation.

The signature variable for this data structure must be SIGNA=L_SAPHYB␣␣␣␣.

The name of each {/caldir/} directory is a `character*12` variable (`text12`) composed using the following FORTRAN instruction:

$$\text{WRITE}(\texttt{text12},'(''\texttt{calc}'',\texttt{I8})')\, J$$

where J is the index of the calculation with $1 \leq J \leq \mathcal{S}_{19}^{\mathbf{sap}}$.

The dimensioning parameters for this data structure, which are stored in the state vector $\mathcal{S}^{\mathbf{sap}}$ named DIMSAP, are defined in the following table:

Values in DIMSAP

	DIMSAP	
$\mathcal{S}_1^{\mathbf{sap}}$	NCOMLI	Number of lines of comment
$\mathcal{S}_2^{\mathbf{sap}}$	NISOTA	Number of isotopes in the reference cross section library
$\mathcal{S}_3^{\mathbf{sap}}$	NCHANN*	Number of types of radioactive decay reactions
$\mathcal{S}_4^{\mathbf{sap}}$	NREA*	Number of neutron–induced reaction
$\mathcal{S}_5^{\mathbf{sap}}$	NISO*	Number of particularized isotopes
$\mathcal{S}_6^{\mathbf{sap}}$	NMAC*	Number of macroscopic sets.
$\mathcal{S}_7^{\mathbf{sap}}$	NMIL	Number of mixtures in the SAPHYB
$\mathcal{S}_8^{\mathbf{sap}}$	NPAR	Number of global parameters
$\mathcal{S}_9^{\mathbf{sap}}$	NPCHR	Number of global parameters linked with isotopes
$\mathcal{S}_{10}^{\mathbf{sap}}$	NPPNT	Number of global parameters linked with MICROLIB objects
$\mathcal{S}_{11}^{\mathbf{sap}}$	NPARL*	Number of local variables.

Values in `DIMSAP` (cntd.)

	DIMSAP	
$\mathcal{S}_{12}^{\mathrm{sap}}$	NPCHRL*	Number of local variables linked with isotopes
$\mathcal{S}_{13}^{\mathrm{sap}}$	NPPNTL*	Number of local variables linked with MICROLIB objects
$\mathcal{S}_{14}^{\mathrm{sap}}$	NISOF*	Number of particularized fissile isotopes
$\mathcal{S}_{15}^{\mathrm{sap}}$	NISOP*	Number of particularized fission products
$\mathcal{S}_{16}^{\mathrm{sap}}$	NMGY	Number of macrogroups for the fission yields $(= 1)$
$\mathcal{S}_{17}^{\mathrm{sap}}$	NVP	Number of nodes in the global parameter tree
$\mathcal{S}_{18}^{\mathrm{sap}}$	NADRX*	Number of address sets in array ADRX
$\mathcal{S}_{19}^{\mathrm{sap}}$	NCALS	Number of elementary calculations
$\mathcal{S}_{20}^{\mathrm{sap}}$	NG	Number of energy groups in the SAPHYB
$\mathcal{S}_{21}^{\mathrm{sap}}$	NISOY*	Number of particularized isotopes and macroscopic sets for which fission yields are provided.
$\mathcal{S}_{22}^{\mathrm{sap}}$	NVERS	Level of SAPHYB specification $(= 2)$
$\mathcal{S}_{23}^{\mathrm{sap}}$		(not used)
$\mathcal{S}_{24}^{\mathrm{sap}}$	NSURFS	Number of surfaces in the SAPHYB
$\mathcal{S}_{25}^{\mathrm{sap}}$		(not used)
$\mathcal{S}_{26}^{\mathrm{sap}}$		(not used)
$\mathcal{S}_{27}^{\mathrm{sap}}$		(not used)
$\mathcal{S}_{28}^{\mathrm{sap}}$	NRT	Number of unknowns in the reference geometry
$\mathcal{S}_{29}^{\mathrm{sap}}$		(not used)
$\mathcal{S}_{30}^{\mathrm{sap}}$	NGA	Number of energy groups in the reference MICROLIB
$\mathcal{S}_{31}^{\mathrm{sap}}$	NPRC*	Number of delayed neutron precursors groups
$\mathcal{S}_{32}^{\mathrm{sap}}$	NISOTS	Maximum number of isotopes in output tables (NISOTS $\leq$ NISOTA)
$\mathcal{S}_{33}^{\mathrm{sap}}$	NMILNR*	Number of mixtures in the SAPHYB with delayed neutron data

Elements of array `DIMSAP` identified with "*" may be equal to zero. Consequently, any array using these dimensions is optional.

15.2 The `constphysiq` sub-directory in /saphyb/

Table 84: Contents of sub-directory `constphysiq` in /saphyb/

Name	Type	Condition	Units	Comment
`ISOTA`	$C(\mathcal{S}_2^{\mathtt{sap}}) * 8$			Alias names of isotopes in the reference MICROLIB.
`ISOTYP`	$C(\mathcal{S}_2^{\mathtt{sap}}) * 4$			Types of isotopes in the reference MICROLIB. $=$'FISS': fissile isotope; $=$'F.P.': fission product; $=$' ': otherwise.
`NOMLAM`	$C(\mathcal{S}_3^{\mathtt{sap}}) * 8$	$\mathcal{S}_3^{\mathtt{sap}} \geq 1$		Character identification of the available radioactive decay reactions.
`ENRGA`	$R(\mathcal{S}_{30}^{\mathtt{sap}} + 1)$		MeV	Limits of the reference multigroup energy mesh.
`ENRGS`	$R(\mathcal{S}_{20}^{\mathtt{sap}} + 1)$		MeV	Limits of the SAPHYB multigroup energy mesh.
`FGYS`	$I(\mathcal{S}_{16}^{\mathtt{sap}} + 1)$			Indices limits in array `ENERGS` of the multigroup energy mesh for the fission yields.

