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A Description of the Data Structures for DRAGON 3.06

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SUMMARY

The computer code DRAGON contains a collection of models that can simulate the neutron behavior of a unit cell or a fuel assembly in a nuclear reactor. It includes all of the functions that characterize a lattice cell code, namely: the interpolation of microscopic cross sections supplied by means of standard libraries; resonance self-shielding calculations in multidimensional geometries; multigroup and multidimensional neutron flux calculations that can take into account neutron leakage; transport-transport or transport-diffusion equivalence calculations as well as editing of condensed and homogenized nuclear properties for reactor calculations; and finally isotopic depletion calculations.

The transfer of information between the various DRAGON execution modules is ensured by well-defined data structure. They are generally created or modified by one of the modules of DRAGON. Here we give a description of the contents of these data structures.

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1 INTRODUCTION

The transfer of information between the various DRAGON execution modules is ensured by well defined data structures.[1–4] These data structures are the DRAGON equivalent of UNIX directories which can contain either files (here records) or sub-directory. They can be stored directly in memory (`LINKED_LIST`) or on a direct access binary file (`XSM_FILE`) via the LCM utilities available in the GANLIB library of utilities.[5,6]

The main difference between a data structure and a UNIX directory is that the concept of file is now replaced by that of record where each record contains a specific number of elements of a fixed type. For example, consider an array $\vec{V}$ of dimension $N = 5$ that contains real valued elements. This array can be saved in the record named `VOLUME` of a data structure identified by `IPDATA` using the FORTRAN instruction:

```
INTEGER    LENGTH,ITREC,IPDATA,NVOL
PARAMETER (NVOL=5)
REAL       VOL(NVOL)
ITREC=2
LENGHT=NVOL
CALL LCMPUT(IPDATA,'VOLUME',LENGTH,ITREC,VOL)
```

where `NVOL=5` is the length of the real array `VOL=`$\vec{V}$. The variable `ITREC` is the record type which in this case takes the value of `ITREC=2` to indicate that the information to be saved is of type `REAL`.[6] Such a record will be described in this report by the following table.

Table 1: The `VOLUME` record in the `IPDATA` structure

Name	Type	Condition	Units	Comment
`VOLUME`␣␣␣␣␣␣	R(N)		m^3	Contents of the volume vector V_i.

In the general case we will have

Table 2: Example of records saved in a data structure

Name	Type	Condition	Units	Comment
`INTEGERARRAY`	I(3)			array containing 3 `INTEGER` valued elements.
`REALARRAY`␣␣␣	R(N)	$F \geq 1$	m^3	optional array containing N `REAL` valued elements. This array is present in the data structure only if $F \geq 1$. The elements in the array have dimensions of cm^3 .
`NAMESARRAY`␣␣	C(N) $*$ 12			array of `CHARACTER*12` variables.
`DIRECTORY`␣␣␣	Dir			Sub-directory.

Here the first column contains a `CHARACTER*12` variable identifying the record, the second column (I(1), R(N), C(N) $*$ 12 and Dir) describes the type of record and its length, the third column provides the condition required

for the record to be present in the data structure (present only if $F \geq 1$), the fourth column describes the units (m^3) and finally the last column provides a brief description of the record contents. For `INTEGER`, `REAL` and `DOUBLE PRECISION` records of length N, we will use respectively I(N), R(N), and D(N) to identify the type of record and its length while for a `CHARACTER*`L record of dimension N the notation C(N) $*$ L has been selected. The presence of a sub-directory is indicated by the type "Dir" as seen in the above table.

In this report we will sometime mix the concept of data structure (denoted DDS) and directory (/DIR/) even if they represent different object. In fact, both concepts are identical form the storage point of view. The main difference is then the fact that a data structure always contains the `SIGNATURE␣␣␣` and `STATE-VECTOR` records on the first level while the presence of these records is generally optional in directories. Moreover, from the point of view of code execution a data structure also refers to an object located in memory or stored on a file which can be transferred from one execution module to the next while a directory refers to the various hierarchical sublevels found inside this data structure.

1.1 Notation used in this report

␣	represents a hard blank space required in a FORTRAN character variable.
DDS	represents a data structure.
/DIR/	represents a directory.
{/dir/}	represents a list of directory.
`RECORD␣DIR␣␣`	The explicit name of a record or directory including the hard blanks.

1.2 Units used in this report

cm	centimeters, a unit of distance.
b	barn, a unit of surface or microscopic cross section with 1 b=10^{-24} cm^2.
Kb	kilobarn, a unit of surface or microscopic cross section with 1 Kb=10^3 b.
s	second, a unit of time.
d	day, a unit of time with 1 d=86400 s.
J	joule, an unit of energy.
eV	electron volt, a unit of energy with 1 eV=1.602×10^{-19} J.
MeV	Mega-electron volt, a unit of energy with 1 MeV=10^6 eV.
W	watt, a unit of power with 1 W= 1 J/s.
MW	Megawatt, a power unit with 1 MW= 10^6 W.
g	gram, a unit of mass.
au	atomic unit, a unit of mass with 1 au=1.660381×10^{-24} g.
nau	neutron atomic unit, a unit of mass with 1 nau=1.008665 au.
T	tonne, a unit of mass with 1 T=10^6 g=10^3 kg.
K	Kelvin, a unit of temperature.

2 DESCRIPTION OF THE DRAGON DATA STRUCTURES

In this section we will provide a brief description of the contents of the various data structures used or generated by DRAGON. The explicit records and directories present in each structure will be described in later sections. We will also mention the DRAGON module that will interact with the different data structures.[4]

2.1 The MACROLIB data structure

The standard data structure that contains group ordered macroscopic cross sections. It can be a stand-alone structure or it can be included into a larger structure, such as a MICROLIB or an EDITION structure. It can be created by the `MAC:`, `LIB:` and `EDI:` modules. It can also be modified by the `SHI:` and `EVO:` modules. Such a structure (either stand-alone or as part of a MICROLIB) is also required for a successful execution of the `ASM:` and `FLU:` modules. The information stored on this data structure is described in /MACROLIB/ (see Section 3).

2.2 The MICROLIB data structure

The standard data structure that contains microscopic and macroscopic cross sections libraries. It always include a MACROLIB substructure. It can be a stand-alone structure or included into a larger structure, such as an EDITION structure. It can be created by the `LIB:` and `EDI:` modules. It can also be modified by the `MAC:`, `SHI:` and `EVO:` modules. Such a structure (the /MACROLIB/) is required for a successful execution of the `ASM:` and `FLU:` modules. The information stored on this data structure is described in /MICROLIB/ (see Section 4).

2.3 The GEOMETRY data structure

The standard data structure that contains a block description of a geometry. It can be a stand-alone structure or included into a larger structure, such as in a /GEOMETRY/ sub-directory. It is created by the `GEO:` module. Such a structure is required for a successful execution of the modules `JPMT:`, `SYBILT:`, `EXCELT:`, `EXCELL:`, `NXT:`, `BIVACT:` and `PSP:`. The information stored on this data structure is described in /GEOMETRY/ (see Section 5).

2.4 The TRACKING data structure

The standard data structure that contains the general tracking information. In fact, the TRACKING data structure generated by the `EXCELT:`, `EXCELL:` and `NXT:` also contains a compact description of the geometry that can be used for illustration purpose. It can be created by the `JPMT:`, `SYBILT:`, `EXCELT:`, `EXCELL:` and `NXT:` modules. A new TRACKING data structure can also be created from an old TRACKING using the `MRG:` module. Such a structure is also required for a successful execution of the `ASM:`, `FLU:`, `MOCC`, `MCU:`, `EDI:`, `EVO:`, `MRG:`, `PSP:`, `SAD:` and `PER:` modules. The information stored on this data structure is described in /TRACKING/ (see Section 6).

2.5 The ASMPIJ data structure

The standard data structure that contains the multigroup response and collision probability matrices. It can be created using the `ASM:` and `EXCELL:` module. Such a structure is required for a successful execution of the `FLU:` module. The information stored on this data structure is described in /ASMPIJ/ (see Section 7).

2.6 The FLUXUNK data structure

The standard data structure that contains the problem eigenvalue and the multigroup fluxes and adjoints. It is created by the `FLU:`, `MOCC:`, `MCU:` and `SAD:` modules. Such a structure is required for a successful execution of the `EDI:` and `EVO:` modules. It can also be used by the `PSP:` module. The information stored on this data structure is described in /FLUXUNK/ (see Section 8).

2.7 The EDITION data structure

The standard data structure that contains condensed and merged microscopic and macroscopic cross section libraries. It can contain /MACROLIB/ (see Section 3) and /MICROLIB/ (see Section 4) sub-directories. It is created by the `EDI:` module. Such a structure is required for a successful execution of the `CPO:` module. The information stored on this data structure is described in /EDITION/ (see Section 9).

2.8 The BURNUP data structure

The standard data structure that contains the burnup information. It is created by the `EVO:` module. Such a structure is also required for a successful execution of the `CPO:` module. It can also be used by the `LIB:` module. The information stored on this data structure is described in /BURNUP/ (see Section 10).

2.9 The CPO data structure

The standard data structure that contains a basic, burnup dependent, reactor database It is created by the `CPO:` module in DRAGON for use in finite reactor diffusion codes (DONJON[7] for example). Such a structure is required for a successful execution of the `CFC:` module. The information stored on this data structure is described in /CPO/ (see Section 11).

2.10 The FBMXSDB data structure

The standard data structure that contains a full reactor cross section database with Feedback coefficients. It is created by the `CFC:` module in DRAGON for use in finite reactor diffusion codes (DONJON[7] for example). The information stored on this data structure is described in /FBM/ (see Section 12).

2.11 The HISTORY data structure

This data structure contains the information required to ensure a smooth coupling of DRAGON with DONJON when a history based full reactor calculation is to be performed.[8] It is used only by the `HST:` module. The information stored on this data structure is described in /HST/ (see Section 13).

3 CONTENTS OF A /MACROLIB/ DIRECTORY

A /MACROLIB/ directory contains the set of macroscopic multigroup cross sections associated with a list of mixtures. The structure of this directory, is quite different from that associated with an /ISOTOPE/ directory (see Section 14). First, it is multi level, namely, it contains sub-directories. Moreover, the information on this directory is primarily classified according to a multigroup hierarchy rather than a mixture hierarchy. In general, the contents of this structure will vary depending on the module that was used to create it.

In the case where the `MAC:` module is used to create this directory ($\mathcal{M} = 0$), it appears on the first level of the MACROLIB data structure. When `LIB:` is used ($\mathcal{M} = 1$), it embedded as a sub-directory in a /MICROLIB/ directory. Finally, when `EDI:` is used ($\mathcal{M} = 2$), it embedded as a sub-directory in a /EDITION/ directory.

3.1 The main directory

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

Table 3: Main records and sub-directories in /MACROLIB/

Name	Type	Condition	Units	Comment
`SIGNATURE␣␣␣`	C∗12			parameter SIGNA containing the signature of the data structure.
`STATE-VECTOR`	I(40)			array $\mathcal{S}_i^M$ containing various parameters that are required to describe this data structure.
`ADDXSNAME␣␣␣`	C($\mathcal{S}_5^M$) ∗ 6	$\mathcal{S}_5^M \geq 1$		array ADDXS$_k$ containing the name of the additional editing cross sections available in this /MACROLIB/.
`FISSIONNAMES`	C($\mathcal{S}_4^M$) ∗ 8	$\mathcal{S}_4^M \geq 1$		array FISNAM$_j$ containing the names of the fissile isotopes associated with fission spectrum j.
`FISSIONINDEX`	I($\mathcal{S}_2^M, \mathcal{S}_4^M$)	$\mathcal{S}_4^M \geq 1$		array $f_{m,j}$ that contains an index to associate an isotope in the MICROLIB with fission spectrum j in mixture m.
`FGWITHUPSCAT`	I($\mathcal{S}_2^M, \mathcal{S}_3^M$)			array $u_{m,l}$ that contains the maximum number of group number for which upscattering takes place in m for Legendre scattering order l.
`TIMESTAMP␣␣␣`	R(3)			array T_j containing the time in days ($T_1 = t$), the burnup in MW d T^{-1} ($T_2 = B$) and the irradiation in Kb^{-1} ($T_3 = w$) associated with this set of cross sections.
`ENERGY␣␣␣␣␣␣`	R($\mathcal{S}_1^M + 1$)	$\mathcal{M} \geq 1$	eV	array E_g containing the energy group limits.
`DELTAU␣␣␣␣␣␣`	R($\mathcal{S}_1^M$)	$\mathcal{M} \geq 1$		array U_g containing the group lethargy width.
`EFISS␣␣␣␣␣␣␣`	R($\mathcal{S}_2^M, \mathcal{S}_4^M$)		MeV	array $E_{m,j}$ that contains the average energy produced by per fission for fission spectrum j in mixture m.
`PHYSALBEDO␣␣`	R($\mathcal{S}_8^M$)	$\mathcal{M} = 0$	cm^3	array $\beta_{p,j}$ containing the surface ordered and energy independent physical albedo.
`VOLUME␣␣␣␣␣␣`	R($\mathcal{S}_2^M$)	$\mathcal{M} = 2$	cm^3	array V_m that contains the volume of the region containing mixture m.
`SPH-FACTORS␣`	R($\mathcal{S}_2^M, \mathcal{S}_1^M$)	$\mathcal{M} = 2$		array μ_m^g that contains the multiregion and multigroup SPH factors.

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

Name	Type	Condition	Units	Comment
`MATCOD␣␣␣␣␣␣`	I($\mathcal{S}_2^M$)	$\mathcal{M}=2$		array M_r that contains the mixture number associated with each region r.
`KEYFLX␣␣␣␣␣␣`	I($\mathcal{S}_2^M$)	$\mathcal{M}=2$		array K_r that contains the flux array index associated with each region r.
`K-EFFECTIVE␣`	R(1)	$\mathcal{M}=2$		parameter k_{eff} that contains the ffective multiplication constant.
`FLUXDISAFACT`	R($\mathcal{S}_1^M$)	$\mathcal{M}=2$		array F_g that contains the ratio of the flux in the fuel to the flux in the cell for group g.
`DIFFB1HOM␣␣␣`	R($\mathcal{S}_1^M$)	$\mathcal{S}_9^M=2$	cm	array D^g that contain the homogeneous diffusion coefficients for group g.
`B2␣␣B1HOM␣␣␣`	R(1)	$\mathcal{S}_9^M\geq 2$	cm^{-2}	parameter B_{hom} that contains the homogeneous buckling.
`B2␣␣HETE␣␣␣`	R(3)	$\mathcal{S}_9^M=2$	cm^{-2}	array B_j containing the directional buckling components. Here $j=1,2,3$ are for direction x, y and z respectively.
{*/GRPDIR/*}	Dir			List of $G=\mathcal{S}_1^M$ sub-directories which contain the cross section information associated with a specific group g.

The signature for this data structure is `SIGNA=L_MACROLIB␣␣`. The array $\mathcal{S}_i^M$ contains the following information:

- $\mathcal{S}_1^M = G$ is the number of groups in this library.
- $\mathcal{S}_2^M = N_m =$ is the number of mixtures in this library.
- $\mathcal{S}_3^M = L+1$ where L is the maximum order for the Legendre expansion for the scattering cross section used in the library.
- $\mathcal{S}_4^M = N_f$ is the number of fission spectrum mixtures in this library.
- $\mathcal{S}_5^M = N_{\text{add}}$ is the number of additional editing cross sections in this library.
- $\mathcal{S}_6^M = I_{tr}$ is the transport correction option used when processing this library where:

$$I_{tr} = \begin{cases} 0 & \text{do not use a transport correction;} \\ 1 & \text{transport correction from } P_1 \text{ scattering;} \\ 2 & \text{recover transport correction from the MACROLIB.} \end{cases}$$

- $\mathcal{S}_7^M = N_d$ is the number of precursor groups for delayed neutron in this library.
- $\mathcal{S}_8^M = N_A$ is the number of physical albedo in this library.
- $\mathcal{S}_9^M = I_l$ the type of leakage cross sections stored in this library.

The list of group directory {/GRPDIR/} names `GRPDIR` is composed using the following FORTRAN instructions

`WRITE(GRPDIR,'(A5,I3,A1,I3)') 'GROUP',`g`,'/',`G

for $1 \leq g \leq G$. For example, in the case where two group cross sections are considered ($G = 2$), two such directory would be generated, namely

Table 4: Example of group sub-directories in /MACROLIB/

Name	Type	Condition	Units	Comment
`GROUP␣␣1/␣␣2`	Dir			Sub-directory that contains the information associated with group $g = 1$.
`GROUP␣␣2/␣␣2`	Dir			Sub-directory that contains the information associated with group $g = 2$.

3.2 The group sub-directory

Inside each group g directory, records associated with vector reaction cross sections will be found.