15.3 The `contenu` sub-directory in /saphyb/

Table 85: Contents of sub-directory `contenu` in /saphyb/

Name	Type	Condition	Units	Comment
`NOMISO`	$C(\mathcal{S}_5^{\mathtt{sap}}) * 8$	$\mathcal{S}_5^{\mathtt{sap}} \geq 1$		Names of the particularized isotopes.
`NOMMAC`	$C(\mathcal{S}_6^{\mathtt{sap}}) * 8$	$\mathcal{S}_6^{\mathtt{sap}} \geq 1$		Names of the macroscopic sets.
`TYPMAC`	$I(\mathcal{S}_6^{\mathtt{sap}})$	$\mathcal{S}_6^{\mathtt{sap}} \geq 1$		Types of the macroscopic sets. $= 1$: select all the available isotopes in the macroscopic set; $= 2$: remove all the particularized isotope contributions from the macroscopic set.
`NOMREA`	$C(\mathcal{S}_4^{\mathtt{sap}}) * 12$	$\mathcal{S}_4^{\mathtt{sap}} \geq 1$		Names of the neutron–induced reactions (e.g.: `TOTALE`, `ABSORPTION`, `FISSION`, etc.).
`TOTMAC`	$I(\mathcal{S}_7^{\mathtt{sap}})$			Indices in array `NOMMAC` corresponding to total macroscopic sets (with *all* isotopic contributions). $= 0$ if a total macroscopic set is not defined.
`RESMAC`	$I(\mathcal{S}_7^{\mathtt{sap}})$			Indices in array `NOMMAC` corresponding to residual macroscopic sets (with isotopic contributions for the non–particularized isotopes). $= 0$ if a residual macroscopic set is not defined.

15.4 The `adresses` sub-directory in /saphyb/

Table 86: Contents of sub-directory `adresses` in /saphyb/

Name	Type	Condition	Units	Comment
`ISADRC␣␣␣␣␣␣`	$I(\mathcal{S}_7^{\text{sap}})$			Equal to array `ISADRX` (in directory `info`) for the last elementary calculation.
`NISOMN␣␣␣␣␣␣`	$I(\mathcal{S}_7^{\text{sap}})$			Number of particularized isotopes in each output mixture for which cross section information is available in at least one elementary calculation.
`ISOMIL␣␣␣␣␣␣`	$I(N^{\text{iso}})$	$N^{\text{iso}} \geq 1$		Array containing the particularized isotope indices in each output mixture. $N^{\text{iso}} = (\mathcal{S}_5^{\text{sap}} + \mathcal{S}_6^{\text{sap}}) \times \mathcal{S}_7^{\text{sap}}$
`ADRX␣␣␣␣␣␣␣␣`	$I(N^{\text{adrx}})$	$N^{\text{adrx}} \geq 1$		Offsets in the array `RDATAX` containing cross section information. If the first index corresponds to reaction `PROFILE`, then `ADRX` is the offset in the array `IDATAP` containing the profile information of the transfer matrix. $N^{\text{adrx}} = (\mathcal{S}_4^{\text{sap}} + 2) \times (\mathcal{S}_5^{\text{sap}} + \mathcal{S}_6^{\text{sap}}) \times \mathcal{S}_{18}^{\text{sap}}$

The array `ADRX` gives the position of the first value of a cross section in array `RDATAX` or the first value of profile information in array `IDATAP`. `RDATAX` and `IDATAP` are located in sub-directory `mili//' m'` of the sub-directory `calc//' n'`. For a given reaction with index `irea` in array `NOMREA` (in sub-directory `contenu`), for a particularized isotope with index `isot` in array `NOMISO` (in sub-directory `contenu`), and for an output mixture with index `imil`, the first cross section value is located at position `ADRX(irea,isot,ISADRX(imil))` of array `RDATAX`. `ISADRX` is defined in the sub-directory `info` of an elementary calculation. If the address is zero, then the corresponding cross sections are not defined.

Information related to Legendre–dependent scattering information is given in the two extra locations of the `ADRX` array: `ADRX(NREA+1,:,:)` contains the number of components for the vectorial scattering cross sections (order of anisotropy +1); `ADRX(NREA+2,:,:)` contains the number of components for the (matrix) transfer cross sections (order of anisotropy +1).

This system is designed in such a way to keep the value of $\mathcal{S}_{18}^{\text{sap}} =$`NADRX` as small as possible.

15.5 The `geom` sub-directory in /saphyb/

Table 87: Contents of sub-directory `geom` in /saphyb/

Name	Type	Condition	Units	Comment
NOMMIL␣␣␣␣␣␣	$C(\mathcal{S}_7^{\mathrm{sap}}) * 20$			Names of the output mixtures.
XVOLMT␣␣␣␣␣␣	$R(\mathcal{S}_7^{\mathrm{sap}})$		cm^3	Volumes of the output mixtures.
SURFS␣␣␣␣␣␣	$R(\mathcal{S}_{24}^{\mathrm{sap}})$	$\mathcal{S}_{24}^{\mathrm{sap}} \geq 1$	cm^2	Surfaces of the output geometry.
outgeom␣␣␣␣␣	Dir	*		Surfacic data related to discontinuity factor information.

Table 88: Contents of sub-directory `outgeom` in /geom/

Name	Type	Condition	Units	Comment
SURF␣␣␣␣␣␣␣␣	$R(N_{\mathrm{nsurfd}})$		cm^2	Surface assigned to each discontinuity factor.

15.6 The `paramdescrip` sub-directory in /saphyb/

Table 89: Contents of sub-directory `paramdescrip` in /saphyb/

Name	Type	Condition	Units	Comment
NPAR␣␣␣␣␣␣␣␣	$I(1)$			Number of global parameters.
NPCHR␣␣␣␣␣␣␣	$I(1)$			Number of global parameters linked with isotopes.
PARNAM␣␣␣␣␣␣	$C(\mathcal{S}_8^{\mathrm{sap}}) * 80$			User–defined names for the global parameters.
PARKEY␣␣␣␣␣␣	$C(\mathcal{S}_8^{\mathrm{sap}}) * 4$			User–defined key-words for the global parameters.
PARTYP␣␣␣␣␣␣	$C(\mathcal{S}_8^{\mathrm{sap}}) * 4$			Character identification for the types of global parameters (eg: `TEMP`, `CONC`, `IRRA`, etc.).
PARFMT␣␣␣␣␣␣	$C(\mathcal{S}_8^{\mathrm{sap}}) * 8$			User–defined names for the global parameters (eg: `FLOTTANT`, `CHAINE`, `ENTIER`, etc.).
PARCHR␣␣␣␣␣␣	$C(\mathcal{S}_9^{\mathrm{sap}}) * 8$	$\mathcal{S}_9^{\mathrm{sap}} \geq 1$		Isotope names linked to type–`CONC` global parameters.
NVALUE␣␣␣␣␣␣	$I(\mathcal{S}_8^{\mathrm{sap}})$			Number of specific values for a global parameters.
PARCAD␣␣␣␣␣␣	$I(\mathcal{S}_8^{\mathrm{sap}} + 1)$			Address of the first element in array `PARCHR`.

Contents of sub-directory `paramdescrip` in /saphyb/

Name	Type	Condition	Units	Comment
PARPAD␣␣␣␣␣␣	$I(\mathcal{S}_8^{\mathrm{sap}}+1)$			Address of the first element in array PARBIB.
PARMIL␣␣␣␣␣␣	$I(\mathcal{S}_{10}^{\mathrm{sap}})$	$\mathcal{S}_{10}^{\mathrm{sap}} \geq 1$		Mixture indices linked to type–TEMP or –CONC global parameters.
PARBIB␣␣␣␣␣␣	$C(\mathcal{S}_{10}^{\mathrm{sap}}) * 12$	$\mathcal{S}_{10}^{\mathrm{sap}} \geq 1$		MICROLIB names linked to type–TEMP or –CONC global parameters.

Types and units of global parameters are defined as follows:

	unit	description
TEMP	°C	Temperature
CONC	$10^{24}/\mathrm{cm}^3$	Number density
IRRA	MW-day/tonne	Burnup
FLUB	n/kb	Neutron exposure
TIME	s	Time
PUIS	MeV/s	Normalization power
MASL	g/cm^3	Mass density of heavy elements
FLUX		Volume-averaged, energy-integrated flux
VALE	(not defined)	User-defined parameter

15.7   The `paramvaleurs` sub-directory in /saphyb/

Table 90: Contents of sub-directory `paramvaleurs` in /saphyb/

Name	Type	Condition	Units	Comment
{/*pvaldir*/}	R(NVALUE(J))	*		Set of real global parameter arrays. Each element of {/pvaldir/} contains a real array containing the tabulated values of the J–th global parameter.
{/*pvaldir*/}	I(NVALUE(J))	*		Set of integer global parameter arrays. Each element of {/pvaldir/} contains an integer array containing the tabulated values of the J–th global parameter.
{/*pvaldir*/}	C(NVALUE(J)) $* 12$	*		Set of character$*12$ global parameter arrays. Each element of {/pvaldir/} contains a character$*12$ array containing the tabulated values of the J–th global parameter.

{/pvaldir/} is a set of $\mathcal{S}_8^{\mathrm{sap}}$ real, integer or character*12 records. The name of each {/pvaldir/} record is a `character*12` variable (`text12`) composed using the following FORTRAN instruction:

$$\mathrm{WRITE}(\mathtt{text12},' \,(''\mathtt{pval}'',\mathtt{I8})')\ J$$

where J is the index of the global parameter with $1 \leq J \leq \mathcal{S}_8^{\text{sap}}$. The global parameter values of type `REAL` or `INTEGER` are sorted.

15.8   The `paramarbre` sub-directory in /saphyb/

The global parameter tree has the same number of stages as global parameters. For each value of the i–th global parameter, the tree indicates the beginning position of the $(i+1)$–th parameter. The arrays `DEBARB` and `ARBVAL` are set to localize the results of an elementary calculation identified by a specific parameter tuple.

Table 91: Contents of sub-directory `paramarbre` in /saphyb/

Name	Type	Condition	Units	Comment
NCALS␣␣␣␣␣␣␣	I(1)			Number of elementary calculations.
DEBARB␣␣␣␣␣␣	I($\mathcal{S}_{17}^{\text{sap}} + 1$)			- If the node does not correspond to the last parameter: index in `DEBARB` of the first daughter of the node. - If the node correspond to the last parameter: index in `DEBARB` where we recover the index of an elementary calculation.
ARBVAL␣␣␣␣␣␣	I($\mathcal{S}_{17}^{\text{sap}}$)			Index of the corresponding parameter in the `pval//'  n'` record.
ORIGIN␣␣␣␣␣␣	I($\mathcal{S}_{19}^{\text{sap}}$)			Index of the mother elementary calculation. This information is useful to follow the historical relation between calculations.

An example of a global parameter tree is represented here:

```
dn = value in DEBARB,  (m) = value in ARBVAL

Root                            *(0)
                                 !
Param. Nb 1                    d2(1)
                     -------------------
                     !                 !
Param. Nb 2       d3(1)              4(2)
                  ---------         ---------
                  !       !         !   !   !
Param. Nb 3    d5(1)    6(3)     d7(1) 8(2) 9(3)   d10

Calculation Nb:  4        5        1   2   3

DEBARB:     2  3  5  7 10  4  5  1  2  3
ARBVAL:     0  1  1  2  1  3  1  2  3
```

The dimensions of variables `DEBARB`, `ARBVAL` and `ORIGIN` in Table 91 represent the useful size, not the allocated size which may be bigger. The allocated size of these arrays may be obtained using the LCM API (`LCMLEN` with the Fortran API).