Table 5: Vector reaction cross section records in /GRPDIR/

Name	Type	Condition	Units	Comment
`TOTAL␣␣␣␣␣␣␣␣`	R(N_m)		cm^{-1}	array Σ_m^g containing the total cross section associated with mixture m.
`TRANC␣␣␣␣␣␣␣␣`	R(N_m)	$\mathcal{S}_6^M = 2$	cm^{-1}	array $\Sigma_{tc,m}^g$ containing the transport correction cross section associated with mixture m.
`NUSIGF␣␣␣␣␣␣`	R(N_m, N_f)	$N_f \geq 1$	cm^{-1}	array $\nu\Sigma_{f,m,I}^g$ containing the product of the fission cross section $\Sigma_{f,m,I}^g$ with $\nu_{m,I}^g$, the averaged number of neutron produced per fission $\nu\Sigma_{f,m,I}^g$ associated with fission spectrum I and mixture m.
`NFTOT␣␣␣␣␣␣␣`	R(N_m, N_f)	$N_f \geq 1$	cm^{-1}	array $\Sigma_{f,m,I}^g$ containing the fission cross section associated with fission spectrum I and mixture m.
`FIXE␣␣␣␣␣␣␣␣`	R(N_m)		$\text{s}^{-1}\text{cm}^{-3}$	array S_m^g containing the fixed neutron source density associated with mixture m .
`FIXA␣␣␣␣␣␣␣␣`	R(N_m)		$\text{s}^{-1}\text{cm}^{-2}$	array $S_m^{*,g}$ containing the adjoint neutron source density associated with mixture m .
`CHI␣␣␣␣␣␣␣␣␣␣`	R(N_m, N_f)	$N_f = 1$		array χ_{mI}^g containing the energy spectrum associated with fission spectrum I and mixture m.
`FLUX-INTG␣␣␣`	R(N_m)	$\mathcal{M} = 2$	cm s^{-1}	array Φ_m^g containing the integrated flux associated with mixture m.
`ABS␣␣␣␣␣␣␣␣␣␣`	R(N_m)	$\mathcal{M} = 2$	cm^{-1}	array $\Sigma_{a,m}^g$ containing the absorption cross section associated with mixture m.

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Vector reaction cross section records in /GRPDIR/ continued from last page

Name	Type	Condition	Units	Comment
`OVERV␣␣␣␣␣␣␣`	R(N_m)	$\mathcal{M}=2$	cm^{-1}s	array containing the inverse of the average neutron velocity $1/v_m^g$ associated with mixture m.
`PRODUCTION␣␣`	R(N_m)	$\mathcal{M}=2$	cm^{-1}	array $\Sigma_{p,m}^g$ containing the total production cross section associated with mixture m.
`DIFFHOM␣␣␣␣␣`	R(N_m)	$\mathcal{M}=2$	cm	array D_m^g containing the homogeneous diffusion coefficient associated with mixture m.
`DIFFX␣␣␣␣␣␣␣`	R(N_m)	$\mathcal{M}=2$	cm	array $D_{x,m}^g$ containing the x directed diffusion coefficient associated with mixture m.
`DIFFY␣␣␣␣␣␣␣`	R(N_m)	$\mathcal{M}=2$	cm	array $D_{y,m}^g$ containing the y directed diffusion coefficient associated with mixture m.
`DIFFZ␣␣␣␣␣␣␣`	R(N_m)	$\mathcal{M}=2$	cm	array $D_{z,m}^g$ containing the z directed diffusion coefficient associated with mixture m.
{*xsname*}	R(N_m)	$N_{\text{add}} \geq 1$	cm^{-1}	List of cross section records specified by ADDXS_k.
`PHYSALBEDO␣␣`	R($\mathcal{S}_8^M$)	$\mathcal{M}=0$	cm^3	array $\beta_{p,j}^g$ containing the surface ordered and energy independent physical albedo.

In the case where $N_{\text{add}}=2$ and

$$\mathsf{ADDXS}_k = \begin{cases} \texttt{NG} & \text{for } k=1, \\ \texttt{N2N} & \text{for } k=2. \end{cases}$$

the following cross section records will also be present in each group directory:

Table 6: Additional cross section records

Name	Type	Condition	Units	Comment
`NG␣␣␣␣␣␣␣␣␣␣`	R(N_m)		cm^{-1}	array containing the neutron capture cross section associated with mixture m.
`N2N␣␣␣␣␣␣␣␣␣`	R(N_m)		cm^{-1}	array containing the (n,2n) cross section associated with mixture 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:

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

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 $\Sigma_{s,m}^{h\to g}(\vec{\Omega}\cdot\to\Omega')$ 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, an array that contains a compress form of the scattering matrix will be considered. We will also define three integer arrays $n_{l,m,d}^g$, $h_{l,m,d}^g$ and $p_{l,m,d}^g$ 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 number 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 $p_{l,m,d}^g$ is directly related to $n_{l,m,d}^g$ by

$$p_{l,m,d}^g=1+\sum_{k=1}^{m-1}n_{l,k,d}^g$$

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

	Mixture $m=1$				Mixture $m=2$			
$\sigma_{0,m}^{h\to g}$	$g=1$	$g=2$	$g=3$	$g=4$	$g=1$	$g=2$	$g=3$	$g=4$
$h=1$	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
$h_{0,m,d}^g$	1	4	3	4	2	3	4	4
$n_{0,m,d}^g$	1	4	2	3	2	3	3	1
$p_{0,m,d}^g$	1	1	1	1	2	5	3	4
$h_{0,m,a}^g$	2	4	3	4	2	3	3	4
$n_{0,m,a}^g$	2	3	2	3	2	3	2	2
$p_{0,m,a}^g$	1	1	1	1	3	4	3	4

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

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

Finally, we will also save independently the diagonal element of the scattering matrix:

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

and the total scattering vector

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

For the case where the adjoint transport problem is to be solved, the group transpose of the scattering matrix is required. Since $\Sigma^g_{0,k,d}$ is stored group by group, evaluating the transpose of this matrix requires a full reconstruction of the scattering matrix.

One way to bypass this problem is to store, in addition to $\Sigma^g_{0,k,d}$ which is associated with the scattering to group g, a compress matrix $\Sigma^g_{0,k,a}$ associated with diffusion from group g. We will again define three integer vectors $n^g_{l,m,a}$, $h^g_{l,m,a}$ and $p^g_{l,m,a}$ in a way similar to $n^g_{l,m,d}$, $h^g_{l,m,d}$ and $p^g_{l,m,d}$. They will contain respectively the number of final energy groups h for which the scattering cross section from group g does not vanish, the maximum energy group number for which scattering from the initial 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. As before $p^g_{l,m,a}$ is directly related to $n^g_{l,m,a}$ by

$$p^g_{l,m,a} = 1 + \sum_{k=1}^{m-1} n^g_{l,k,a}$$

For the 4 groups isotropic scattering cross section matrix associated with mixture 1 and 2 ($N_m = 2$) defined above we will have:

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

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 7: Scattering cross section records in /GRPDIR/

Name	Type	Condition	Units	Comment
`SIGW␣0␣␣␣␣␣␣`	R(N_m)		cm^{-1}	array $\Sigma^g_{0,m,w}$ that contains the isotropic component ($l = 0$) of the within group scattering cross section for mixture m.
`SIGS␣0␣␣␣␣␣␣`	R(N_m)		cm^{-1}	array $\Sigma^g_{0,m}$ that contains the isotropic component ($l = 0$) of the total group scattering cross section for mixture m.
`IJJD␣0␣␣␣␣␣␣`	I(N_m)			array $h^g_{0,m,d}$ that contains the highest energy group number for which the isotropic component of the scattering cross section to group g for mixture m does not vanish, .
`NJJD␣0␣␣␣␣␣␣`	I(N_m)			array $n^g_{0,m,d}$ that contains the number of energy group number for which the isotropic component of the scattering cross section to group g for mixture m does not vanish, .
`IPOD␣0␣␣␣␣␣␣`	I(N_m)			array $p^g_{0,m,d}$ that contains the location in the compressed scattering matrix of the information associated with mixture m.

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Scattering cross section records in /GRPDIR/ continued from last page

Name	Type	Condition	Units	Comment
SCAD␣0␣␣␣␣␣␣	R($N^g_{0,m,d}$)		cm^{-1}	array ($\Sigma^g_{0,k,d}$) that contains the compressed component of the scattering matrix for scattering to group g for mixture m.
IJJA␣0␣␣␣␣␣␣	I(N_m)			array $h^g_{0,m,a}$ that contains the highest energy group number for which the isotropic component of the scattering cross section from group g for mixture m does not vanish, .
NJJA␣0␣␣␣␣␣␣	I(N_m)			array $n^g_{0,m,a}$ that contains the number of energy group number for which the isotropic component of the scattering cross section from group g for mixture m does not vanish, .
IPOA␣0␣␣␣␣␣␣	I(N_m)			array $p^g_{0,m,a}$ that contains the location in the compressed scattering matrix of the information associated with mixture m.
SCAA␣0␣␣␣␣␣␣	R($N^g_{0,m,d}$)		cm^{-1}	array ($\Sigma^g_{0,k,a}$) that contains the compressed component of the scattering matrix for scattering from group g for mixture m.
SIGW␣1␣␣␣␣␣␣	R(N_m)		cm^{-1}	array $\Sigma^g_{1,m,w}$ that contains the linearly anisotropic component ($l = 1$) of the within group scattering cross section for mixture m.
SIGS␣1␣␣␣␣␣␣	R(N_m)		cm^{-1}	array $\Sigma^g_{1,m}$ that contains the linearly anisotropic component ($l = 1$) of the within total scattering cross section for mixture m.
IJJD␣1␣␣␣␣␣␣	I(N_m)			array $h^g_{1,m,d}$ that contains the highest energy group number for which the linearly anisotropic component of the scattering cross section to group g for mixture m does not vanish, .
NJJD␣1␣␣␣␣␣␣	I(N_m)			array $n^g_{1,m,d}$ that contains the number of energy group number for which the linearly anisotropic component of the scattering cross section to group g for mixture m does not vanish, .
IPOD␣1␣␣␣␣␣␣	I(N_m)			array $p^g_{1,m,d}$ that contains the location in the compressed scattering matrix of the information associated with mixture m.
SCAD␣1␣␣␣␣␣␣	R($N^g_{1,m,d}$)		cm^{-1}	array ($\Sigma^g_{1,k,d}$) that contains the compressed component of the linearly anisotropic component of the scattering matrix for scattering to group g for mixture m.
IJJA␣1␣␣␣␣␣␣	I(N_m)			array $h^g_{1,m,a}$ that contains the highest energy group number for which the linearly anisotropic component of the scattering cross section from group g for mixture m does not vanish, .

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Scattering cross section records in /GRPDIR/ continued from last page

Name	Type	Condition	Units	Comment
`NJJA␣1␣␣␣␣␣␣`	I(N_m)			array $n^g_{1,m,a}$ that contains the number of energy group number for which the linearly anisotropic component of the scattering cross section from group g for mixture m does not vanish, .
`IPOA␣1␣␣␣␣␣␣`	I(N_m)			array $p^g_{1,m,a}$ that contains the location in the compressed scattering matrix of the information associated with mixture m.
`SCAA␣1␣␣␣␣␣␣`	R($N^g_{0,m,d}$)		cm^{-1}	array ($\Sigma^g_{1,k,a}$) that contains the compressed component of the linearly anisotropic components of the scattering matrix for scattering from group g for mixture m.

Here we have used:

$$N^g_{l,m,d} = \sum_{m=1}^{N_m} n^g_{l,m,d}$$

$$N^g_{l,m,a} = \sum_{m=1}^{N_m} n^g_{l,m,a}$$

4 CONTENTS OF A /MICROLIB/ DIRECTORY

A /MICROLIB/ directory contains the set of multigroup microscopic cross sections associated with a list 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 3). Finally it may contain a /DEPLETION/ directory (see Section 4.2) which is required for burnup calculation and a /SELFSHIELD/ directory which is generated by the `SHI:` module (see Section 4.3). Note that the contents of the /MICROLIB/ will vary depending on the module that was used to create or modify it.

In the case where the `LIB:` module is used to create this directory, it appears on the first level of the MACROLIB data structure. When `LIB:` is used ($\mathcal{M} = 1$), it embedded as a sub-directory in a /MICROLIB/ directory. Finally, when `EDI:` is used ($\mathcal{M} = 2$), it embedded as a sub-directory in a /EDITION/ directory.

Here for convenience we will define the variable $\mathcal{M}$ to identify the creation module:

$$\mathcal{M} = \begin{cases} 1 & \text{if the directory is created or modified by the } \texttt{LIB:} \text{ or } \texttt{EVO:} \text{ module;} \\ 2 & \text{if the directory is created or modified by the } \texttt{EDI:} \text{ module;} \\ 3 & \text{if the directory is modified by the } \texttt{SHI:} \text{ module.} \end{cases}$$

In the case where the `LIB:` ($\mathcal{M} = 1$) or `SHI:` ($\mathcal{M} = 3$), module are used to create or modify this directory, it appears on the first level of the MICROLIB data structure. Otherwise the `EDI:` ($\mathcal{M} = 2$) module is used and /MICROLIB/ represents a sub-directory in an EDITION data structure.

4.1 The main directory

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

Table 8: Main records and sub-directories in /MICROLIB/

Name	Type	Condition	Units	Comment
`SIGNATURE␣␣␣`	C∗12			parameter SIGNA containing the signature of the data structure.
`STATE-VECTOR`	I(40)			array $\mathcal{S}_i^m$ containing various parameters that are required to describe this data structure.
`ENERGY␣␣␣␣␣␣`	R($\mathcal{S}_3^m + 1$)		eV	array E_g containing the groups limits g.
`DELTAU␣␣␣␣␣␣`	R($\mathcal{S}_3^m$)			array U_g containing the lethargy width of each energy group g.
`ISOTOPESUSED`	C($\mathcal{S}_2^m$) ∗ 12			array NALIAS_i containing the alias name of the isotopes i.
`ISOTOPERNAME`	C($\mathcal{S}_2^m$) ∗ 12			array NISO_i containing the reference names of the isotopes i.
`ISOTOPESMIX␣`	I($\mathcal{S}_2^m$)			array M_i containing the mixture number associated with each isotope i.
`ISOTOPESTODO`	I($\mathcal{S}_2^m$)			array J_{todo} containing the flag for processing each depleting isotope i. A value of 0 indicates automatic processing while a value of 1 forces the isotope to be non depleting..

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

Name	Type	Condition	Units	Comment
ISOTOPESTYPE	I($\mathcal{S}_2^m$)			array P_i containing the type number associated with each isotope i. A value of $P_i = 3$ indicates a fission product. A value of $P_i = 2$ indicates a fissile isotope. For all other cases $P_i = 1$.
ISOTOPESDENS	R($\mathcal{S}_2^m$)		(cm b)$^{-1}$	array ρ_i containing the density of isotope i.
ISOTOPESTEMP	R($\mathcal{S}_2^m$)		K	array T_i containing the temperature of the isotope i.
ISOTOPESAWR$_\sqcup$	R($\mathcal{S}_2^m$)		nau	array m_i containing the weight of the isotope i.
ISOTOPESVOL$_\sqcup$	R($\mathcal{S}_2^m$)	$\mathcal{M} = 2$	cm^3	array V_i containing the volume occupied by the isotope i.
ILIBRARYTYPE	C($\mathcal{S}_2^m$) $* 8$	$\mathcal{S}_8^m \geq 1$		array NLTY$_i$ containing the library type associated with each isotope i.
ILIBRARYNAME	C($\mathcal{S}_2^m$) $* 8$	$\mathcal{S}_8^m \geq 1$		array NLIB$_i$ containing the library name associated with each isotope i.
ILIBRARYINDX	I(M_I)	$N_{\text{lib}} \geq 1$		Index of the cross-section library associated with each isotope $1 \leq$ LLIB$_i \leq N_{\text{lib}}$.
ISOTOPESCOH$_\sqcup$	C($\mathcal{S}_2^m$) $* 8$	$\mathcal{S}_8^m \geq 1$		array NCOH$_i$ containing the name of the coherent scattering type at thermal energies associated with each isotope i.
ISOTOPESINC$_\sqcup$	C($\mathcal{S}_2^m$) $* 8$	$\mathcal{S}_8^m \geq 1$		array NINC$_i$ containing the name of the incoherent scattering type at thermal energies associated with each isotope i.
ISOTOPESNTFG	I($\mathcal{S}_2^m$)	$\mathcal{S}_8^m \geq 1$		array $G_{s,i}$ containing the number of thermal groups involved in coherent or incoherent scattering for isotope i.
ISOTOPESHIN$_\sqcup$	C($\mathcal{S}_2^m$) $* 8$	$\mathcal{S}_8^m * \mathcal{S}_{15}^m \geq 1$		array NSHI$_i$ containing the name of the resonant isotope associated with each isotope i.
ISOTOPESSHI$_\sqcup$	I($\mathcal{S}_2^m$)	$\mathcal{S}_8^m * \mathcal{S}_{15}^m \geq 1$		array $I_{R,i}$ containing the resonant mixture number associated with each isotope i.
ISOTOPESDSN$_\sqcup$	R($\mathcal{S}_2^m$)	$\mathcal{S}_8^m * \mathcal{S}_{15}^m \geq 1$	b	array $\sigma_{\text{LJ},i}$ containing the standard dilution cross section for isotope i.
ISOTOPESGIR$_\sqcup$	R($\mathcal{S}_2^m$)	$\mathcal{S}_8^m \geq 1$		array $P_{\text{GC},i}$ containing the Goldstein-Cohen intermediate resonance parameter for isotope i.
ISOTOPESNIR$_\sqcup$	I($\mathcal{S}_2^m$)	$\mathcal{S}_8^m \geq 1$		array $G_{\text{GC},i}$ containing the energy group cutoff for Goldstein-Cohen intermediate resonance parameter for isotope i.
ADDXSNAME$_{\sqcup\sqcup\sqcup}$	C($\mathcal{S}_{13}^m$) $* 6$	$\mathcal{S}_{13}^m \geq 1$		array ADDXS$_i$ containing the name of additional editing cross sections stored on /MACROLIB/.
TIMESPER$_{\sqcup\sqcup\sqcup\sqcup}$	R(2, 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 d T^{-1} and irradiation in Kb^{-1} respectively for which the perturbative expansion is valid.
MACROLIB$_{\sqcup\sqcup\sqcup\sqcup}$	Dir			name of directory containing the macroscopic library associated with this microscopic library.