Each elementary calculation is fully identified by a global parameter tuple, an integer array of dimension $\mathcal{S}_8^{\text{sap}}$ =NPAR. A recursive program can be used to search the elementary calculation index ICAL corresponding to a parameter tuple represented in the Fortran array MUPLET(NPAR). The recursive function is called using

```
ICAL=NICAL(1,NVP,NPAR,DEBARB,ARBVAL,MUPLET)
```

and is implemented in Fortran-90 as

```
RECURSIVE INTEGER FUNCTION NICAL(II,NVP,NPAR,DEBARB,ARBVAL,MUPLET) RESULT(ICAL)
   INTEGER II,NVP,NPAR,DEBARB(NVP+1),ARBVAL(NVP),MUPLET(NPAR)
   IF(NPAR==0) THEN
      ICAL=DEBARB(II+1)
      RETURN
   ENDIF
   NBOK=0
   IKEEP=0
   DO I=DEBARB(II),DEBARB(II+1)-1
      IF((MUPLET(1)==0).OR.(MUPLET(1)==ARBVAL(I))) THEN
         JICAL=NICAL(I,NVP,NPAR-1,DEBARB,ARBVAL,MUPLET(2))
         IF(JICAL > 0) THEN
            IKEEP=JICAL
            NBOK=NBOK+1
         ELSE IF(JICAL==-1) THEN
            NBOK=2
         ENDIF
      ENDIF
   ENDDO
   IF(NBOK > 1) THEN
      ! Many elementary calculation exist for this tuple.
      ICAL=-1
   ELSE IF(NBOK==0) THEN
      ! No elementary calculation exists for this tuple.
      ICAL=0
   ELSE
      ICAL=IKEEP
   ENDIF
END FUNCTION NICAL
```

Similarly, a Fortran program can be used to search the global parameter tuple corresponding to the elementary calculation index ICAL:

```
SUBROUTINE COMUPL(NVP,NPAR,ICAL,NCALS,DEBARB,ARBVAL,MUPLET)
INTEGER DEBARB(NVP+1),ARBVAL(NVP),MUPLET(NPAR)
DO I=NVP-NCALS+1,NVP
   IF(DEBARB(I+1).EQ.ICAL) THEN
      I0=I
      EXIT
   ENDIF
ENDDO
MUPLET(NPAR)=ARBVAL(I0)
DO IPAR=NPAR-1,1,-1
   DO I=1,NVP-NCALS
      IF(DEBARB(I+1).GT.I0) THEN
         I0=I
```

```
            EXIT
         ENDIF
      ENDDO
      MUPLET(IPAR)=ARBVAL(IO)
   ENDDO
   END
```

15.9 The `varlocdescri` sub-directory in /saphyb/

Table 92: Contents of sub-directory `varlocdescri` in /saphyb/

Name	Type	Condition	Units	Comment
NPAR␣␣␣␣␣␣␣␣	I(1)			Number of local variables.
NPCHR␣␣␣␣␣␣␣	I(1)			Number of local variables linked with isotopes.
PARNAM␣␣␣␣␣␣	$C(\mathcal{S}_{11}^{sap}) * 80$	$\mathcal{S}_{11}^{sap} \geq 1$		User–defined names for the local variables.
PARKEY␣␣␣␣␣␣	$C(\mathcal{S}_{11}^{sap}) * 4$	$\mathcal{S}_{11}^{sap} \geq 1$		User–defined key-words for the local variables.
PARTYP␣␣␣␣␣␣	$C(\mathcal{S}_{11}^{sap}) * 4$	$\mathcal{S}_{11}^{sap} \geq 1$		Character identification for the types of local variables (eg: TEMP, IRRA, FLUB, EQUI, etc.).
PARFMT␣␣␣␣␣␣	$C(\mathcal{S}_{11}^{sap}) * 8$	$\mathcal{S}_{11}^{sap} \geq 1$		User–defined names for the local variables (eg: FLOTTANT, CHAINE, ENTIER, etc.).
PARCHR␣␣␣␣␣␣	$C(\mathcal{S}_{12}^{sap}) * 8$	$\mathcal{S}_{12}^{sap} \geq 1$		Isotope names linked to type–CONC local variables.
PARCAD␣␣␣␣␣␣	$I(\mathcal{S}_{11}^{sap} + 1)$	$\mathcal{S}_{11}^{sap} \geq 1$		Address of the first element in array PARCHR.

15.10 The elementary calculation sub-directory /caldir/ in /saphyb/

For each elementary calculation, we define a directory `calc//' n'`, where `n` is the index of the calculation in the global parameter tree. The results for each output mixture are stored in a directory `mili//' m'` where `m` is the position index of the mixture in the array `NOMMIL` of the sub-directory `geom`. Inside each elementary calculation directory /caldir/, the following records and sub-directories will be found:

Table 93: Contents of sub-directory /caldir/ in /saphyb/

Name	Type	Condition	Units	Comment
info␣␣␣␣␣␣␣␣	Dir			General informations about the elementary calculation
divers␣␣␣␣␣␣	Dir			Results not related to a specific mixture: interface currents, k_∞, k_{eff}, B^2, etc.
outflx␣␣␣␣␣␣	Dir	$N_{nsurfd} > 0$		Discontinuity factor information.

Contents of sub-directory /caldir/ in /saphyb/

Name	Type	Condition	Units	Comment
{/mixdir/}	Dir			Set of $\mathcal{S}_7^{\texttt{sap}}$ sub-directories containing the cross section information associated with a specific mixture.

The name of each {/mixdir/} directory is a `character*12` variable (`text12`) composed using the following FORTRAN instruction:

$$\texttt{WRITE(text12,}'\,(''\texttt{mili}'',\texttt{I8})')\, J$$

where J is the index of the mixture with $1 \leq J \leq \mathcal{S}_7^{\texttt{sap}}$.