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

Name	Type	Condition	Units	Comment
`DEPL-CHAIN␣␣`	Dir	$\mathcal{S}_{11}^m \geq 1$		name of directory containing the depletion chain associated with this microscopic library.
`SHIBA␣␣␣␣␣␣␣␣`	Dir	$\mathcal{M} = 3$		name of directory containing the self-shielding data associated with this microscopic library.
{*/ISOTOPE/*}	Dir			array $\mathcal{S}_2^m$ of sub-directories that contain the cross section information associated with a specific isotope. The name of these directories is specified by NALIAS$_i$.

The signature for this data structure is `SIGNA=L_LIBRARY␣␣␣␣`. The array $\mathcal{S}_i^m$ contains the following information:

- $\mathcal{S}_1^m = M_m$ is the maximum number of mixtures in the library.
- $\mathcal{S}_2^m = N_I$ is the maximum number of isotopes in the library.
- $\mathcal{S}_3^m = G$ is the number of groups in the library.
- $\mathcal{S}_4^m = L+1$ where L is the maximum order for the Legendre expansion for the scattering cross section used in the library.
- $\mathcal{S}_5^m = I_{tr}$ is the transport correction option used when processing this library where

$$I_{tr} = \begin{cases} 0 & \text{do not use a transport correction;} \\ 1 & \text{transport correction from } P_1 \text{ scattering;} \\ 2 & \text{recover transport correction from the MICROLIB.} \end{cases}$$

- $\mathcal{S}_7^m = I_d$ is the type of delay neutron data included in this library such that

$$I_d = \begin{cases} 1 & \text{include the delayed and prompt neutron effect;} \\ 2 & \text{consider only the prompt neutrons.} \end{cases}$$

- $\mathcal{S}_8^m = N_{\text{lib}} =$ is the number of independent microscopic cross section libraries used to create this library.
- $\mathcal{S}_9^m = G_f$ is the number of fast groups in this library. This represents the number of energy groups above 4.0 eV where resonance self-shielding effects will not be considered. It is automatically known for isotopes coming from WIMS-D4 or WIMS-AECL format libraries. For the other types of libraries, this value is initialized to 0. This value, which is only used by the `SHI:` module, can be modified using the keyword `GRMAX`.
- $\mathcal{S}_{10}^m = G_e$ is the number of epithermal groups in this library. This represents the total number of energy groups above 4.0 eV. This value is first used for the evaluation of the transport correction when it is not given explicitly in the original library. It is also used by the `SHI:` module and can be modified locally in this module using the keyword `GRMIN` if the last energy for which self-shielding calculations will take place is different from 4.0 eV.
- $\mathcal{S}_{11}^m = N_d$ is the number of depleting isotopes that can be found in this library.

- $\mathcal{S}_{12}^m = N_{d,f}$ is the number of depleting mixtures that can be found in this library.
- $\mathcal{S}_{13}^m = N_{\text{add}}$ is the number of additional editing cross sections found in this library.
- $\mathcal{S}_{14}^m = N_m$ is the number of mixtures found in this library.
- $\mathcal{S}_{15}^m = N_r$ is the number of resonant mixtures found in this library.
- $\mathcal{S}_{17}^m = I_{\text{proc}}$ is the option for processing the cross-section libraries

$$I_{\text{proc}} = \begin{cases} -1 & \text{skip the library processing (i.e., no interpolation).} \\ 0 & \text{perform an interpolation in temperature and dilution.} \\ 2 & \text{perform an interpolation in temperature and build a new temperature-independent cross-section library in DRAGON format.} \end{cases}$$

- $\mathcal{S}_{18}^m = I_{\text{mac}}$ is the option for computing the macrolib

$$I_{\text{mac}} = \begin{cases} 0 & \text{do not build an embedded macrolib.} \\ 1 & \text{build an embedded macrolib.} \end{cases}$$

- $\mathcal{S}_{19}^m = N_{\text{del}}$ is the number of precursor groups producing delayed neutrons.
- $\mathcal{S}_{20}^m = N_{\text{dfi}}$ is the number of fissile isotopes producing fission products.
- $\mathcal{S}_{17}^m = 20 + \mathcal{S}_4^m = N_x$ is the number of cross section types to process in this library.
- $\mathcal{S}_{18}^m = N_e$ is the number of energy producing mixtures without burnup found in this library.
- $\mathcal{S}_{19}^m = N_p$ is the maximum order for time dependent perturbations in this library.
- $\mathcal{S}_{20}^m = N_p$ is the maximum order for time dependent perturbations in this library.
- $\mathcal{S}_{21}^m = I_{\text{cmp}}$ is the decay chain completion option.

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

- $\mathcal{S}_{22}^m = M_I$ is the maximum number of isotopes per mixture for the mixtures found in this library.

One can find in Section 3 a description of the /MACROLIB/ directory and in Section 14 the contents of an /ISOTOPE/ directory. Note that if $N_I = 2$ and

$$\text{NALIAS}_i = \begin{cases} \texttt{235} \quad \texttt{0001} & \text{for } i = 1, \\ \texttt{Pu239} \quad \texttt{0003} & \text{for } i = 2. \end{cases}$$

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

Table 9: 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.

4.2 The depletion sub-directory

The following records and sub-directories will be found on a /DEPLETION/ directory:

Table 10: Main records in /DEPLETION/

Name	Type	Condition	Units	Comment
`STATE-VECTOR`	I(40)			array $\mathcal{S}_i^d$ containing the control parameters required for building the depletion chain from the information stored in this directory.
`ISOTOPESDEPL`	C($\mathcal{S}_1^d$) $*$ 12			array NISOD_i containing the reference name for the isotopes included in the depletion chain.
`CHARGEWEIGHT`	I($\mathcal{S}_1^d$)			array K_i^{aze} containing an identifier composed of the atomic number, charge and excitation mode for isotope i.
`DEPLETE-IDEN`	C($\mathcal{S}_8^d$) $*$ 8			array NREAD_r containing the name of the depletion reactions r.
`DEPLETE-REAC`	I($\mathcal{S}_8^d, \mathcal{S}_1^d$)			array $K_{r,i}^d$ containing the list of valid depletion reaction for isotope i.
`DEPLETE-ENER`	R($M_{\text{R}} \times N_{\text{depl}}$)		Mev	array $E_{r,i}$ containing the energy per reaction associated with each depletion reaction r and isotope i.
`DEPLETE-DECA`	R($\mathcal{S}_1^d$)		10^{-8} s^{-1}	array λ_i containing the rasioactive decay constant for isotope i.
`PRODUCE-REAC`	I($\mathcal{S}_9^d, \mathcal{S}_1^d$)			array $K_{s,i}^p$ containing the list of valid production reaction s for isotope i.
`PRODUCE-RATE`	R($\mathcal{S}_9^d, \mathcal{S}_1^d$)			array $R_{s,i}^p$ containing the branching ratio associated with each production reaction s for isotope i.
`FISSIONYIELD`	R($\mathcal{S}_2^d, \mathcal{S}_3^d$)			array $Y_{i\to j}$ containing the yield for the production of the direct fission product j by a fission og the direct fissile isotope i.

The array $\mathcal{S}_i^d$ contains the following information:

- $\mathcal{S}_1^d = N_{\text{depl}}$ is the number of depleting isotopes in this library.
- $\mathcal{S}_2^d = N_{\text{dfi}}$ is the number of direct fissile isotopes in this library.
- $\mathcal{S}_3^d = N_{\text{dfp}}$ is the number of direct fission product in this library.
- $\mathcal{S}_4^d = N_{\text{H}}$ is the number of heavy isotopes in this library. This represents the combination of fissile isotopes and the other isotopes produced from these isotopes by reactions other than fission.
- $\mathcal{S}_5^d = N_{\text{fp}}$ is the number of fission products in this library. This number represents the combination of fission fragments and the other isotopes produced from these isotopes by any reaction (decay or neutron induced).
- $\mathcal{S}_6^d = N_{\text{O}}$ is the number of other isotopes in this library. This number represents the other isotopes that are not produced by fission or by reaction with fission isotopes or fission products but have a depletion chain.
- $\mathcal{S}_7^d = N_{\text{E}}$ is the number of 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.
- $\mathcal{S}_8^d = M_{\text{R}}$ is the maximum number of independent depletion reaction considered in the depletion chain.
- $\mathcal{S}_9^d = M_{\text{S}}$ is the maximum number of parent isotopes leading to the production of an isotope in the depletion chain.

Note that contrarily to the information stored in the main /MICROLIB/ directory where the reference name of an isotope (NISO_i) is represented by a `CHARACTER*12` variable, here a `CHARACTER*8` variable is considered for NISOD_i. As a result, an isotope specified by NISO_i will be considered as being part of the depletion chain only if one can find a value of $1 \leq j \leq N_{\text{depl}}$ such that $\mathsf{NISO}_i(1:8) = \mathsf{NISOD}_j$.

In general, the reaction types NREAD_r associated with a given depletion mechanism will be identified by the microscopic cross section name associated with this reaction. Typically, the contents of the NREAD_r will be the following:

- NREAD_1=`DECAY␣␣␣` to identify a radioactive decay reaction.
- NREAD_2=`NG␣␣␣␣␣␣` to identify a capture reaction

$$ {}_0^1n + {}_Z^A X \longrightarrow {}_Z^{A+1}X + \gamma \, . $$

- NREAD_3=`NFTOT␣␣␣` to identify a fission reaction

$$ {}_0^1n + {}_Z^A X \longrightarrow \eta \, {}_0^1n + {}_{Z-Y}^{A+1-\eta-B} U + {}_Y^B V + \gamma \, . $$

- NREAD_4=`N2N␣␣␣␣␣` to identify the reaction

$$ {}_0^1n + {}_Z^A X \longrightarrow 2 \, {}_0^1n + {}_Z^{A-1} X + \gamma \, . $$

- NREAD_5=`N3N␣␣␣␣␣` to identify the reaction

$$ {}_0^1n + {}_Z^A X \longrightarrow 3 \, {}_0^1n + {}_Z^{A-2} X + \gamma \, . $$

- NREAD$_6$=N4N$\sqcup\sqcup\sqcup\sqcup\sqcup$ to identify the reaction
$$ {}^1_0n + {}^A_Z X \longrightarrow 4\,{}^1_0n + {}^{A-3}_Z X + \gamma\,. $$
- NREAD$_7$=NA$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$ to identify the reaction
$$ {}^1_0n + {}^A_Z X \longrightarrow {}^4_2\alpha + {}^{A-3}_{Z-2} Y + \gamma\,. $$
- NREAD$_8$=NP$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$ to identify the reaction
$$ {}^1_0n + {}^A_Z X \longrightarrow {}^1_1p + {}^A_{Z-1} Y + \gamma\,. $$
- NREAD$_9$=N2A$\sqcup\sqcup\sqcup\sqcup\sqcup$ to identify the reaction
$$ {}^1_0n + {}^A_Z X \longrightarrow 2\,{}^4_2\alpha + {}^{A-7}_{Z-4} Y + \gamma\,. $$
- NREAD$_{10}$=NNP$\sqcup\sqcup\sqcup\sqcup\sqcup$ to identify the reaction
$$ {}^1_0n + {}^A_Z X \longrightarrow {}^1_1p + {}^1_0\,n + {}^{A-1}_{Z-1} Y + \gamma\,. $$
- NREAD$_{10}$=ND$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$ to identify the reaction
$$ {}^1_0n + {}^A_Z X \longrightarrow {}^2_1D + {}^{A-1}_{Z-1} Y + \gamma\,. $$
- NREAD$_{10}$=NT$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$ to identify the reaction
$$ {}^1_0n + {}^A_Z X \longrightarrow {}^3_1T + {}^{A-2}_{Z-1} Y + \gamma\,. $$

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

$$ d(r) = K^d_{r,i} \bmod 100 $$
$$ i(r) = \frac{K^d_{r,i}}{100} $$

where

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

and $i(r) = 0$ unless $4 \leq d(r) \leq 5$. When $d(r) = 4$, $i(r)$ represents the fissile isotope number while for $d(r) = 5$, $i(r)$ represents the direct fission fragment number. The fractional yield for the production of the direct fission product $i(r)$ from the fissile isotope $j(r)$ is stored in the matrix $Y_{i(r)\rightarrow j(r)}$. The array $R^d_{r,i}$,contains the energy generated by reaction in MeV.

The contents of the variables $K^p_{s,i}$ is used to identify explicitly the parent isotope that generated the current isotope i. The maximum number of parent reaction for the depletion chain is $M_{\rm S}$. As in the case of $K^d_{r,i}$, $K^p_{s,i}$ also contains two different types of information namely $r(s)$ and $i(s)$ that are defined as follows:

$$ r(s) = K^p_{s,i} \bmod 100 $$
$$ i(s) = \frac{K^p_{s,i}}{100} $$

where $r(s) = 0$ indicates that the list of parent reaction is complete while $r_p > 0$ refers to the reaction type $\mathsf{NREAD}_{r(s)}$. In the case where $r(s) > 0$, $i(s)$ refers to the parent isotope $\mathsf{NISOD}_{i(s)}$ and can take the following values

$$r(s) = \begin{cases} 0 & \text{isotope } i \text{ produced by radioactive decay;} \\ 1 & \text{isotope } i \text{ produced by fission (this contribution is kept apart from record 'FISSIONYIELD');} \\ 2 & \text{isotope } i \text{ produced by neutron capture;} \\ 3 & \text{isotope isotope } i \text{ produced by } \mathsf{NREAD}_{r(s)} \text{ reaction;} \\ \text{otherwise} & \text{isotope is fissile with fission yield (valid only for } r \text{ such that } \mathsf{NREAD}_r = \texttt{NFTOT}. \end{cases}$$

The array $R^p_{s,i}$ is the fractional branching ratio for the production of isotope $\mathsf{NISOD}_{i(s)}$ via reaction $r(s)$.

4.3 The self-shielding sub-directory

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

Table 11: Main records in /SELFSHIELD/

Name	Type	Condition	Units	Comment
`STATE-VECTOR`	I(40)			array $\mathcal{S}^s_i$ containing the various parameters associated with the self-shielding process.
`EPS-SHIBA␣␣␣`	R(1)			constant ϵ_r that contains the relative convergence criterion for the self-shielding iterations.

The array $\mathcal{S}^s_i$ contains the following information:

- $\mathcal{S}^s_1 = G_{\text{min}}$ is the first group for which self-shielding takes place. By default $G_{\text{min}} = N_{g,f} + 1$.
- $\mathcal{S}^s_2 = G_{\text{max}}$ is the last group for which self-shielding takes place. By default $G_{\text{max}} = N_{g,e}$.
- $\mathcal{S}^s_3 = M_r$ is the maximum number of iteration in the self-shielding calculation
- $\mathcal{S}^s_4 = I_{\text{LJ}}$ is the Livolant-Jeanpierre self-shielding option activation key where:

$$I_{\text{LJ}} = \begin{cases} 0 & \text{for standard self-shielding;} \\ 1 & \text{for self-shielding with Livolant-Jeanpierre equivalence.} \end{cases}$$

- $\mathcal{S}^s_5 = I_{\text{GC}}$ is the option Goldstein-Cohen approximation activation key where:

$$I_{\text{GC}} = \begin{cases} 0 & \text{do not use the Goldstein-Cohen approximation;} \\ 1 & \text{activate the Goldstein-Cohen approximation.} \end{cases}$$

- $\mathcal{S}^s_6 = I_{\text{TC}}$ is the transport correction activation key where:

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

- $\mathcal{S}_7^s = I_{\text{level}}$ is the of self-shielding model where

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

5 CONTENTS OF A /GEOMETRY/ DIRECTORY

This directory contains a compact description of a geometry.

5.1 The main directory

On its first level, the following records and sub-directories can be found:

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

Name	Type	Condition	Units	Comment
SIGNATURE	C∗12			parameter SIGNA containing the signature of the data structure.
STATE-VECTOR	I(40)			array $\mathcal{S}_i^G$ containing various parameters that are required to describe this data structure.
MIX	I($\mathcal{S}_6^G$)			array M_r containing the mixture associated with each region r in the geometry.
RADIUS	R(N_r+1)	$N_r \geq 1$	cm	array R_i containing the radial mesh in the geometry. The first element of this vector is identical to 0.0.
OFFCENTER	R(3)	$N_r \geq 1$	cm	array d_R containing the displacement of the center of the annular mesh with respect to the center of the Cartesian cell.
MESHX	R(N_x+1)	$N_x \geq 1$	cm	array X_i that contains the X directed mesh.
MESHY	R(N_y+1)	$N_y \geq 1$	cm	array Y_j that contains the Y directed mesh.
MESHZ	R(N_z+1)	$N_z \geq 1$	cm	array Z_k that contains the Z directed mesh.
SIDE	R(1)	$F_h = 1$	cm	value H containing he width of the side of the hexagon. The flag $F_h = 0$ by default. It takes the value $F_h = 1$ when $\mathcal{S}_1^G = 8$ or 9.
SPLITR	I(N_r+1)	$N_r \geq 1$		array $S_{r,i}$ containing the radial mesh splitting. A negative value indicates that the radial mesh must be subdivided into regions of equal volumes; a positive value indicates that the radial mesh must be subdivided into regions of equal radial thickness.
SPLITX	I(N_x)	$N_x \geq 1$		array $S_{x,i}$ containing the X directed mesh splitting.
SPLITY	I(N_y)	$N_y \geq 1$		array $S_{y,j}$ containing the Y directed mesh splitting.
SPLITZ	I(N_z)	$N_z \geq 1$		array $S_{z,k}$ containing the Z directed mesh splitting.
IHEX	I(1)	$F_h = 1$		value S_h that contains the hexagonal symmetry factor. The flag $F_h = 0$ by default. It takes the value $F_h = 1$ when $\mathcal{S}_1^G = 8$ or 9.
NCODE	I(6)			array $N_{\beta,j}$ containing the types of boundary conditions associated with each surface.
ZCODE	R(6)			array β_j containing the albedo value associated with each surface.