15.10.1 The `info` sub-directory in /caldir/

Table 94: Contents of sub-directory `info` in /caldir/

Name	Type	Condition	Units	Comment
NLOC⎵⎵⎵⎵⎵⎵⎵	I(1)			Number of local variables (0 ≤NLOC≤NPARL).
NISOTS⎵⎵⎵⎵⎵	I(1)			Number of isotopes in output tables ($\mathcal{S}_{32}^{\texttt{sap}} \equiv$ NISOTS≤NISOTA).
NISF⎵⎵⎵⎵⎵⎵⎵	I(1)			Number of particularized fissile isotopes (NISF≤NISOF).
NISP⎵⎵⎵⎵⎵⎵⎵	I(1)			Number of particularized fission products (NISP≤NISOP).
NISY⎵⎵⎵⎵⎵⎵⎵	I(1)			Number of particularized isotopes and macroscopic sets used for computing the fission yields (NISY≤NISOY).
LOCNAM⎵⎵⎵⎵⎵	C(NLOC) ∗ 80	NLOC≥ 1		User–defined names for the local variables.
LOCKEY⎵⎵⎵⎵⎵	C(NLOC) ∗ 4	NLOC≥ 1		User–defined key-words for the local variables.
LOCTYP⎵⎵⎵⎵⎵	C(NLOC) ∗ 4	NLOC≥ 1		Character identification for the types of local variables (eg: TEMP, IRRA, FLUB, EQUI, etc.).
LOCADR⎵⎵⎵⎵⎵	I(NLOC+1)	NLOC≥ 1		Address of the first element in array RVALOC (sub-directory mili//' m') corresponding to a local variable.
ISOTS⎵⎵⎵⎵⎵⎵	C($\mathcal{S}_{32}^{\texttt{sap}}$) ∗ 8			Alias names of isotopes in output tables.
ADRY⎵⎵⎵⎵⎵⎵⎵	I(NISY)	NISY≥ 1		Indices of fissile isotopes (positive values) and fission products (negative values) in array YLDS (sub-directory mili//' m').
ISADRX⎵⎵⎵⎵⎵	I($\mathcal{S}_7^{\texttt{sap}}$)			Used to recover the third index in array ADRX (sub-directory adresses).

Contents of sub-directory `info` in /caldir/

Name	Type	Condition	Units	Comment
LENGDX␣␣␣␣␣␣	$I(\mathcal{S}_7^{\mathrm{sap}})$			Length of the cross section array `RDATAX` (sub-directory `mili`//' m').
LENGDP␣␣␣␣␣␣	$I(\mathcal{S}_7^{\mathrm{sap}})$			Length of the transfer matrix profile array `IDATAP` (sub-directory `mili`//' m').

15.10.2 The `divers` sub-directory in /caldir/

Table 95: Contents of sub-directory `divers` in /caldir/

Name	Type	Condition	Units	Comment
NVDIV␣␣␣␣␣␣	$I(1)$			Number of values in arrays `IDVAL` and `VALDIV`.
IDVAL␣␣␣␣␣␣	$C(\mathrm{NVDIV}) * 4$	$\mathrm{NVDIV} \geq 1$		Character identification for the values in array `VALDIV` (`KEFF`, `KINF` or `B2`).
VALDIV␣␣␣␣␣␣	$R(\mathrm{NVDIV})$	$\mathrm{NVDIV} \geq 1$		Values given in the order of the `IDVAL` array.
FLXREF␣␣␣␣␣␣	$R(\mathcal{S}_{28}^{\mathrm{sap}} \times \mathcal{S}_{30}^{\mathrm{sap}})$	$\mathcal{S}_{28}^{\mathrm{sap}} \geq 1$		Neutron flux values (region– and group–ordered) in the reference calculation.
SCURM␣␣␣␣␣␣	$R(\mathcal{S}_{24}^{\mathrm{sap}} \times \mathcal{S}_{20}^{\mathrm{sap}})$	$\mathcal{S}_{24}^{\mathrm{sap}} \geq 1$		Entering partial currents on the surfaces surrounding the geometry. The values are given in the order of the `SURF` array (in sub-directory `geom`).

Table 96: Contents of sub-directory `outflx` in /caldir/

Name	Type	Condition	Units	Comment
REGFLX␣␣␣␣␣␣	R(NG)			Averaged flux in the complete geometry.
SURFLX␣␣␣␣␣␣	R($N_{\text{nsurfd}} \times$NG)			Surfacic fluxes (N_{nsurfd} values per energy group) integrated over surface. The averaged values are obtained by dividing these components by those of SURF record in `outgeom` sub-directory (see Section 15.5).

15.10.3 The mixture sub-directory /mixdir/ in /caldir/

Table 97: Contents of mixture sub-directory /mixdir/ in /caldir/

Name	Type	Condition	Units	Comment
CONCES␣␣␣␣␣␣	R($\mathcal{S}_{32}^{\text{sap}}$)		$10^{24}cm^{-3}$	Number density of each isotope in the output tables. Correspond to isotopes names ISOTS in Sect. 15.10.1.
RVALOC␣␣␣␣␣␣	R(NVLC)	NLOC≥ 1		Values of the local variables. NVLC=LOCADR(NLOC+1)-1
FLUXS␣␣␣␣␣␣␣	R($\mathcal{S}_{20}^{\text{sap}}$)			Volume– and energy–integrated neutron fluxes in the output tables.
YLDS␣␣␣␣␣␣␣␣	R(N^{ylds})	NISP≥ 1		The fission product i yield from fissile isotope k is given as YLDS(ADRY(k),-ADRY(i)). Indices i and k are given in the order of array NOMISO (in sub-directory `contenu`). A macroscopic set with a non–vanishing fission cross section is considered as an averaged fissile isotope. $N^{\text{ylds}} = (\text{NISF}+\mathcal{S}_6^{\text{sap}})\times$NISP.
DECAYC␣␣␣␣␣␣	R($\mathcal{S}_3^{\text{sap}} \times \mathcal{S}_{32}^{\text{sap}}$)	$\mathcal{S}_3^{\text{sap}} \geq 1$	s^{-1}	Radioactive decay constants for each type of decay reaction and each isotope of the output tables.
RDATAX␣␣␣␣␣␣	R(N^{datax})	$N^{\text{datax}} \geq 1$		Cross section data. N^{datax} =LENGDX(m) where m is the mixture index.
IDATAP␣␣␣␣␣␣	I(N^{datap})	$N^{\text{datap}} \geq 1$		Profile information of the transfer matrix. N^{datap} =LENGDP(m) where m is the mixture index.
cinetique␣␣␣	Dir	$\mathcal{S}_{33}^{\text{sap}} \geq 1$		Delayed neutron data for the mixture.