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

Name	Type	Condition	Units	Comment
`ICODE␣␣␣␣␣␣␣`	I(6)			array $I_{\beta,j}$ containing albedo index associated with each surface $I_{\beta,j}$. The information stored in this array 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)	$\mathcal{S}_1^G = 3$		Number N_{pin} of identical pins in the cluster ring.
`RPIN␣␣␣␣␣␣␣␣`	R(1)	$\mathcal{S}_1^G = 3$	cm	array $R_{\text{pin},j}$ containing the radial position at which each of the pin in the cluster ring is located with respect to the center of the cell. In the case where $R_{\text{pin},j}$ contains a single element, it is assumed that the pins are all located at the same radial position.
`APIN␣␣␣␣␣␣␣␣`	R(1)	$\mathcal{S}_1^G = 3$		array $\theta_{\text{pin},j}$ containing the angular position at which each of the pin in the cluster ring is located with respect to the X, Y or Z axis respectively for `TUBEX`, `TUBEY` and `TUBEZ` geometry. In the case where $\theta_{\text{pin},j}$ contains a single element, it is assumed that the first pin is located at θ_{pin}, the remaining pins being located at $\theta_{\text{pin},j} + 2(j-1)\pi/N_{\text{pin}}$.
`MICRO␣␣␣␣␣␣␣`	I(1)	$\mathcal{S}_{12}^G = 1$		number F_{micro} indicating the type of micro structure included in the geometry.
`NS␣␣␣␣␣␣␣␣␣␣`	I($\mathcal{S}_{14}^G$)	$\mathcal{S}_{12}^G = 1$		array $N_{\text{micro},i}$ containing the number of regions in the micro structures.
`RS␣␣␣␣␣␣␣␣␣␣`	R($\mathcal{S}_{15}^G, \mathcal{S}_{14}^G$)	$\mathcal{S}_{12}^G = 1$	cm	array $R_{\text{micro},i,j}$ containing the radii of the tubes or spherical shells making up the micro structures.
`MILIE␣␣␣␣␣␣␣`	I($\mathcal{S}_{16}^G$)	$\mathcal{S}_{12}^G = 1$		array $C_{\text{micro},i,j}$ containing the composite mixture number associated with each region in the micro structures.
`MIXDIL␣␣␣␣␣␣`	I($\mathcal{S}_{16}^G$)	$\mathcal{S}_{12}^G = 1$		array $D_{\text{micro},i,j}$ containing the mixture number associated with each region of the geometry where the micro structure is to be inserted.
`MIXGR␣␣␣␣␣␣␣`	I($\mathcal{S}_{17}^G, \mathcal{S}_{16}^G$)	$\mathcal{S}_{12}^G = 1$		array $M_{\text{micro},i,j}$ containing the mixture number associated with each region of the micro structures.
`FRACT␣␣␣␣␣␣␣`	R($\mathcal{S}_{16}^G, \mathcal{S}_{14}^G$)	$\mathcal{S}_{12}^G = 1$		array $\rho_{\text{micro},i,j}$ containing the volumetric concentration of each micro structure.
`POURCE␣␣␣␣␣␣`	R($\mathcal{S}_3^G$)	$\mathcal{S}_1^G = 30$		array P_j containing the proportion of each cell type in the lattice.
`PROCEL␣␣␣␣␣␣`	R($\mathcal{S}_3^G, \mathcal{S}_3^G$)	$\mathcal{S}_1^G = 30$		array $P_{i,j}$ containing 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.
`CELL␣␣␣␣␣␣␣␣`	C($\mathcal{S}_9^G$) $* 12$	$\mathcal{S}_8^G = 1$		array CELL_k containing the names of the sub-geometry.
`GENERATING␣␣`	I($\mathcal{S}_6^G$)	$\mathcal{S}_8^G = 1$		array $G_{c,i}$ containing the generating sub-geometry index corresponding to each region.
`MERGE␣␣␣␣␣␣␣`	I($\mathcal{S}_6^G$)	$\mathcal{S}_{10}^G = 1$		array $G_{m,i}$ containing the merging index corresponding to each region.

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

Name	Type	Condition	Units	Comment
TURN␣␣␣␣␣␣␣␣	I($\mathcal{S}_6^G$)	$\mathcal{S}_{11}^G = 1$		array $G_{t,i}$ containing the orientation index corresponding to each region.
CLUSTER␣␣␣␣␣	C($\mathcal{S}_{13}^G$) $* 12$	$\mathcal{S}_{13}^G \geq 1$		array CLUSTER$_k$ containing the names of the subgeometry making up the cluster.
{*/SUBGEO/*}	Dir			List of sub-directories that contain a subgeometry.

The signature for this data structure is SIGNA=L_GEOM␣␣␣␣␣␣. The array $\mathcal{S}_i^G$ contains the following information:

- $\mathcal{S}_1^G$ identifies the type of geometry where:

$$\mathcal{S}_1^G = \begin{cases} 0 & \text{virtual geometry;} \\ 1 & \text{homogeneous geometry;} \\ 2 & \text{Cartesian 1–D geometry;} \\ 3 & \text{annular 1–D geometry;} \\ 4 & \text{spherical 1–D geometry;} \\ 5 & \text{Cartesian 2–D geometry;} \\ 6 & Z \text{ directed cylindrical 2–D geometry;} \\ 7 & \text{Cartesian 3–D geometry;} \\ 8 & \text{hexagonal 2–D geometry;} \\ 9 & \text{hexagonal 3–D geometry;} \\ 10 & X \text{ directed cylindrical 2–D geometry;} \\ 11 & Y \text{ directed cylindrical 2–D geometry;} \\ 20 & \text{Cartesian 2–D geometry containing an annular mesh;} \\ 21 & \text{Cartesian 3–D geometry containing a } X \text{ directed cylindrical mesh;} \\ 22 & \text{Cartesian 3–D geometry containing a } Y \text{ directed cylindrical mesh;} \\ 23 & \text{Cartesian 3–D geometry containing a } Z \text{ directed cylindrical mesh;} \\ 24 & \text{hexagonal 2–D geometry containing an annular mesh;} \\ 25 & \text{hexagonal 3–D geometry containing a } Z \text{ directed cylindrical mesh;} \\ 30 & \text{do-it-yourself geometry.} \end{cases}$$

- $\mathcal{S}_2^G = N_r$ is the number of radial mesh intervals in the geometry. By default, $N_r = 0$.
- $\mathcal{S}_3^G = N_x$ is the number of X directed mesh intervals or hexagon in the geometry. By default, $N_x = 1$.
- $\mathcal{S}_4^G = N_y$ is the number of Y directed mesh intervals or hexagon in the geometry. By default, $N_y = 1$.
- $\mathcal{S}_5^G = N_z$ is the number of Z directed mesh intervals or hexagon in the geometry. By default, $N_z = 1$.
- $\mathcal{S}_6^G = N_k$ is the total number of regions in the geometry. In the case where $20 \leq \mathcal{S}_1^G \leq 25$, N_k takes the value:

$$N_k = (N_r + 1) \times N_x \times N_y \times N_x$$

When $\mathcal{S}_1^G = 3,\ 6,\ 10$ and 11, N_k takes the value:

$$N_k = N_r \times N_x \times N_y \times N_x$$

- $\mathcal{S}_7^G = M_m$ is the maximum mixtures number used in this geometry.
- $\mathcal{S}_8^G = F_C$ is the `CELL` activation option where:

$$F_c = \begin{cases} 0 & \text{the } \texttt{CELL} \text{ option is not activated;} \\ 1 & \text{the } \texttt{CELL} \text{ option is activated.} \end{cases}$$

- $\mathcal{S}_9^G = N_s$ is the number of sub-geometries defined in this geometry.
- $\mathcal{S}_{10}^G = F_m$ is the `MERGE` activation option where:

$$F_m = \begin{cases} 0 & \text{the } \texttt{MERGE} \text{ option is not activated;} \\ 1 & \text{the } \texttt{MERGE} \text{ option is activated.} \end{cases}$$

- $\mathcal{S}_{11}^G = F_s$ is the `SPLIT` activation option where:

$$F_m = \begin{cases} 0 & \text{the } \texttt{SPLIT} \text{ option is not activated;} \\ 1 & \text{the } \texttt{SPLIT} \text{ option is activated.} \end{cases}$$

- $\mathcal{S}_{12}^G = F_{\text{dh}}$ is the double heterogeneity activation option where:

$$F_{\text{dh}} = \begin{cases} 0 & \text{the double heterogeneity option is not activated;} \\ 1 & \text{Double heterogeneity option present.} \end{cases}$$

- $\mathcal{S}_{13}^G = N_{\text{cl}}$ is the number of cluster sub-geometry.
- $\mathcal{S}_{14}^G$ is the number of regions in the micro structures,
- $\mathcal{S}_{15}^G$ is the maximum number of annular regions in any micro structure.
- $\mathcal{S}_{16}^G$ is the number of micro structures.
- $\mathcal{S}_{17}^G$ is the total number of annular regions in the micro structure.

The hexagonal symmetry factor S_h is defined as:

$$S_h = \begin{cases} 1 & \text{for an assembly with a } \texttt{S30} \text{ symmetry;} \\ 2 & \text{for an assembly with a } \texttt{SA60} \text{ symmetry;} \\ 3 & \text{for an assembly with a } \texttt{SB60} \text{ symmetry;} \\ 4 & \text{for an assembly with a } \texttt{S90} \text{ symmetry;} \\ 5 & \text{for an assembly with a } \texttt{R120} \text{ symmetry;} \\ 6 & \text{for an assembly with a } \texttt{R180} \text{ symmetry;} \\ 7 & \text{for an assembly with a } \texttt{SA180} \text{ symmetry;} \\ 8 & \text{for an assembly with a } \texttt{SB180} \text{ symmetry;} \\ 9 & \text{for an assembly without symmetry (} \texttt{COMPLETE}\text{).} \end{cases}$$

where the description of the symmetries can be found in the DRAGON users guide. Similarly the type of boundary conditions used will be defined in the following way:

$$N_{\beta,j} = \begin{cases} 0 & \text{not used;} \\ 1 & \text{void boundary condition;} \\ 2 & \text{reflection boundary condition;} \\ 3 & \text{diagonal reflection boundary condition;} \\ 4 & \text{periodic (translation) boundary condition;} \\ 5 & \text{symmetric reflection boundary condition;} \\ 6 & \text{albedo boundary condition.} \end{cases}$$

The type of micro structure F_{micro} is defined as:

$$F_{\text{micro}} = \begin{cases} 3 & \text{annular micro structure;} \\ 4 & \text{spherical micro structure.} \end{cases}$$

In the case where $\mathcal{S}_8^G = 1$, the list of directory {/SUBGEO/} will have the same name as the variable CELL_k. For example, in the case where $\mathcal{S}_9^G = 2$ and

$$\mathsf{CELL}_k = \begin{cases} \texttt{GEO1} & \text{for } k = 1, \\ \texttt{GEO2} & \text{for } k = 2. \end{cases}$$

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

Table 13: Cell sub-geometry directory

Name	Type	Condition	Units	Comment
`GEO1␣␣␣␣␣␣␣␣`	Dir			a `CELL` /GEOMETRY/ directory.
`GEO2␣␣␣␣␣␣␣␣`	Dir			another `CELL` /GEOMETRY/ directory.

In the case where $\mathcal{S}_{13}^G \geq 1$, the list of directory {/SUBGEO/} will have the same name as the variable $\mathsf{CLUSTER}_k$. For example, in the case where $\mathcal{S}_{13}^G = 2$ and

$$\mathsf{CLUSTER}_k = \begin{cases} \texttt{RODS1} & \text{for } k = 1, \\ \texttt{RODS2} & \text{for } k = 2. \end{cases}$$

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

Table 14: Cluster sub-geometry directory

Name	Type	Condition	Units	Comment
`RODS1␣␣␣␣␣␣␣␣`	Dir			a `CLUSTER` /GEOMETRY/ directory.
`RODS2␣␣␣␣␣␣␣␣`	Dir			another `CLUSTER` /GEOMETRY/ directory.

6 CONTENTS OF A /TRACKING/ DIRECTORY

This directory contains the information generated after the geometry has been analyzed by the DRAGON tracking modules.

6.1 The main directory

The following records and sub-directories will be found in the /TRACKING/ directory:

Table 15: Main records in /TRACKING/

Name	Type	Condition	Units	Comment
`SIGNATURE␣␣␣`	C∗12			parameter SIGNA containing the signature of the data structure.
`STATE-VECTOR`	I(40)			array $\mathcal{S}_i^t$ containing various parameters that are required to describe this data structure.
`TRACK-TYPE␣␣`	C∗12			parameter TRKT containing the name of the tracking model used to create this structure.
`TITLE␣␣␣␣␣␣␣`	C∗72			parameter TITLE containing a title associated with data structure (see DRAGON input option `TITL`).
`MATCOD␣␣␣␣␣␣`	I($\mathcal{S}_1^t$)			array M_r containing the mixture number associated with each region r.
`KEYFLX␣␣␣␣␣␣`	I($\mathcal{S}_1^t$)			array I_r containing the location in the array containing unknown where one can find the volume averaged flux associated with region r.
`VOLUME␣␣␣␣␣␣`	R($\mathcal{S}_1^t$)		cm^3	array V_r containing the volume associated with each region r.

The signature for this data structure is SIGNA=`L_TRACK␣␣␣␣␣`. The tracking model TRKT can take the following values:

$$\text{TRKT} = \begin{cases} \texttt{EXCELL} & \text{for tracking by the } \texttt{EXCELT:}, \texttt{EXCELL:} \text{ or } \texttt{NXT:} \text{ modules;} \\ \texttt{SYBIL} & \text{for tracking by the } \texttt{SYBILT:} \text{ module;} \\ \texttt{JPM} & \text{for tracking by the } \texttt{JPMT:} \text{ module;} \\ \texttt{BIVAC} & \text{for tracking by the } \texttt{BIVACT:} \text{ module.} \end{cases}$$

The array $\mathcal{S}_i^t$ contains the following information:

- $\mathcal{S}_1^t = N_r$ is the number of independent regions in the problem.
- $\mathcal{S}_2^t = N_u$ is the number of independent unknowns in the problem.
- $\mathcal{S}_3^t = I_L$ is the leakage flag where:

$$I_L = \begin{cases} 0 & \text{indicates that some leakage is present;} \\ 1 & \text{indicates that no leakage is present.} \end{cases}$$

- $\mathcal{S}_4^t = \mathcal{S}_7^G = M_m$ is the maximum number of mixture used in the problem.
- $\mathcal{S}_5^t = N_s$ is the number of independent outer surfaces in the problem.
- $\mathcal{S}_6^t$ is the anisotropy level for flux calculation in the problem where:

$$\mathcal{S}_6^t = \begin{cases} 0 & \text{only the isotropic flux components are considered;} \\ 1 & \text{the isotropic and linearly anisotropic flux components are considered.} \end{cases}$$

In addition to the above records, the main /TRACKING/ directory also contains information that is specific to each tracking module. This information will be described in the following subsections. Also note that the contents of the $\mathcal{S}_i^t$ vector for $i \geq 7$ will depend on the specific tracking module and will be defined in the next three subsections.

6.2 The `EXCELL` records and sub-directories

When TRKT=`EXCELL` the following elements of $\mathcal{S}_i^t$ are also defined.

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

$$\mathcal{S}_7^t = \begin{cases} 1 & \text{for the tracking of Cartesian assemblies using } \texttt{EXCELT:} \text{ or } \texttt{EXCELL:}; \\ 2 & \text{for the tracking of hexagonal assemblies using } \texttt{EXCELT:}; \\ 3 & \text{for the tracking of 2-D cluster geometries using } \texttt{EXCELT:}; \\ 4 & \text{for the tracking of 2-D and 3-D Cartesian assemblies with clusters using } \texttt{NXT:}. \end{cases}$$

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

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

  The default is $\mathcal{S}_8^t = 0$. The option $\mathcal{S}_8^t = -1$ can only be activated using the `RENO` keyword in the `EXCELT:` and `EXCELL:` modules.

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

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

- $\mathcal{S}_{10}^t$ is the type of boundary conditions to be used for the collision probability calculations where:

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

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

- the number of equal sectors (trapezoidal quadrature) in the $[0, \max(\mathcal{S}^t_{12}, 2)\pi]$ range when the **EXCELT:** modules 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 ($0 \leq \varphi \leq \pi/2$ and $0 \leq \theta \leq \pi/2$) when the **EXCELT:** and **EXCELL:** modules are used for Cartesian assemblies for $\mathcal{S}^t_{16} = n(n+2)/8$ direction in each quadrant;
- the number of equal sectors (trapezoidal quadrature) in the $[0, 2\pi/]$ range when the **EXCELT:** modules is used for hexagonal geometries;
- not used for the **EXCELT:** modules in cluster geometries;
- the order n of the EQ_n, LC_n or LT_n quadrature in a quadrant:

  $$0 \leq \varphi \leq \pi/2$$
  $$0 \leq \theta \leq \pi/2$$

  When the **NXT:** modules is used this results in $\mathcal{S}^t_{16} = n(n+2)/8$ directions for the EQ_n quadrature, $\mathcal{S}^t_{16} = 3 \times n(n+2)/8$ for the LC_n quadrature and $\mathcal{S}^t_{16} = 3 \times n^2/2$ for the LT_n quadrature.