ADRX (in sub-directory `adresses`) contains the offset used to recover information from arrays `RDATAX` and `IDATAP`:

- Starting from this offset, we recover $\mathcal{S}_{20}^{\text{sap}}$ cross section values in `RDATAX`, except for the scattering cross section where we recover $\mathcal{S}_{20}^{\text{sap}}$ values for each available Legendre order, and except for the scattering transfer matrix where we recover N^{scat} values for each available Legendre order. N^{scat} is defined with the `IDATAP` array.

- For a `PROFILE`–type reaction, starting from this offset, we recover $2 \times \mathcal{S}_{20}^{\text{sap}} + 7$ integer values in `IDATAP`.

The transfer matrix elements are stored in the following way. The non-zero values are stored in the order of the secondary group and, for each secondary group, in the order of the primary groups. The $2 \times \mathcal{S}_{20}^{\text{sap}} + 7$ values describing the profile of the transfer matrix are stored in the following order:

> `FAGG, LAGG, FDGG, WGAL, FAG, LAG, (FDG(g),g=1,NG), (ADR(g),g=1,NG+1)`

where

`FAGG`	(not used)
`LAGG`	(not used)
`FDGG`	(not used)
`WGAL`	set to 0
`FAG`	First secondary group
`LAG`	Last secondary group
`FDG`	First primary group in each secondary group
`ADR`	Address in the cross section array where data for secondary group g is beginning (the address is relative to the isotope). The number of elements in a transfer matrix is $N^{\text{scat}} =$`ADR(NG+1)-1`.

For an energy transfer g' → g and for a Legendre order L(≥ 0), the transfer cross section is identified in the cross section array `RDATAX` as

$$\sigma_{s\ell}^{g' \to g} = \text{RDATAX(ADRX(irea,isot,ISADRX(imil)) + L*(ADR(NG+1)-1) + I-1)}$$

with `I = ADR(g)+g'-FDG(g)`.

15.10.4 The `cinetique` *sub-directory in /mixdir/*

Table 98: Contents of sub-directory `cinetique` in /mixdir/

Name	Type	Condition	Units	Comment
NPR␣␣␣␣␣␣␣␣␣␣	I(1)			Number of delayed neutron precursors groups in the mixture.
LAMBRS␣␣␣␣␣␣	R(NPR)	NPR≥ 1	s^{-1}	Radioactive decay constants of the delayed neutron precursors groups.
CHIRS␣␣␣␣␣␣␣	R($\mathcal{S}_{20}^{\mathtt{sap}} \times$NPR)	NPR≥ 1	1	Delayed neutron emission spectrums.
BETARS␣␣␣␣␣␣	R(NPR)	NPR≥ 1	1	Delayed neutron fractions.
INVELS␣␣␣␣␣␣	R($\mathcal{S}_{20}^{\mathtt{sap}}$)	NPR≥ 1	$cm^{-1}s$	Group average of the inverse neutron velocity.
TGENRS␣␣␣␣␣␣	R(1)	NPR≥ 1	s	Prompt–neutron lifetime.

16 Contents of a /mc/ Directory

This directory contains information generated by the `MC:` multigroup Monte Carlo module.

16.1   State vector content for the /mc/ data structure

The dimensioning parameters for the /mc/ data structure, which are stored in the state vector $\mathcal{S}^{mc}$, represent:

- Nominal number of source histories M per K_{eff} cycle $N_{\text{nsrck}} = \mathcal{S}_1^{mc}$

- Number of source cycles I_c to skip before K_{eff} accumulation $N_{\text{ikz}} = \mathcal{S}_2^{mc}$

- Total number of cycles N in the problem $N_{\text{kct}} = \mathcal{S}_3^{mc}$

- Initial seed for the random number generator $S = \mathcal{S}_4^{mc}$

- N2N processing flag $F = \mathcal{S}_5^{mc}$

$$F = \begin{cases} 0 & \text{do not use information in the 'N2N and 'N3N records} \\ 1 & \text{use information in the 'N2N and 'N3N records to perform the random walk} \end{cases}$$

- Type of tallies $T = \mathcal{S}_6^{mc}$

$$T = \begin{cases} 0 & \text{no tallies} \\ 1 & \text{effective multiplication factor tally} \\ 2 & \text{effective multiplication factor } and \text{ macrolib tallies} \end{cases}$$

- The number of homogenized mixtures in the macrolib tally $M_{\text{out}} = \mathcal{S}_7^{mc}$

- The number of condensed energy groups in the macrolib tally $G_{\text{out}} = \mathcal{S}_8^{mc}$

- The number of regions in the initial geometry $N_{\text{in}} = \mathcal{S}_9^{mc}$

16.2   The main /mc/ directory

The following records and sub-directories will be found on the first level of a /mc/ directory:

Table 99: Main records and sub-directories in /mc/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C*12			Signature of the /mc/ data structure (SIGNA =L_MC␣␣␣␣␣␣␣␣).
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}_i^{mc}$, as defined in Section 16.1.
K-EFFECTIVE␣	R(1)			Effective multiplication factor K_{eff}
K-EFFECTI-SD	R(1)			Standard deviation of the effective multiplication factor ΔK_{eff}

Main records and sub-directories in /mc/

Name	Type	Condition	Units	Comment
`REF:IMERGE␣␣`	$I(N_{\text{in}})$	$T = 2$		Merged region number associated with each of the original region number in the macrolib tally M_r
`REF:IGCOND␣␣`	$I(G_{\text{out}})$	$T = 2$		Reference group limits associated with the condensed groups in the macrolib tally C_g
`MACROLIB␣␣␣␣`	Dir	$T = 2$		Directory containing the /macrolib/ structure associated with the macrolib tally, following the specification presented in Section 1.2.