- $\mathcal{S}^t_{12}$ is the angular symmetry factor.
- $\mathcal{S}^t_{13}$ is the polar angle quadrature type where:

$$\mathcal{S}^t_{13} = \begin{cases} 1 & \text{for a Gauss quadrature;} \\ 2 & \text{for a CACTUS type A quadrature;} \\ 3 & \text{for a CACTUS type B quadrature;} \\ 4 & \text{for an optimized Bickley quadrature.} \end{cases}$$

- $\mathcal{S}^t_{14}$ is the polar angle quadrature order.
- $\mathcal{S}^t_{15}$ is the azimuthal (2-D) or solid (3-D) angle quadrature type where:

$$\mathcal{S}^t_{15} = \begin{cases} 1 & \text{for a } EQ_n \text{ (3-D) or trapezoidal (2-D) quadrature;} \\ 2 & \text{for a Gauss quadrature (2-D hexagonal geometries);} \\ 3 & \text{for a median angle quadrature;} \\ 4 & \text{for a } LC_n \text{ 3-D quadrature;} \\ 5 & \text{for a } LT_n \text{ 3-D quadrature.} \end{cases}$$

- $\mathcal{S}^t_{16}$ is the number of directions for the azimuthal (2-D) or solid (3-D) angle quadrature.
- $\mathcal{S}^t_{17}$ is the number of tracking points on a line.
- $\mathcal{S}^t_{18}$ is the maximum length of a track.
- $\mathcal{S}^t_{19}$ is the total number of tracks generated.
- $\mathcal{S}^t_{20}$ is the total number of track directions processed.

The following records will also be present on the main level of a /TRACKING/ directory:

Table 16: Additionnal records for `EXCELL` tracking

Name	Type	Condition	Units	Comment
`EXCELTRACKOP`	R(40)			array $\mathcal{R}_i$ containing additional `EXCELL` tracking parameters.
`ICODE␣␣␣␣␣␣␣␣`	I(6)			array $I_{\beta,k}$ containing the surface albedo index (geometric surface albedo $\beta_{g,k}$ are used if $I_{\beta,k} < 0$ while physical surface albedo $\beta_{p,k}$ are used if $I_{\beta,k} > 0$).
`ALBEDO␣␣␣␣␣␣␣`	R(6)			array $\beta_{g,k}$ containing the geometric surface albedo (used only if $I_{\beta,k} \geq 0$).
`EXCELL␣␣␣␣␣␣␣`	Dir	$\mathcal{S}_7^t < 4$		directory containing additional `EXCELT:` and `EXCELL:` 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.

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 2–D and 3–D 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 2–D and 3–D 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 $\mathcal{S}_7^t = 4$).

The `/NXTRecords/` directory contains the information required to track the geometry using the `NXT:` based procedures once it has been analyzed. This information is in the following format:

Table 17: 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^{GG})			array $D_{i,j}^{GG}$ containing the assembly description of the geometry in terms of cells and rotation. The first element ($i = 1$) identifies the cell number while the second element identifies the cell rotation.
`G00000001CIS`	I(4, N_4^{GG})			array $S_{i,j}^{GG}$ containing the cell intrinsic symmetry properties. A value of 1 indicates that the symmetry is present while a value of 0 indicates that the symmetry is not considered. The order of the symmetry is X, Y, $X = Y$ and Z respectively for $i = 1,\ 2,\ 3,$ and 4.
`G00000001CFE`	I(7, N_4^{GG})			array $F_{i,j}^{GG}$ containing the cell external surface identification. A value of 1 indicates that this face is an external surface while a value of 0 indicates that the face represents an internal surface. The order of the external faces is $X_-, X_+, Y_-, Y_+, Z_-, Z_+$ and R_+ respectively for $i = 1,\ 2,\ 3,\ 4,\ 5,\ 6,$ and 7.
`G00000001SMX`	D(N_{13}^{GG})		cm	array x^{GG} containing the X directed mesh for the cell assembly.
`G00000001SMY`	D(N_{14}^{GG})		cm	array y^{GG} containing the Y directed mesh for the cell assembly.
`G00000001SMZ`	D(N_{15}^{GG})		cm	array z^{GG} containing the Z directed mesh for the cell assembly.
`G00000001SMR`	D(1)	$N_2^{GG} = 1$	cm	the radius of the outer assembly boundary.

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

- N_1^{GG} is the number of dimensions for the problem.
- N_2^{GG} is the type of boundary. A value of 0 indicates a Cartesian geometry and a value of 1 indicates a cylindrical geometry.
- N_3^{GG} is the 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 geometry a value of 1 (x-axis) is selected by default.
- N_4^{GG} is the number of cells in the original geometry (before unfolding).
- N_5^{GG} is the total number of cells in the geometry after the original geometry is unfolded according to the symmetries.
- N_6^{GG} in the diagonal symmetry flag. A value of 0 indicates that this symmetry is not used. A value of -1 indicates that the symmetry is used along the $X_- = Y_+$ and a value of 1 that the symmetry is used along $X_+ = Y$ axis.
- N_7^{GG} in the flag to identify symmetries with respect to the x-axis (X_- or X_+). A value of 0 indicates that no symmetry is present, $N_7^{GG} = \pm 1$ is for a `SYME` symmetry at the $X_\pm$ plane, $N_7^{GG} = \pm 2$ represents a `SSYM` symmetry at the $X_\pm$ plane and $N_7^{GG} = 3$ implies a translation symmetry is the x direction ($X_- = X_+$).

- N_8^{GG} in the flag to identify symmetries with respect to the y-axis (Y_- or Y_+). A value of 0 indicates that no symmetry is present, $N_7^{\text{GG}} = \pm 1$ is for a `SYME` symmetry at the $Y_\pm$ plane, $N_7^{\text{GG}} = \pm 2$ represents a `SSYM` symmetry at the $Y_\pm$ plane and $N_7^{\text{GG}} = 3$ implies a translation symmetry is the y direction ($Y_- = Y_+$).
- N_9^{GG} in the flag to identify symmetries with respect to the z-axis (Z_- or Z_+). A value of 0 indicates that no symmetry is present, $N_7^{\text{GG}} = \pm 1$ is for a `SYME` symmetry at the $Z_\pm$ plane, $N_7^{\text{GG}} = \pm 2$ represents a `SSYM` symmetry at the $Z_\pm$ plane and $N_7^{\text{GG}} = 3$ implies a translation symmetry is the z direction ($Z_- = Z_+$).
- N_{10}^{GG} is the number of x mesh subdivisions in the original geometry.
- N_{11}^{GG} is the number of y mesh subdivisions in the original geometry.
- N_{12}^{GG} is the number of z mesh subdivisions in the original geometry.
- N_{13}^{GG} is the number of x mesh subdivisions in the unfolded geometry.
- N_{14}^{GG} is the number of y mesh subdivisions in the unfolded geometry.
- N_{15}^{GG} is the number of z mesh subdivisions in the unfolded geometry.
- N_{16}^{GG} is the maximum number cells required to represent this geometry.
- N_{17}^{GG} is the maximum number of region for this geometry.
- N_{18}^{GG} is the total number of clusters in this geometry.
- N_{19}^{GG} is the maximum number of pins in this geometry.
- N_{20}^{GG} is the maximum dimension of any mesh array for a cell in this geometry.
- N_{21}^{GG} is not maximum dimension of any mesh array for a pin in this geometry.
- N_{22}^{GG} is the number of external surfaces for this geometry.
- N_{23}^{GG} is the number of regions for this geometry.
- N_{24}^{GG} is the maximum number of external surfaces in a sub-geometry included in this geometry.
- N_{25}^{GG} is the maximum number of regions in a sub-geometry included in this geometry.

The array x^{GG} contains the following information:

- x_{-1}^{GG} 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:

  $$x_c = \frac{x_{n^x}^{\text{GG}} + x_0^{\text{GG}}}{2}$$

  where we have used $n^x = N_3^{\text{GG}}$
- $x_{i-1}^{\text{GG}} \leq x \leq x_i^{\text{GG}}$ gives the position in x of mesh element i with $i = 1, n^x$

The array y^{GG} contains the following information:

- y_{-1}^{GG} 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:

  $$y_c = \frac{y_{n^y}^{\text{GG}} + y_0^{\text{GG}}}{2}$$

  where we have used $n^y = N_4^{\text{GG}}$

- $y_{i-1}^{\mathrm{GG}} \leq y \leq y_i^{\mathrm{GG}}$ gives the position in y of mesh element i with $i = 1, n^y$.

The array z^{GG} contains the following information:

- z_{-1}^{GG} 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:

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

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

- $z_{i-1}^{\mathrm{GG}} \leq z \leq z_i^{\mathrm{GG}}$ gives the position in z of mesh element i with $i = 1, n^z$

As we noted above, the global geometry is described in terms of cells. For cell $i = 1$ the following records will be stored on the `/NXTRecords/` directory.

Table 18: Cell $i = 1$ records in `/NXTRecords/`

Name	Type	Units	Comment
`C00000001DIM`	I(40)		array $N_{j,i}^{\mathrm{GC}}$ containing the dimensioning information required to rebuilt cell i.
`C00000001SMR`	D(N_2^{GC})	cm	array $r_{j,i}^{\mathrm{GC}}$ containing the radial mesh description for cell i.
`C00000001SMX`	D(N_3^{GC})	cm	array $x_{j,i}^{\mathrm{GC}}$ containing X directed mesh description for cell i.
`C00000001SMY`	D(N_4^{GC})	cm	array $y_{j,i}^{\mathrm{GC}}$ containing Y directed mesh description for cell i.
`C00000001SMZ`	D(N_5^{GC})	cm	array $z_{j,i}^{\mathrm{GC}}$ containing Z directed mesh description for cell i.
`C00000001MIX`	I(N_6^{GC})		array $M_{j,i}^{\mathrm{GC}}$ containing the mixture associated with each region j in cell i.
`C00000001VSE`	D($-N_9^{\mathrm{GC}} : N_8^{\mathrm{GC}}$)		array $\mathrm{SV}_{j,i}^{\mathrm{GC}}$ containing surface area j ($\mathrm{SV}_{-j,i}^{\mathrm{GC}} = S_j^{\mathrm{GC}}$ in cm for 2-D and cm^2 for 3-D problems) and regional volumes j ($\mathrm{SV}_{j,i}^{\mathrm{GC}} = V_{j,i}^{\mathrm{GC}}$ cm^2 for 2-D and cm^3 for 3-D problems) associated with cell i.
`C00000001VSI`	I($4, -N_9^{\mathrm{GC}} : N_8^{\mathrm{GC}}$)		array $\mathrm{VSI}_{k,j,i}^{\mathrm{GC}}$ containing the location of a geometrical surface and region j position (j is negative for surfaces and positive for regions) in cell i.
`C00000001RID`	I(N_8^{GC})		array $\mathrm{RID}_{j,i}^{\mathrm{GC}}$ containing the final region number associated with a geometrical region position in cell i.
`C00000001SID`	I(N_9^{GC})		array $\mathrm{SID}_{j,i}^{\mathrm{GC}}$ containing the final surface number associated with a geometrical surface position in cell i.
`C00000001PNT`	I($3, N_{18}^{\mathrm{GC}}$)		array $\mathrm{PC}_{k,j,i}^{\mathrm{GC}}$ containing the pin content of cell i.
`C00000001PIN`	D($-1 : 4, N_{18}^{\mathrm{GC}}$)		array $\mathrm{p}_{k,j,i}^{\mathrm{GC}}$ containing the location of the pins in cell i.

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

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

with i, the cell number and `NAMEXT` the record extention name (for example `NAMEXT=STA` for the cell dimensioning array N_i^{GC}).

The cell dimensioning array N_i^{GC} for each cell geometry contains the following information:

- $N_{1,i}^{\mathrm{GC}}$ contains the cell geometry type (see the definition of $\mathcal{S}_1^G$ in Section 5.1)
- $N_{2,i}^{\mathrm{GC}}$ contains the dimensions of the radial mesh array.
- $N_{3,i}^{\mathrm{GC}}$ contains the dimensions of the x directed mesh array.
- $N_{4,i}^{\mathrm{GC}}$ contains the dimensions of the y directed mesh array.
- $N_{5,i}^{\mathrm{GC}}$ contains the dimensions of the z directed mesh array.
- $N_{6,i}^{\mathrm{GC}}$ contains the dimensions of the mixture record.
- $N_{7,i}^{\mathrm{GC}}$ contains the geometry level (1 for cell).
- $N_{8,i}^{\mathrm{GC}}$ contains the number of regions in the cell before symmetry considerations.
- $N_{9,i}^{\mathrm{GC}}$ contains the number of surfaces in the cell before symmetry considerations.
- $N_{10,i}^{\mathrm{GC}}$ contains the number of regions in the cell after symmetry considerations.
- $N_{11,i}^{\mathrm{GC}}$ contains the number of surfaces in the cell after symmetry considerations.
- $N_{12,i}^{\mathrm{GC}}$ contains the first region number associated with this cell.
- $N_{13,i}^{\mathrm{GC}}$ contains the last region number associated with this cell.
- $N_{14,i}^{\mathrm{GC}}$ contains the first surface number associated with this cell.
- $N_{15,i}^{\mathrm{GC}}$ contains the last surface number associated with this cell.
- $N_{16,i}^{\mathrm{GC}}$ contains the number of pin cluster geometries in this cell.
- $N_{17,i}^{\mathrm{GC}}$ contains the first pin cluster geometry associated with this cell.
- $N_{18,i}^{\mathrm{GC}}$ contains the total number of pins in this cell.
- $N_{19,i}^{\mathrm{GC}}$ contains the number of times this cell is used in the global cell.

while the remaining elements are not used. The array $x_{j,i}^{\mathrm{GC}}$ contains the following information:

- $x_{-1,i}^{\mathrm{GC}}$ 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:

  $$x_{c,i} = \frac{x_{n_i^x,i}^{\mathrm{Gc}} + x_{0,i}^{\mathrm{GC}}}{2}$$

  where we have used $n_i^x = N_{3,i}^{\mathrm{GC}}$.
- $x_{j-1,i}^{\mathrm{GC}} \leq x \leq x_{j,i}^{\mathrm{GC}}$ gives the position in x of mesh element j with $j = 1, n_i^x$.

The array $y_{j,i}^{\mathrm{GC}}$ contains the following information:

- $y^{\text{GC}}_{-1,i}$ 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:

$$y_{c,i} = \frac{y^{\text{GC}}_{n^y_i,i} + y^{\text{GC}}_{0,i}}{2}$$

  where we have used $n^y_i = N^{\text{GC}}_{4,i}$.

- $y^{\text{GC}}_{j-1,i} \leq y \leq y^{\text{GC}}_{j,i}$ gives the position in y of mesh element j with $j = 1, n^y_i$.

The array $z^{\text{GC}}_{j,i}$ contains the following information:

- $z^{\text{GC}}_{-1,i}$ 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:

$$z_{c,i} = \frac{z^{\text{GC}}_{n^z_i,i} + z^{\text{GC}}_{0,i}}{2}$$

  where we have used $n^z_i = N^{\text{GC}}_{5,i}$.

- $z^{\text{GC}}_{j-1,i} \leq z \leq z^{\text{GC}}_{j,i}$ gives the position in z of mesh element j with $j = 1, n^z_i$.

The array $r^{\text{GC}}_{j,i}$ contains the following information:

- $r^{\text{GC}}_{-1,i} = r^{\text{GC}}_{0,i} = 0$.

- $r^{\text{GC}}_{j-1,i} \leq r \leq r^{\text{GC}}_{j,i}$ describes the position in r of mesh element j with $j = 1, N^{\text{GC}}_{2,i}$.

The array $p^{\text{GC}}_{j,i}$ contains the following information:

- $p^{\text{GC}}_{-1,i}$ is the angular position of z, x or y directed pin with respect to the x, y or z axis.

- $p^{\text{GC}}_{0,i}$ 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.

- $p^{\text{GC}}_{1,i}$ is the height of a x directed pin.

- $p^{\text{GC}}_{2,i}$ is the height of a y directed pin.

- $p^{\text{GC}}_{3,i}$ is the height of a z directed pin.

- $p^{\text{GC}}_{4,i}$ is the outer radius of the pin.

The cells may also contain pin clusters geometry that overlap the cell. For pin $i = 1$ the following records will be available on the `/NXTRecords/` directory.

Table 19: Pin $i = 1$ records in `/NXTRecords/`

Name	Type	Units	Comment
`P00000001DIM`	I(40)		array $N^{\text{GP}}_{j,i}$ containing the dimensioning information required to rebuilt pin i.

continued on next page

Pin $i = 1$ records in `/NXTRecords/` continued from last page

Name	Type	Units	Comment
`P00000001SMR`	D(N_2^{GP})	cm	array $r_{j,i}^{\text{GP}}$ containing the radial mesh description for pin i.
`P00000001SMX`	D(N_3^{GP})	cm	array $x_{j,i}^{\text{GP}}$ containing X directed mesh description for pin i.
`P00000001SMY`	D(N_4^{GP})	cm	array $y_{j,i}^{\text{GP}}$ containing Y directed mesh description for pin i.
`P00000001SMZ`	D(N_5^{GP})	cm	array $z_{j,i}^{\text{GP}}$ containing Z directed mesh description for pin i.
`P00000001MIX`	I(N_6^{GP})		array $M_{j,i}^{\text{GP}}$ containing the mixture associated with each region j in pin i.
`P00000001VSE`	D($-N_9^{\text{GP}} : N_8^{\text{GP}}$)		array $\text{SV}_{j,i}^{\text{GP}}$ containing surface area j ($\text{SV}_{-j,i}^{\text{GP}} = S_j^{\text{GP}}$ in cm for 2-D and cm^2 for 3-D problems) and regional volumes j ($\text{SV}_{j,i}^{\text{GP}} = V_{j,i}^{\text{GP}}$ cm^2 for 2-D and cm^3 for 3-D problems) associated with pin i.
`P00000001VSI`	I($4, -N_9^{\text{GP}} : N_8^{\text{GP}}$)		array $\text{VSI}_{k,j,i}^{\text{GP}}$ containing the location of a geometrical surface and region j position (j is negative for surfaces and positive for regions) in pin i.
`P00000001RID`	I(N_8^{GP})		array $\text{RID}_{j,i}^{\text{GP}}$ containing the final region number associated with a geometrical region position in pin i.
`P00000001SID`	I(N_9^{GP})		array $\text{SID}_{j,i}^{\text{GP}}$ containing the final surface number associated with a geometrical surface position in pin i.