17 Contents of a /draglib/ directory

The DRAGLIB format provide an efficient way to store burnup data and multigroup isotopic nuclear data to be used in a lattice code. A DRAGLIB file is a persistent LCM object (an XSM–formatted file) used to organize the data in a hierarchical format. Therefore, it will be easy to convert back and forth between the binary direct access format (efficient during a lattice calculation) and the ASCII export format (usefull for backup and exchange purposes). A library in DRAGLIB format is generally built using the `dragr` module available in an inhouse version of NJOY.[3] The optional capability to define energy-dependent fission spectra is available, as described in Ref. 2.

A DRAGLIB is an LCM object with a depletion chain and a set of isotopic sub-directories located on the root directory. Each isotopic sub-directory contains infinite dilution nuclear data for a set of absolute temperatures. Incremental values corresponding to finite dilutions are given on the last directory level.

The first group corresponds to highest energy neutrons. Every cross section is given in barn. Finally, note that the lagging zeros of any cross section record can be removed from that record in order to save space on the DRAGLIB. The lattice code will therefore have to pack any uncomplete cross section record with zeros.

17.1 The main /draglib/ directory

On its first level, the following records and sub-directories will be found in the /draglib/ directory:

Table 100: Main records and sub-directories in /draglib/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			Signature of the data structure (SIGNA =L␣DRAGLIB␣␣␣).
VERSION␣␣␣␣␣	C∗12			Version identification. Currently equal to 'RELEASE␣2003'. This value will change if the DRAGLIB specification is to be modified in the future.
README␣␣␣␣␣␣	$C(N^{\text{dgl}}) * 80$			User–defined comments about the library.
ENERGY␣␣␣␣␣␣	$R(G + 1)$		eV	$E(g)$: Group energy limits in eV. Group g is defined as $E(g) < E \le E(g-1)$.
CHI-ENERGY␣␣	$R(G_{\text{chi}} + 1)$	$G_{\text{chi}} \neq 0$	eV	$E_{\text{chi}}(g)$: Group energy limits defining the energy-dependent fission spectra. By default, a unique fission spectra is used.
CHI-LIMITS␣␣	$I(G_{\text{chi}} + 1)$	$G_{\text{chi}} \neq 0$		$N_{\text{chi}}(g)$: Group limit indices defining the energy-dependent fission spectra. By default, a unique fission spectra is used.
DEPL-CHAIN␣␣	Dir	*		directory containing the /depletion/ associated with this library, following the specification presented in Section 2.4. (*) This data is required if the library is to be used for burnup calculations.
{*/isotope/*}	Dir			Set of sub-directories containing the cross section information associated with a specific isotope.

where G is the number of energy groups. For design reasons, the DRAGLIB object has no state vector record.

17.2 Contents of an /isotope/ directory

Each /isotope/ directory contains information related to a single isotope. This information is written using one of the following formats:

- a temperature–independent isotopic data is written using the format described in Tables 14 to 20 of the MICROLIB specification. Such isotopic data is typically produced by the EDI: module.

- a temperature–dependent isotopic data, tabulated for $N_{\rm tmp}$ temperatures, is written using the format presented in Table 101.

Table 101: Temperature-dependent isotopic records

Name	Type	Condition	Units	Comment
README␣␣␣␣␣␣	$C(N^{\rm iso}) * 80$			User–defined comments about the isotope.
AWR␣␣␣␣␣␣␣␣␣	$R(1)$		nau	Ratio of the isotope mass divided by the neutron mass
TEMPERATURE␣	$R(N_{\rm tmp})$		K	Set of temperatures, expressed in Kelvin.
{/tmpdir/}	Dir			Set of $N_{\rm tmp}$ sub-directories, each containing the cross section information associated with a specific temperature.
BIN-NFS␣␣␣␣␣	$I(G)$	*		Number of fine energy groups $n_{{\rm bin},g}$ in each group g. May be set to zero in some groups. (*) This data is optional and is useful when advanced self-shielding models are used in the lattice calculation.
BIN-ENERGY␣␣	$R(N_{\rm bin} + 1)$	*	eV	Fine group energy limits in eV. Here, $N_{\rm bin} = \sum_g n_{{\rm bin},g}$. (*) This data should be given if and only if the record 'BIN-NFS' is present.

The name of each {/tmpdir/} directory is a `character*12` variable (`text12`) composed using the following Fortran instruction:

$$\text{WRITE}(\text{text12},'(''SUBTMP'', \text{I4.4})') \, J$$

where J is the index of the temperature with $1 \le J \le N_{\rm tmp}$.

Each /tmpdir/ directory contains information related to a single isotope at a single temperature. This information is written using one of the following formats:

- If the isotope contains no self-shielding data (i.e., if the isotope is only present at infinite dilution), then the isotopic data is written using the format described in Tables 14 to 20 of the MICROLIB specification.

- If the isotope contains self-shielding data, then the infinite-dilution isotopic data is written using the format described in Tables 14 to 20 of the MICROLIB specification. In this case, additional data is required to represent the dilution dependence of the cross sections. This additional data is presented in Table 102.