Here the record names are built using a procedure similar to that described above for the cell, namely:

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

with i, the pin number and `NAMEXT` the record extention name (for example `NAMEXT=STA` for the pin dimensioning array N_i^{GP}).

The pin dimensioning array N_i^{GP} for each contains the following information:

- $N_{1,i}^{\text{GP}}$ contains the pin geometry type (see the definition of $\mathcal{S}_1^G$ in Section 5.1)
- $N_{2,i}^{\text{GP}}$ contains the dimensions of the radial mesh array.
- $N_{3,i}^{\text{GP}}$ contains the dimensions of the x directed mesh array.
- $N_{4,i}^{\text{GP}}$ contains the dimensions of the y directed mesh array.
- $N_{5,i}^{\text{GP}}$ contains the dimensions of the z directed mesh array.
- $N_{6,i}^{\text{GP}}$ contains the dimensions of the mixture record.
- $N_{7,i}^{\text{GP}}$ contains the geometry level (2 for pins).
- $N_{8,i}^{\text{GP}}$ contains the number of regions in the pin before symmetry considerations.
- $N_{9,i}^{\text{GP}}$ contains the number of surfaces in the pin before symmetry considerations.

- $N^{\text{GP}}_{10,i}$ contains the number of regions in the pin after symmetry considerations.
- $N^{\text{GP}}_{11,i}$ contains the number of surfaces in the pin after symmetry considerations.
- $N^{\text{GP}}_{12,i}$ contains the first region number associated with this pin cluster.
- $N^{\text{GP}}_{13,i}$ contains the last region number associated with this pin cluster.
- $N^{\text{GP}}_{14,i}$ contains the first surface number associated with this pin cluster.
- $N^{\text{GP}}_{15,i}$ contains the last surface number associated with this pin cluster.
- $N^{\text{GP}}_{16,i}$ contains the first pin cluster geometry associated with this pin cluster.
- $N^{\text{GP}}_{17,i}$ contains the total number of pins associated with this pin cluster.

while the remaining elements are not used. The array $x^{\text{GP}}_{j,i}$ contains the following information:

- $x^{\text{GP}}_{-1,i}$ 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:

  $$x_{c,i} = \frac{x^{\text{GP}}_{n^x_i,i} + x^{\text{GP}}_{0,i}}{2}$$

  where we have used $n^x_i = N^{\text{GP}}_{3,i}$.
- $x^{\text{GP}}_{j-1,i} \leq x \leq x^{\text{GP}}_{j,i}$ gives the position in x of mesh element j with $j = 1, n^x_i$.

The array $y^{\text{GP}}_{j,i}$ contains the following information:

- $y^{\text{GP}}_{-1,i}$ 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:

  $$y_{c,i} = \frac{y^{\text{GP}}_{n^y_i,i} + y^{\text{GP}}_{0,i}}{2}$$

  where we have used $n^y_i = N^{\text{GP}}_{4,i}$.
- $y^{\text{GP}}_{j-1,i} \leq y \leq y^{\text{GP}}_{j,i}$ gives the position in y of mesh element j with $j = 1, n^y_i$.

The array $z^{\text{GP}}_{j,i}$ contains the following information:

- $z^{\text{GP}}_{-1,i}$ 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:

  $$z_{c,i} = \frac{z^{\text{GP}}_{n^z_i,i} + z^{\text{GP}}_{0,i}}{2}$$

  where we have used $n^z_i = N^{\text{GP}}_{5,i}$.
- $z^{\text{GP}}_{j-1,i} \leq z \leq z^{\text{GP}}_{j,i}$ gives the position in z of mesh element j with $j = 1, n^z_i$.

The array $r^{\text{GP}}_{j,i}$ contains the following information:

- $r^{\text{GP}}_{-1,i} = r^{\text{GP}}_{0,i} = 0$.
- $r^{\text{GP}}_{j-1,i} \leq r \leq r^{\text{GP}}_{j,i}$ describes the position in r of mesh element j with $j = 1, N^{\text{GP}}_{2,i}$.

Finally the `/NXTRecords/` directory also contains records associated with global identification of the surfaces and volumes.

Table 20: Global geometry records in `/NXTRecords/`

Name	Type	Units	Comment
`TrackingDnsA`	D($\mathcal{S}^t_{20}$)	cm	array D_i containing the track spacing for direction i.
`TrackingDirc`	D($N^{\text{GG}}_1, \mathcal{S}^t_{20}$)		array $\alpha_{j,i}$ containing the director cosine for axis j in direction i.
`TrackingOrig`	D($N^{\text{GG}}_1, N_p, \mathcal{S}^t_{20}$)	cm	array $L_{k,j,i}$ containing the origin in space ($k = 1, N^{\text{GG}}_1$) and the direction of the normal plan for each plane j with direction i.
`TrackingWgtD`	D($\mathcal{S}^t_{20}$)		array W_i containing the integration weight for each track direction i.
`VTNormalize␣`	D(N^{GG}_{22})		array R_i containing the ratio of the analytical and numerical volume for region i.
`VTNormalizeD`	D($N^{\text{GG}}_{22}, \mathcal{S}^t_{20}$)		array R_i containing the ratio of the analytical and numerical volume for region i for each track direction. Valid only if $\mathcal{S}^t_8 = -1$.
`KEYMRG␣␣␣␣␣␣`	I($-N^{\text{GG}}_{23}, N^{\text{GG}}_{22}$)		array MRG$_i$ containing the global merging index.
`MATALB␣␣␣␣␣␣`	I($-N^{\text{GG}}_{23}, N^{\text{GG}}_{22}$)		array containing the albedo number associated with each surface and the mixture number associated with each region.
`SAreaRvolume`	D($-N^{\text{GG}}_{23}, N^{\text{GG}}_{22}$)		array containing the area (S_α in cm for 2-D and cm^2 for 3-D problems) and regional (V_i cm^2 for 2-D and cm^3 for 3-D problems) of each surface and region associated with this.

6.3 The `SYBIL` records and sub-directories

When the `SYBIL` module is used ($\mathcal{M} = 2$), the following elements in the vector $\mathcal{S}^t_i$ are also defined:

- $\mathcal{S}^t_7$ is the main SYBIL model where:

$$\mathcal{S}^t_7 = \begin{cases} 2 & \text{pure geometry;} \\ 3 & \text{do-it-yourself geometry;} \\ 4 & \text{2–D assembly geometry;} \\ 10 & \text{double heterogeneity geometry.} \end{cases}$$

- $\mathcal{S}^t_8$ is the minimum space required to store tracks for assembly geometry.
- $\mathcal{S}^t_9$ is the minimum space required to store interface currents for assembly geometry.

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

Table 21: The `SYBIL` records and directories

Name	Type	Condition	Units	Comment
`PURE-GEOM␣␣␣`	Dir	$\mathcal{S}_7^t = 2$		directory containing the data related to a pure geometry.
`DOITYOURSELF`	Dir	$\mathcal{S}_7^t = 3$		directory containing the data related to a do-it-yourself geometry.
`EURYDICE␣␣␣␣`	Dir	$\mathcal{S}_7^t = 4$		directory containing the data related to an assembly geometry.
`BIHET␣␣␣␣␣␣␣`	Dir	$\mathcal{S}_7^t = 10$		directory containing the data related to a double heterogeneity geometry.

where the directories `/PURE-GEOM/`, `/DOITYOURSELF/`, `/EURYDICE/` and `/BIHET/` contain respectively:

Table 22: The contents of the `SYBILT: /PURE-GEOM/` directory

Name	Type	Units	Comment
`PARAM␣␣␣␣␣␣␣`	I(6)		array $\mathcal{P}_i$ containing the parameters for a SYBIL tracking on a pure geometry.
`XXX␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_4 + 1$)	cm	array containing the 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($\mathcal{P}_5 + 1$)	cm	array containing the Y directed mesh coordinates after mesh splitting for type 5, 6 and 7 geometries.
`ZZZ␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_6 + 1$)	cm	array containing the Z directed mesh coordinates after mesh splitting for type 7 and 9 geometries.
`SIDE␣␣␣␣␣␣␣␣`	R(1)	cm	parameter containing de dimensions of one side of a hexagon for type 8 and 9 geometries.
`NCODE␣␣␣␣␣␣␣`	I(6)		array containing the types of boundary conditions on each surface $N_{\beta,j}$.
`ZCODE␣␣␣␣␣␣␣`	R(6)		arrau containing the albedo value on each surface.

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

- $\mathcal{P}_1$ is the type of geometry where:

$$\mathcal{P}_1 = \begin{cases} 2 & \text{indicates a Cartesian 1–D geometry;} \\ 3 & \text{indicates a tube 1–D geometry;} \\ 5 & \text{indicates a Cartesian 2–D geometry;} \\ 6 & \text{indicates a tube 2–D geometry;} \\ 7 & \text{indicates a Cartesian 3–D geometry;} \\ 8 & \text{indicates a hexagonal 2–D geometry;} \\ 9 & \text{indicates a hexagonal 3–D geometry.} \end{cases}$$

- $\mathcal{P}_2$ is the type of hexagonal symmetry where:

$$\mathcal{P}_2 = \begin{cases} 1 & \text{for an assembly with a } \texttt{S30} \text{ symmetry;} \\ 2 & \text{for an assembly with a } \texttt{SA60} \text{ symmetry;} \\ 3 & \text{for an assembly with a } \texttt{SB60} \text{ symmetry;} \\ 4 & \text{for an assembly with a } \texttt{S90} \text{ symmetry;} \\ 5 & \text{for an assembly with a } \texttt{R120} \text{ symmetry;} \\ 6 & \text{for an assembly with a } \texttt{R180} \text{ symmetry;} \\ 7 & \text{for an assembly with a } \texttt{SA180} \text{ symmetry;} \\ 8 & \text{for an assembly with a } \texttt{SB180} \text{ symmetry;} \\ 9 & \text{for an assembly without symmetry (} \texttt{COMPLETE}\text{).} \end{cases}$$

- $\mathcal{P}_3$ is the quadrature parameter.
- $\mathcal{P}_4$ is the number of X directed or radial mesh intervals in the geometry.
- $\mathcal{P}_5$ is the number of Y directed mesh intervals in the geometry.
- $\mathcal{P}_6$ is the number of Z directed mesh intervals in the geometry.

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

$$N_{\beta,j} = \begin{cases} 0 & \text{not used;} \\ 1 & \text{void boundary condition;} \\ 2 & \text{reflection boundary condition;} \\ 3 & \text{diagonal reflection boundary condition;} \\ 4 & \text{periodic (translation) boundary condition;} \\ 5 & \text{symmetric reflection boundary condition;} \\ 6 & \text{albedo boundary condition.} \end{cases}$$

Table 23: The contents of the `SYBILT: /DOITYOURSELF/` directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣␣`	I(3)			array $\mathcal{P}_i$ containing the parameters for a SYBIL tracking on a do-it-yourself geometrY.
`NMC␣␣␣␣␣␣␣␣␣␣`	I(M)			array containing the offset of the first region in each cell.
`RAYRE␣␣␣␣␣␣␣␣`	R(N, M)		cm	array containing the radius of the tubes in each cell.
`PROCEL␣␣␣␣␣␣␣`	R(M, M)			array containing the geometric matrix.
`POURCE␣␣␣␣␣␣␣`	R(M)			array containing the weight assign to each cell.
`SURFA␣␣␣␣␣␣␣␣`	R(M)		cm^2	array containing the surface of each cell .

with the array $\mathcal{P}_i$ containing:

- $\mathcal{P}_1 = M - 1$ is the number of cell.
- $\mathcal{P}_2$ is the quadrature parameter.
- $\mathcal{P}_3$ is the statistical option.
- $\mathcal{P}_4 = N$ is the maximum number of region per cell.

Table 24: The contents of the `SYBILT: /EURYDICE/` directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣␣`	I(15)			array $\mathcal{P}_i$ containing the parameters for a SYBIL tracking on an assembly geometry.
`XX␣␣␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_6$)		cm	array containing the X thickness of the generating cells.
`YY␣␣␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_6$)		cm	array containing the Y thickness of the generating cells.
`NMC␣␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_6$)			array containing the offset of the first region in each generating cell.
`RAYRE␣␣␣␣␣␣␣␣`	R(M)		cm	array containing the radius of the tubes in each generating cell.
`MAIL␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_6$)			array containing the offset of the first tracking information in each generating cell.
`ZMAILI␣␣␣␣␣␣␣`	I($\mathcal{P}_{15}$)			array containing the integer tracking information.
`ZMAILR␣␣␣␣␣␣␣`	R($\mathcal{P}_{15}$)		cm	array containing the tracking length.
`IFR␣␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_4, \mathcal{P}_{14}$)			array containing the index numbers of incoming currents.
`ALB␣␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_4, \mathcal{P}_{14}$)			array containing the albedo or transmission factors corresponding to incoming currents.
`INUM␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_4$)			array containing the index number of the merge cell associated to each cell of the assembly.

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The contents of the `SYBILT: /EURYDICE/` directory continued from last page

Name	Type	Condition	Units	Comment
`MIX␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_5, \mathcal{P}_{14}$)			array containing the index numbers of outgoing currents.
`DVX␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_5, \mathcal{P}_{14}$)			array containing the weights corresponding to outgoing currents.
`IGEN␣␣␣␣␣␣␣␣`	I($\mathcal{P}_5$)			array containing the index number of the generating cell associated to each merged cell.

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

- $\mathcal{P}_1$ is the type of hexagonal symmetry where:

$$\mathcal{P}_2 = \begin{cases} 1 & \text{for an assembly with a } \texttt{S30} \text{ symmetry;} \\ 2 & \text{for an assembly with a } \texttt{SA60} \text{ symmetry;} \\ 3 & \text{for an assembly with a } \texttt{SB60} \text{ symmetry;} \\ 4 & \text{for an assembly with a } \texttt{S90} \text{ symmetry;} \\ 5 & \text{for an assembly with a } \texttt{R120} \text{ symmetry;} \\ 6 & \text{for an assembly with a } \texttt{R180} \text{ symmetry;} \\ 7 & \text{for an assembly with a } \texttt{SA180} \text{ symmetry;} \\ 8 & \text{for an assembly with a } \texttt{SB180} \text{ symmetry;} \\ 9 & \text{for an assembly without symmetry (} \texttt{COMPLETE} \text{).} \end{cases}$$

- $\mathcal{P}_2$ is the type of multicell approximation.
- $\mathcal{P}_3$ is the type of cylindrization.
- $\mathcal{P}_4$ is the total number of cells.
- $\mathcal{P}_5$ is the number of merged cells.
- $\mathcal{P}_6$ is the number of generating cells.
- $\mathcal{P}_7$ is the number of distinct interface currents.
- $\mathcal{P}_8$ is the number of angles for 2–D quadrature.
- $\mathcal{P}_9$ is the number of segments for 2–D quadrature.
- $\mathcal{P}_{10}$ is the number of segments for homogeneous 2–D cells.
- $\mathcal{P}_{11}$ is the number of segments for 1–D cells.
- $\mathcal{P}_{12}$ is the track normalization option where:

$$\mathcal{P}_{12} = \begin{cases} 0 & \text{indicates that the tracks are normalized;} \\ 1 & \text{indicates that the tracks are not ormalized.} \end{cases}$$

- $\mathcal{P}_{13}$ is the type of quadrature in angle and space where:

$$\mathcal{P}_{13} = \begin{cases} 0 & \text{indicates a Gauss quadrature;} \\ 1 & \text{indicates a trapezoidal quadrature.} \end{cases}$$

- $\mathcal{P}_{14}$ is the number of outgoing interface currents per cell.
- $\mathcal{P}_{15}$ is the number of array elements in the tracking arrays.

Table 25: The contents of the `SYBILT: /BIHET/` directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣␣`	I(8)			array $\mathcal{P}_i$ containing the parameters for a SYBIL tracking on a double heterogeneity geometry $\mathcal{P}_i$.
`NS␣␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_4$)			array containing the number of tubes or shells in each kind of micro structure.
`IBI␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_3$)			array containing the type of mixture in each generating region of the macro geometry.
`RS␣␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_4, M$)		cm	array containing the radii of the micro regions.
`FRACT␣␣␣␣␣␣␣`	R($\mathcal{P}_4, \mathcal{P}_2$)			array containing the volume fraction of each type of micro region in each composite mixture.
`VOLK␣␣␣␣␣␣␣␣`	R($\mathcal{P}_4, \mathcal{P}_5$)			array containing the volume fractions of the tubes or shells in the micro regions.

where $\mathcal{P}_i$ contains:

- $\mathcal{P}_1$ is the number of ordinary mixtures pointing to the MACROLIB.
- $\mathcal{P}_2$ is the number of mixtures, including the composite mixtures (i.e., containing micro structures).
- $\mathcal{P}_3$ is the number of regions in the macro geometry,
- $\mathcal{P}_1$ is the number of different kinds of macro structures. 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.
- $\mathcal{P}_5 = M - 1$ is the maximum number of regions (tubes or shells) in each kind of macro structure.
- $\mathcal{P}_6$ is the main SYBIL model for the macro geometry.
- $\mathcal{P}_7$ is the type of micro regions where:

$$\mathcal{P}_7 = \begin{cases} 3 & \text{indicates a cylinder;} \\ 4 & \text{indicates a sphere.} \end{cases}$$

- $\mathcal{P}_8$ is the quadrature parameter for the 1–D collision probability calculation in the micro structures.

6.4 The `JPMT:` records and sub-directories

When the `JPMT:` module is used ($\mathcal{M} = 3$), the following elements in the array $\mathcal{S}_i^t$ will also defined:

- $\mathcal{S}_7^t$ is the main JPM model where:

$$\mathcal{S}_7^t = \begin{cases} 2 & \text{pure geometry;} \\ 3 & \text{do-it-yourself geometry;} \\ 4 & \text{2–D assembly geometry;} \\ 5 & \text{2–D cluster geometry;} \\ 10 & \text{double heterogeneity geometry.} \end{cases}$$

- $\mathcal{S}_8^t$ is the minimum space required to store tracks for assembly geometry.
- $\mathcal{S}_9^t$ is the minimum space required to store interface currents for assembly geometry.
- $\mathcal{S}_{10}^t$ is the flag to specify if the individual cell collision probability must all be recomputed even if the properties of specific cells have not been modified. Here:

$$\mathcal{S}_{10}^t = \begin{cases} 0 & \text{always re-compute all blocks probabilities;} \\ 1 & \text{re-compute probabilities only for modified blocks.} \end{cases}$$

- $\mathcal{S}_{11}^t$ is the total number of blocks in the domain.
- $\mathcal{S}_{12}^t$ is the total number of generating blocks.
- $\mathcal{S}_{13}^t$ is the total number of distinct outgoing currents.
- $\mathcal{S}_{14}^t$ is the total number of incoming currents.
- $\mathcal{S}_{15}^t$ is the total number of outgoing currents,
- $\mathcal{S}_{16}^t$ is the dimension of PSS vector.
- $\mathcal{S}_{17}^t$ is the dimension of ICM vector.

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

Table 26: The `JPM` records and sub-directories

Name	Type	Condition	Units	Comment
`IFR␣␣␣␣␣␣␣␣␣`	I($\mathcal{S}_{14}^t$)			array containing the index numbers of incoming currents.
`ALB␣␣␣␣␣␣␣␣␣`	R($\mathcal{S}_{14}^t$)			array containing the albedo or transmission factors corresponding to incoming currents.
`INUM␣␣␣␣␣␣␣␣`	I($\mathcal{S}_{11}^t$)			array containing the index number of the merge cell associated to each cell of the assembly.
`MIX␣␣␣␣␣␣␣␣␣`	I($\mathcal{S}_{15}^t$)			array containing the index numbers of outgoing currents.
`DVX␣␣␣␣␣␣␣␣␣`	R($\mathcal{S}_{15}^t$)			array containing the weights corresponding to outgoing currents.

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The JPM records and sub-directories continued from last page

Name	Type	Condition	Units	Comment
IGEN$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	I($\mathcal{S}^t_{11}$)			array containing the index number of the generating cell associated to each merged block.
ISURF$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	I($\mathcal{S}^t_{12}$)			array containing the number of surfaces associated with a generating block.
CHORD$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R($\mathcal{S}^t_{4}$)			array containing the mean chord length associated with each block.
MU1$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	I($\mathcal{S}^t_{13}$)			array containing the position of diagonal element in compress response matrix.
IMA$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	I($\mathcal{S}^t_{13}$)			array containing the position of first non zero element in compress response matrix.
/PURE-GEOM/	Dir	$\mathcal{S}^t_7 = 2$		directory containing the data related to a pure geometry.
/DOITYOURSELF/	Dir	$\mathcal{S}^t_7 = 3$		directory containing the data related to a do-it-yourself geometry.
/EURYDICE/	Dir	$\mathcal{S}^t_7 = 4$		directory containing the data related to an assembly geometry.
/CLUSTER/	Dir	$\mathcal{S}^t_7 = 5$		directory containing the data related to a cluster geometry.
/BIHET/	Dir	$\mathcal{S}^t_7 = 10$		directory containing the data related to a double heterogeneity geometry.

where the directories /PURE-GEOM/, /DOITYOURSELF/, /EURYDICE/, /BIHET/ and /CLUSTER/ contain respectively:

Table 27: The contents of the JPMT: /PURE-GEOM/ directory

Name	Type	Condition	Units	Comment
PARAM$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	I(6)			array $\mathcal{P}_i$ containing the containing the parameters for a JPM tracking on a pure geometry.
XX$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R($\mathcal{P}_5$)		cm	array containing the 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.
YY$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R($\mathcal{P}_5$)		cm	array containing the Y directed mesh coordinates after mesh splitting for type 5, 6 and 7 geometries.
ZZ$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R($\mathcal{P}_5$)		cm	array containing the Z directed mesh coordinates after mesh splitting for type 7 and 9 geometries.

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

- $\mathcal{P}_1$ is the type of geometry where:

$$\mathcal{P}_1 = \begin{cases} 2 & \text{indicates a Cartesian 1–D geometry;} \\ 3 & \text{indicates a tube 1–D geometry;} \\ 5 & \text{indicates a Cartesian 2–D geometry;} \\ 6 & \text{indicates a tube 2–D geometry;} \\ 7 & \text{indicates a Cartesian 3–D geometry;} \\ 8 & \text{indicates a hexagonal 2–D geometry;} \\ 9 & \text{indicates a hexagonal 3–D geometry.} \end{cases}$$

- $\mathcal{P}_2$ is the type of hexagonal symmetry where:

$$\mathcal{P}_2 = \begin{cases} 1 & \text{for an assembly with a } \texttt{S30} \text{ symmetry;} \\ 2 & \text{for an assembly with a } \texttt{SA60} \text{ symmetry;} \\ 3 & \text{for an assembly with a } \texttt{SB60} \text{ symmetry;} \\ 4 & \text{for an assembly with a } \texttt{S90} \text{ symmetry;} \\ 5 & \text{for an assembly with a } \texttt{R120} \text{ symmetry;} \\ 6 & \text{for an assembly with a } \texttt{R180} \text{ symmetry;} \\ 7 & \text{for an assembly with a } \texttt{SA180} \text{ symmetry;} \\ 8 & \text{for an assembly with a } \texttt{SB180} \text{ symmetry;} \\ 9 & \text{for an assembly without symmetry (} \texttt{COMPLETE}\text{).} \end{cases}$$

- $\mathcal{P}_3$ is the type of IC approximation between the blocks where:

$$\mathcal{P}_3 = \begin{cases} 1 & \text{use the } DP_0 \text{ approximation for all surfaces;} \\ 2 & \text{use the } DP_1 \text{ approximation for all surfaces;} \\ 3 & \text{use the } DP_1 \text{ approximation for inner and } DP_0 \text{ approximation for outer surfaces.} \end{cases}$$

- $\mathcal{P}_4$ is the quadrature parameter.
- $\mathcal{P}_5$ number of mesh intervals in the geometry.

Table 28: The contents of the `JPMT: /DOITYOURSELF/` directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣␣`	I(5)			array $\mathcal{P}_i$ containing the containing the parameters for a JPM tracking on a do-it-yourself geometry.
`NMC␣␣␣␣␣␣␣␣␣␣`	I(M)			array containing the offset of the first region in each cell.
`RAYRE␣␣␣␣␣␣␣␣`	R(N, M)		cm	array containing the radius of the tubes in each cell.
`PROCEL␣␣␣␣␣␣␣`	R(M, M)			array containing the geometric matrix.

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

- $\mathcal{P}_1$ is the number of cell.
- $\mathcal{P}_2$ is the type of IC approximation between the blocks where:

$$\mathcal{P}_2 = \begin{cases} 1 & \text{use the } DP_0 \text{ approximation for all surfaces;} \\ 2 & \text{use the } DP_1 \text{ approximation for all surfaces;} \\ 3 & \text{use the } DP_1 \text{ approximation for inner and } DP_0 \text{ approximation for outer surfaces.} \end{cases}$$

- $\mathcal{P}_3$ is the quadrature parameter.
- $\mathcal{P}_4$ is the statistical option.
- $\mathcal{P}_5 = N$ is the maximum number of region per cell.

Table 29: The contents of the `JPMT: /EURYDICE/` directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣␣`	I(11)			array $\mathcal{P}_i$ containing the parameters for a JPM tracking on an assembly geometry.
`ITGEN␣␣␣␣␣␣␣␣`	I(M)			array containing the type of generating block.
`COORD␣␣␣␣␣␣␣␣`	R($3, M$)		cm	array containing the dimensions of the generating blocks.
`MAIL␣␣␣␣␣␣␣␣␣`	I(M)			array containing the offset of the first tracking information in each generating cell.
`ZMAILI␣␣␣␣␣␣␣`	I($\mathcal{P}_{10}$)			array containing the integer tracking information.
`ZMAILR␣␣␣␣␣␣␣`	R($\mathcal{P}_{10}$)		cm	array containing the tracking length.

with $\mathcal{P}_i$ containing:

- $\mathcal{P}_1$ is the type of multicell approximation.
- $\mathcal{P}_2$ is the type of cylindrization.
- $\mathcal{P}_3$ is the type of IC approximation between the blocks where:

$$\mathcal{P}_3 = \begin{cases} 1 & \text{use the } DP_0 \text{ approximation for all surfaces;} \\ 2 & \text{use the } DP_1 \text{ approximation for all surfaces;} \\ 3 & \text{use the } DP_1 \text{ approximation for inner and } DP_0 \text{ approximation for outer surfaces.} \end{cases}$$

- $\mathcal{P}_4$ is the number of angles for 2–D quadrature.
- $\mathcal{P}_5$ is the number of segments for 2–D quadrature.
- $\mathcal{P}_6$ is the number of segments for homogeneous 2–D cells.
- $\mathcal{P}_7$ is the number of segments for 1–D cells.

- $\mathcal{P}_8$ is the track normalization option where:

$$\mathcal{P}_8 = \begin{cases} 0 & \text{indicates that the tracks are normalized;} \\ 1 & \text{indicates that the tracks are not ormalized.} \end{cases}$$

- $\mathcal{P}_9$ is the type of quadrature in angle and space.

$$\mathcal{P}_9 = \begin{cases} 0 & \text{indicates a Gauss quadrature;} \\ 1 & \text{indicates a trapezoidal quadrature.} \end{cases}$$

- $\mathcal{P}_{10}$ is the number of array elements in the tracking arrays.
- $\mathcal{P}_{11} = M$ is the number of cell elements.

Table 30: The contents of the `JPMT: /CLUSTER/` directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣`	I(11)			array $\mathcal{P}_i$ containing the parameters for a JPM tracking on a cluster geometry.
`YSIDE␣␣␣␣␣␣␣`	R(1)		cm	array containing the Y directed side of a Cartesian geometry.
`NRINFO␣␣␣␣␣␣`	I($2, \mathcal{P}_6$)			array containing the rod location information.
`RAN␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_6$)		cm	array containing the radii of the annular regions.
`NRODS␣␣␣␣␣␣␣`	I($\mathcal{P}_3, \mathcal{P}_1$)			array containing the rod information.
`ROD␣␣␣␣␣␣␣␣␣`	R($3, \mathcal{P}_7$)			array containing the rod location.
`RODR␣␣␣␣␣␣␣␣`	R($\mathcal{P}_8, \mathcal{P}_7$)		cm	array containing the rod radii.

where $\mathcal{P}_i$ contains:

- $\mathcal{P}_1$ is the type of IC approximation between the blocks where:

$$\mathcal{P}_1 = \begin{cases} 1 & \text{use the } DP_0 \text{ approximation for all surfaces;} \\ 2 & \text{use the } DP_1 \text{ approximation for all surfaces;} \\ 3 & \text{use the } DP_1 \text{ approximation for inner and } DP_0 \text{ approximation for outer surfaces.} \end{cases}$$

- $\mathcal{P}_2$ is the type of cluster reconstruction where:

$$\mathcal{P}_2 = \begin{cases} 1 & \text{use the direct approach;} \\ 2 & \text{use the surface splitting approach.} \end{cases}$$

- $\mathcal{P}_3$ is the number of 2–D quadrature angles.
- $\mathcal{P}_4$ is the number of 2–D integration segments.
- $\mathcal{P}_5$ is the number of 1–D quadrature segments.

- $\mathcal{P}_6$ is the number of annular regions.
- $\mathcal{P}_7$ is the number of rod types.
- $\mathcal{P}_8$ is the maximum number of subrods per rod.
- $\mathcal{P}_9$ is the total number of surfaces.
- $\mathcal{P}_{10}$ is the number of outer surfaces.
- $\mathcal{P}_{11}$ is the maximum track length.

Table 31: The contents of the `JPMT: /BIHET/` directory

Name	Type	Condition	Units	Comment
`PARAM␣␣␣␣␣␣␣`	I(9)			array containing the parameters for a JPM tracking on a double heterogeneity geometry $\mathcal{P}_i$.
`NS␣␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_3$)			array containing the number of tubes or shells in each kind of micro structure.
`IGI␣␣␣␣␣␣␣␣␣`	I($\mathcal{P}_2$)			array containing the type of mixture in each generating region of the macro geometry.
`RS␣␣␣␣␣␣␣␣␣␣`	R($\mathcal{P}_3, M$)		cm	array containing the radii of the micro regions.
`FRACT␣␣␣␣␣␣␣`	R($\mathcal{P}_3, \mathcal{P}_1$)			array containing the volume fraction of each type of micro region in each composite mixture.
`ISURF2␣␣␣␣␣␣`	I($\mathcal{P}_2$)			array containing the number of surfaces associated with a generating block.
`CHORD2␣␣␣␣␣␣`	R($\mathcal{P}_9$)			array containing the mean chord length associated with each block.

where $\mathcal{P}_i$ contains:

- $\mathcal{P}_1$ is the number of ordinary mixtures pointing to the MACROLIB.
- $\mathcal{P}_2$ is the number of regions in the macro geometry.
- $\mathcal{P}_3$ is the number of different kinds of macro structures. 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.
- $\mathcal{P}_4 = M - 1$ is the maximum number of regions (tubes or shells) in each kind of macro structure.
- $\mathcal{P}_5$ is the main JPM model for the macro geometry.
- $\mathcal{P}_6$ is the type of micro regions where

$$\mathcal{P}_6 = \begin{cases} 3 & \text{for cylinder;} \\ 4 & \text{for sphere.} \end{cases}$$

- $\mathcal{P}_7$ is the quadrature parameter for the 1–D collision probability calculation in the micro structures.

- $\mathcal{P}_8$ is the type of IC approximation between the blocks where:

$$\mathcal{P}_8 = \begin{cases} 1 & \text{use the } DP_0 \text{ approximation for all surfaces;} \\ 2 & \text{use the } DP_1 \text{ approximation for all surfaces;} \\ 3 & \text{use the } DP_1 \text{ approximation for inner and } DP_0 \text{ approximation for outer surfaces.} \end{cases}$$

- $\mathcal{P}_9$ is the total number of surfaces.

7 CONTENTS OF A /ASMPIJ/ DIRECTORY

This directory contains the multigroup collision probability and response matrices required for the solution of the transport equation.

7.1 The main directory

The following records and sub-directories will be found in the /ASMPIJ/ directory:

Table 32: Main records and sub-directories in /ASMPIJ/

Name	Type	Condition	Units	Comment
`SIGNATURE␣␣␣`	C∗12			parameter SIGNA containing the signature of the data structure.
`STATE-VECTOR`	I(40)			array $\mathcal{S}_i^a$ containing various parameters that are required to describe this data structure.
{*/GRPDIR/*}	Dir			list of sub-directories that contain the collision probability and response matrices associated with each energy group g.