Table 102: Temperature-dependent isotopic records

Name	Type	Condition	Units	Comment
DILUTION␣␣␣␣	$\mathrm{R}(N_{\mathrm{dil}})$		b	Set of finite dilutions σ_e, expressed in barn. Note: the infinite dilution value (1.0E10) is not given.
{/*dildir*/}	Dir			Set of N_{dil} sub-directories, each containing the *incremental* cross section information associated with a specific dilution.
BIN-NTOTO␣␣␣	$\mathrm{R}(N_{\mathrm{bin}})$	*	b	Microscopic total cross sections $\sigma^{\mathrm{BIN}}(h)$ defined in the fine groups. (*) This data should be given if and only if the records 'BIN-NFS' and 'BIN-ENERGY' are present in the parent directory.
BIN-SIGS00␣␣	$\mathrm{R}(N_{\mathrm{bin}})$	*	b	Microscopic diffusion cross sections $\sigma^{\mathrm{BIN}}_{\mathrm{scat0}}(h)$ for an isotropic collision in the laboratory system defined in the fine groups. (*) This data should be given if and only if the records 'BIN-NFS' and 'BIN-ENERGY' are present in the parent directory.

The name of each {/*dildir*/} directory is a `character*12` variable (`text12`) composed using the following Fortran instruction:

$$\mathrm{WRITE}(\texttt{text12},{}'\,(''\mathrm{SUBMAT}'',\mathrm{I4.4}){}')\ K$$

where K is the index of the finite dilution with $1 \leq K \leq N_{\mathrm{dil}}$.

The fine-group cross sections in records BIN-NTOTO␣␣␣ and BIN-SIGS00␣␣ are normalized to the coarse group values $\sigma(g)$ and $\sigma_{\mathrm{scat0}}(g)$ in such a way that

$$\sigma(g) = \frac{1}{\ln[E(g-1)/E(g)]} \sum_{h=h_{\min}+1}^{h_{\min}+N^{\mathrm{BIN}}(g)} \sigma^{\mathrm{BIN}}(h)\, \ln\left[\frac{E^{\mathrm{BIN}}(h-1)}{E^{\mathrm{BIN}}(h)}\right]$$

and

$$\sigma_{\mathrm{scat0}}(g) = \frac{1}{\ln[E(g-1)/E(g)]} \sum_{h=h_{\min}+1}^{h_{\min}+N^{\mathrm{BIN}}(g)} \sigma^{\mathrm{BIN}}_{\mathrm{scat0}}(h)\, \ln\left[\frac{E^{\mathrm{BIN}}(h-1)}{E^{\mathrm{BIN}}(h)}\right]$$

where

$$h_{\min} = \sum_{i=1}^{g-1} N^{\mathrm{BIN}}(i) \ \ .$$

Nuclear data stored on sub-directory /tmpdir/ is infinite dilution data related to a single isotope at a single temperature. Nuclear data stored on /dildir/ and corresponding to dilution σ_e is incremental data relative to infinite dilution data:

$$\delta\sigma_{\mathrm{x}}(g,\sigma_e) = I_{\mathrm{x}}(g,\sigma_e) - \sigma_{\mathrm{x}}(g,\infty) = \sigma_{\mathrm{x}}(g,\sigma_e)\varphi(g,\sigma_e) - \sigma_{\mathrm{x}}(g,\infty)$$

and

$$\delta\varphi(g,\sigma_e) = \varphi(g,\sigma_e) - 1$$

where $I_{\mathrm{x}}(g,\sigma_e)$ is the effective resonance integral and $\varphi(g,\sigma_e)$ is the averaged fine structure function at dilution σ_e. Note that $\varphi(g,\infty) = 1$.

18 Contents of a /fview/ data structure

This directory contains information generated by the `VAL:` module used to interpolate the diffusion flux computed for Cartesian geometries. The following options of calculations are currently implemented:

- 3D geometries tracked with `TRIVAT:` using `PRIM` (aka, variational collocation) method

- 3D geometries tracked with `TRIVAT:` using `DUAL` (aka, Raviart-Thomas) method

- 3D geometries tracked with `TRIVAT:` using `MCFD` (aka, nodal collocation) method

18.1 The state-vector content

- The total number of energy group $N_g = \mathcal{S}_1$

- The number of mesh along X direction $N_x = \mathcal{S}_2$

- The number of mesh along Y direction $N_y = \mathcal{S}_3$

- The number of mesh along Z direction $N_z = \mathcal{S}_4$

18.2 The main /fview/ directory

Table 103: Records and sub-directories in /fview/ data structure

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			Signature of the /fview/ data structure (SIGNA =L_FVIEW␣␣␣␣␣).
STATE-VECTOR	I(40)			Vector describing the various parameters associated with this data structure $\mathcal{S}$
MXI␣␣␣␣␣␣␣␣␣	R(N_x)			array containing the mesh position along X-direction.
MYI␣␣␣␣␣␣␣␣␣	R(N_y)			array containing the mesh position along Y-direction.
MZI␣␣␣␣␣␣␣␣␣	R(N_z)			array containing the mesh position along Z-direction.
FLUX␣␣␣␣␣␣␣␣	Dir(N_g)			List of real arrays. Each component of this list is a real array of dimension $N_x * N_y * N_z$ containing the interpolated values of the flux in the energy group.

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[2] P. Mosca, C. Mounier, P. Bellier and I. Zmijarevic, "Improvements in Transport Calculations by the Energy-Dependent Fission Spectra and Subgroup Method for Mutual Self-Shielding," *Nucl. Sci. Eng.*, **175**, 266-282 (2013).

[3] A. Hébert and H. Saygin, "Development of DRAGR for the Formatting of DRAGON Cross-section Libraries", paper presented at the *Seminar on NJOY-91 and THEMIS for the Processing of Evaluated Nuclear Data Files*, NEA Data Bank, Saclay, France, April 7-8 (1992).

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