The signature variable for this data structure must be SIGNA=`L_PIJ␣␣␣␣␣␣␣␣`. The array $\mathcal{S}_i^a$ contains the following information:

- $\mathcal{S}_1^a = I_P$ contains the option to indicate the type of system matrix to be stored. It can be an isotropic collision probability a directional collision probability or a response matrix. Here I_P can take the following values:

$$I_P = \begin{cases} -1 & \text{the system responses matrices will be stored;} \\ 0 & \text{only isotropic collision probability matrices will be stored;} \\ 1 & \text{isotropic and directional collision probability matrices will be stored.} \end{cases}$$

- $\mathcal{S}_2^a = I_S$ contains the type of collision probabilities considered where:

$$I_S = \begin{cases} 0 & \text{scattering reduced collision probability or response matrix;} \\ 1 & \text{direct collision probability or response matrix.} \end{cases}$$

- $\mathcal{S}_3^a = I_R$ contains the residual system matrix flag where:

$$I_R = \begin{cases} 0 & \text{residual system matrix is present;} \\ 1 & \text{residual system matrix is not saved.} \end{cases}$$

- $\mathcal{S}_4^a = I_C$ contains the type of collision probability closure relation used where:

$$I_C = \begin{cases} -1 & \text{no closure relation used on cell with leakage;} \\ 0 & \text{no closure relation used on cell without leakage;} \\ 1 & \text{total reflection closure relation;} \\ 2 & \text{Selengut closure relation.} \end{cases}$$

- $\mathcal{S}_5^a = I_N$ contains the type of collision probability normalization method used. Here I_N can take the following values:

$$I_N = \begin{cases} -1 & \text{no normalization;} \\ 0 & \text{HELIOS type normalization;} \\ 1 & \text{Gelbard normalization algorithm;} \\ 2 & \text{diagonal element normalization;} \\ 3 & \text{non-linear normalization.} \end{cases}$$

- $\mathcal{S}_6^a = N_g$ contains the collision probability calculation grouping algorithm. Here N_g is the number of simultaneous groups to process for each integration line.
- $\mathcal{S}_7^a = I_R$ contains the number of groups.
- $\mathcal{S}_8^a = N_u$ contains the number of unknown in flux system.
- $\mathcal{S}_9^a = N_m$ contains the number of mixtures.
- $\mathcal{S}_{10}^a = N_l$ contains the anisotropy order.
- $\mathcal{S}_{11}^a = N_{\text{gen}}$ contains the umber of generating cells.
- $\mathcal{S}_{12}^a = N_r$ contains the number of regions.
- $\mathcal{S}_{13}^a = N_s$ contains the number of surfaces.
- $\mathcal{S}_{14}^a = N_{\text{pss}}$ contains the dimension of the P_{ss} matrix,
- $\mathcal{S}_{15}^a = N_{\text{icm}}$ contains the dimension of the interface current matrix.
- $\mathcal{S}_{1?}^a = I_{\text{leak}}$ contains flag indicating the presence of absence of the complete leakage matrix where

$$I_{\text{leak}} = \begin{cases} 0 & \text{the complete leakage matrix is absent;} \\ 1 & \text{the complete leakage matrix is present.} \end{cases}$$

The list of group directory {/GRPDIR/} names GRPDIR will be composed using the following FORTRAN instructions

`{WRITE(`GRPDIR`,'(A5,I3,A1,I3)') 'GROUP'`,g,`'/'`,G

for $1 \leq g \leq G$. For example, in the case where two group collision probability matrices are considered ($G = 2$), two such directory would be generated, namely

Table 33: Example of collision probability directories

Name	Type	Condition	Units	Comment
`GROUP␣␣1/␣␣2`	Dir	$G = 2$		sub-directory that contains the information associated with group $g = 1$.
`GROUP␣␣2/␣␣2`	Dir	$G = 2$		sub-directory that contains the information associated with group $g = 2$.

7.2 The group sub-directory

Inside each group g directory the following records will be found

Table 34: Collision probability directories

Name	Type	Condition	Units	Comment
`DRAGON-TXSC␣`	R$(0:N_m)$		cm^{-1}	array Σ_m^g containing the total cross section for the mixtures assuming that the first mixture represents void ($\Sigma_0^g = 0$).
`DRAGON-S0XSC`	R$(0:N_m)$		cm^{-1}	array $\Sigma_{0,m,w}^g$ containing the within group scattering cross section for the mixtures assuming that the first mixture represents void ($\Sigma_{0,0,w}^g = 0$).
`DRAGON-PCSCT`	R(N_r, N_r)	$I_P \geq 0$		array $P_{s,i,j}^g$ containing the scattering modified or direct collision probability matrix.
`DRAGON1PCSCT`	R(N_r, N_r)	$I_P = 1$		array $P_{s,x,i,j}^g$ containing the X directed scattering modified or direct collision probability matrix.
`DRAGON2PCSCT`	R(N_r, N_r)	$I_P = 1$		array $P_{s,y,i,j}^g$ containing the Y directed scattering modified or direct collision probability matrix.
`DRAGON3PCSCT`	R(N_r, N_r)	$I_P = 1$		array $P_{s,z,i,j}^g$ containing the Z directed scattering modified or direct collision probability matrix.
`DRAGON1P*SCT`	R(N_r, N_r)	$I_P = 1$		array $P_{s,x,i,j}^{g,*}$ containing the isotropic current X directed scattering modified or direct collision probability matrix.
`DRAGON2P*SCT`	R(N_r, N_r)	$I_P = 1$		array $P_{s,y,i,j}^{g,*}$ containing the isotropic current Y directed scattering modified or direct collision probability matrix.
`DRAGON3P*SCT`	R(N_r, N_r)	$I_P = 1$		array $P_{s,z,i,j}^{g,*}$ containing the isotropic current Z directed scattering modified or direct collision probability matrix.
`DRAGON-PIS␣␣`	R(N_r)	$I_C \neq 0, 1$		array $P_i^{g,l}$ containing the total leakage matrix.
`DRAGON-PCFUI`	D(N_r, N_s)	$I_{\text{leak}} = 1$		array $P_{\text{leak},i,j}^{g,l}$ containing the complete leakage matrix.

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.

8.1 The main directory

The following records and sub-directories will be found in the /FLUXUNK/ directory:

Table 35: Main records and sub-directories in /FLUXUNK/

Name	Type	Condition	Units	Comment
SIGNATURE␣␣␣	C∗12			parameter SIGNA containing the signature of the data structure.
STATE-VECTOR	I(40)			array $\mathcal{S}_i^f$ containing various parameters that are required to describe this data structure.
EPS-CONVERGE	R(5)			array Δ_i^ϵ containing the convergence parameters for the flux solution algorithm.
K-EFFECTIVE␣	R(1)	$1 \leq \mathcal{S}_1^f \leq 5$		parameter containing the computed or imposed effective multiplication constant for eigenvalue problem.
FLUXDIRECT␣␣	Dir			/FLUX/ directory containing the direct solution to the transport equation.
PSEUDOADJ␣␣␣	Dir	$\mathcal{S}_i^f \geq 1$		/FLUX/ directory containing the pseudo-adjoint solution to the transport equation.
FLUXADJ␣␣␣␣␣	Dir	$\mathcal{S}_i^f \geq 2$		/FLUX/ directory containing the adjoint solution to the transport equation.
PSEUDOGENADJ	Dir	$\mathcal{S}_i^f \geq 3$		/FLUX/ directory containing the generalized pseudo-adjoint solution to the transport equation.
FLUXGENADJ␣␣	Dir	$\mathcal{S}_i^f \geq 4$		/FLUX/ directory containing the generalized adjoint solution to the transport equation.

where each /FLUX/ directory contains:

Table 36: Contents of a /FLUX/ directory

Name	Type	Condition	Units	Comment
1/EIGENVALUE	R(1)	$1 \leq \mathcal{S}_1^f \leq 5$		parameter k_{eff} containing the inverse of the eigenvalue for the problem.
B2␣␣B1HOM␣␣␣	R(1)	$2 \leq \mathcal{S}_1^f \leq 5$	cm^{-2}	parameter B^2 containing the homogeneous buckling.

continued on next page

Contents of a /FLUX/ directory continued from last page

Name	Type	Condition	Units	Comment
`DIFFB1HOM␣␣␣`	R(G)	$2 \leq \mathcal{S}_1^f \leq 5$	cm	array d^g containing the multigroup homogeneous leakage coefficients.
`PNL␣␣␣␣␣␣␣␣␣`	R(G)	$\mathcal{S}_8^f = 0$		array P_{NL}^g containing the non-leakage probabilities.
`B2␣␣HETE␣␣␣␣`	R(3)	$\mathcal{S}_2^f \geq 5$	cm^{-2}	array B_i^2 containing the directional buckling.
{*flxcur*}	R(N_U)		$\text{cm}^{-2}\text{s}^{-1}$	array $\Phi_{u,i}$ containing the unknowns.
{*funsur*}	R(N_U)	$\mathcal{S}_{12}^f = 1$	$\text{cm}^{-2}\text{s}^{-1}$	array $\Phi_{s,i}$ containing the surface flux.

The signature for this data structure is `SIGNA=L_FLUX␣␣␣␣␣␣`. The array $\mathcal{S}_i^f$ contains the following information:

- $\mathcal{S}_1^f = I_s$ contains the type of solution considered where:

$$I_s = \begin{cases} 0 & \text{no flux calculation, fluxes taken from input file;} \\ 1 & k_{\mathit{eff}} \text{ eigenvalue problem with fission and no leakage;} \\ 2 & k_{\mathit{eff}} \text{ eigenvalue problem with fission and fixed leakage } (dB^2); \\ 3 & k_{\mathit{eff}} \text{ eigenvalue problem with fission and fixed } B^2; \\ 4 & \text{Buckling eigenvalue problem with fission and leakage;} \\ 5 & \text{Buckling eigenvalue problem without fission but with leakage;} \\ 6 & \text{fixed source problem, no eigenvalue.} \end{cases}$$

- $\mathcal{S}_2^f = I_l$ contains the type of leakage model where:

$$I_l = \begin{cases} 0 & \text{no leakage model;} \\ 1 & \text{homogeneous } \texttt{PNLR} \text{ calculation;} \\ 2 & \text{homogeneous } \texttt{PNL} \text{ calculation;} \\ 3 & \text{homogeneous } \texttt{SIGS} \text{ calculation;} \\ 4 & \text{homogeneous } \texttt{ALSB} \text{ calculation;} \\ 5 & \text{heterogeneous leakage with imposed buckling;} \\ 6 & \text{heterogeneous leakage with } X \text{ Buckling search;} \\ 7 & \text{heterogeneous leakage with } Y \text{ Buckling search;} \\ 8 & \text{heterogeneous leakage with } Z \text{ Buckling search;} \\ 9 & \text{heterogeneous leakage with radial Buckling search;} \\ 10 & \text{heterogeneous leakage with total Buckling search.} \end{cases}$$

- $\mathcal{S}_3^f = N_f$ contains the number of free iteration per variational acceleration cycle.
- $\mathcal{S}_4^f = N_a$ contains the number of accelerated iteration per variational acceleration cycle.
- $\mathcal{S}_5^f = I_r$ contains the thermal rebalancing option where:

$$I_r = \begin{cases} 0 & \text{no thermal iteration rebalancing;} \\ 1 & \text{thermal iteration rebalancing activated.} \end{cases}$$

- $\mathcal{S}_6^f = M_{\text{in}}$ contains the maximum number of inner (thermal) iterations.
- $\mathcal{S}_7^f = M_{\text{out}}$ contains the maximum number of outer iterations.
- $\mathcal{S}_8^f = I_A$ contains the adjoint calculation option where:

$$I_A = \begin{cases} 0 & \text{no adjoint calculation;} \\ 1 & \text{pseudo-adjoint calculation;} \\ 2 & \text{pseudo-adjoint and adjoint calculation;} \\ 3 & \text{generalized pseudo-adjoint calculation;} \\ 4 & \text{generalized pseudo-adjoint and adjoint calculation.} \end{cases}$$

- $\mathcal{S}_9^f = N_G$ contains the number of groups.
- $\mathcal{S}_{10}^f = N_U$ contains the number of unknowns.
- $\mathcal{S}_{11}^f = N_S$ contains the number of outer surfaces.
- $\mathcal{S}_{12}^f = I_S$ contains the surface flux calculation option where:

$$I_r = \begin{cases} 0 & \text{the surface flux are not computed;} \\ 1 & \text{the surface flux are computed.} \end{cases}$$

The array Δ_i^ϵ contains:

- Δ_1^ϵ is the inner 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 outer generalized adjoint convergence factor.
- Δ_5^ϵ is the generalized adjoint contamination parameter.

In the case of a G group calculation, G *flxcur* and *funsur* records can be present on this directory, one for each group g. The explicit name of these records is created using the following FORTRAN instruction:

```
WRITE(flxcur,'(A4,I3)')   'FLUX',g
WRITE(funsur,'(A6,I3)')   'FUNSUR',g
```

In the case of a two group calculation ($N_G = 2$) we will then find on /FLUXUNK/ the following records:

Table 37: Two groups flux/current records on /FLUXUNK/

Name	Type	Condition	Units	Comment
`FLUX␣␣1␣␣␣␣␣`	R(N_U)		$\text{cm}^{-2}\text{s}^{-1}$	array Φ_i^1 containing the unknown for group $g = 1$.
`FLUX␣␣2␣␣␣␣␣`	R(N_U)		$\text{cm}^{-2}\text{s}^{-1}$	array Φ_i^2 containing the unknown for group $g = 2$.
`FUNSUR␣␣2␣␣␣`	R(N_S)	$\mathcal{S}_{12}^f = 1$	$\text{cm}^{-2}\text{s}^{-1}$	array $\Phi_{s,i}^1$ containing the surface flux for group $g = 1$.
`FUNSUR␣␣2␣␣␣`	R(N_S)	$\mathcal{S}_{12}^f = 1$	$\text{cm}^{-2}\text{s}^{-1}$	array $\Phi_{s,i}^2$ containing the surface flux for group $g = 2$.

9 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 FLIB 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 `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/.

9.1 The main directory

The following records and sub-directories will be found in the /EDITION/ directory:

Table 38: Main records and sub-directories in /EDITION/

Name	Type	Condition	Units	Comment
`SIGNATURE␣␣␣`	C∗12			parameter SIGNA containing the signature of the data structure.
`STATE-VECTOR`	I(40)			array $\mathcal{S}_i^e$ containing various parameters that are required to describe this data structure.
`TITLE␣␣␣␣␣␣␣`	C∗72			parameter TITLE containing the title associated with the last TRACKING processed.
`LAST-EDIT␣␣␣`	C∗12			parameter LAST containing the name of the last editing sub-directory generated.
`REF-IMERGE␣␣`	I($\mathcal{S}_{15}^e$)			array M_r containing the merged region number associated with each region number in the last TRACKING processed.
`REF-IGCOND␣␣`	I($\mathcal{S}_2^e$)			array C_g containing the old group limits associated with the merged groups.
`CARISO␣␣␣␣␣␣`	C($\lvert\mathcal{S}_9^e\rvert - 1$) ∗ 12	$\lvert\mathcal{S}_9^e\rvert \geq 2$		array NAMI containing the name of the isotopes save during the last editing.
`IACTI␣␣␣␣␣␣␣`	I($\mathcal{S}_5^e$)	$\lvert\mathcal{S}_5^e\rvert \geq 1$		array A_m containing the mixture numbers for which activation data was generated.
{*/micdir/*}	Dir			list of sub-directories that contain the editing information.

The signature for this data structure is SIGNA=`L_EDIT␣␣␣␣␣␣`. The array $\mathcal{S}_i^e$ contains the following information:

- $\mathcal{S}_1^e = N_H$ contains the number of homogeneous mixtures saved for the last editing step.
- $\mathcal{S}_2^e = M_G$ contains the number of condensed groups considered for the last editing step.

- $\mathcal{S}_3^e = I_{4f}$ contains a flag to indicate whether or not the 4 factor were generated. Here:

$$I_{4f} = \begin{cases} 1 & \text{if the 4 factor are generated;} \\ 0 & \text{otherwise.} \end{cases}$$

- $\mathcal{S}_4^e = I_U$ contains a flag to indicate whether or not the scattering cross-section matrix was been modified in such a way that it does not contain up-scattering contributions. Here:

$$I_U = \begin{cases} 1 & \text{if the scattering matrix is modified to get rid of up-scattering contribution;} \\ 0 & \text{otherwise.} \end{cases}$$

- $\mathcal{S}_5^e = N_A$ contains the number of mixture activated.
- $\mathcal{S}_6^e = I_S$ contains a flag to identify the types of statistics to be generated.

$$I_S = \begin{cases} 0 & \text{no statistics generated;} \\ 1 & \text{relative differences in the fluxes;} \\ 2 & \text{relative differences in the reaction rates;} \\ 3 & \text{relative differences in the fluxes and reaction rates;} \\ -1 & \text{absolute differences in the cross sections.} \end{cases}$$

- $\mathcal{S}_7^e = I_{EF}$ contains a flag to identify the type of SPH equivalence factor to be computed.

$$I_{EF} = \begin{cases} 0 & \text{no SPH correction;} \\ 1 & \text{the SPH factors already stored on the data structure are used;} \\ 2 & \text{transport-transport SPH equivalence for an homogeneous macro geometry;} \\ 3 & \text{transport-transport SPH equivalence for a user defined GEOMETRY;} \\ 4 & \text{transport-diffusion SPH equivalence for a user defined GEOMETRY;} \\ 5 & \text{transport-transport SPH equivalence for a user defined TRACKING.} \end{cases}$$

- $\mathcal{S}_8^e = I_{EN}$ contains a flag to identify the type of SPH equivalence normalization considered.

$$I_{EN} = \begin{cases} 0 & \text{no SPH correction;} \\ 1 & \text{an average flux normalization is selected;} \\ 1 & \text{a Selengut normalization is selected;} \\ 1 & \text{a Selengut normalization with surface leakage is selected.} \end{cases}$$

- $\mathcal{S}_9^e = I_m$ contains the type of microscopic library generated.

$$I_m = \begin{cases} -1 & \text{a complete MICROLIB is generated including the depletion chain;} \\ 0 & \text{no MICROLIB is generated;} \\ 1 & \text{a complete MICROLIB is generated without the depletion chain.} \end{cases}$$

- $\mathcal{S}_{10}^e = I_p$ contains the print level considered.
- $\mathcal{S}_{11}^e = I_x$ contains a flag to identify the types of cross section saved.

$$I_x = \begin{cases} 0 & \text{cross section are neither computed nor saved;} \\ 1 & \text{cross section are computed but not saved;} \\ 2 & \text{cross section are computed and saved;} \\ 3 & \text{cross section are computed and perturbation parameters are saved} \end{cases}$$

- $\mathcal{S}^e_{12} = I_w$ contains flag to identify the types of weighting used for the homogenization and condensation of the linearly anisotropic contribution to the scattering matrix.

$$I_w = \begin{cases} 0 & \text{flux/volume;} \\ 1 & \text{current/volume;} \\ 2 & \text{buckling weighted coherent current/volume;} \\ 2 & \text{buckling weighted coherent current/volume with directional correction.} \end{cases}$$

- $\mathcal{S}^e_{13} = M_I$ contains the maximum number of isotopes per mixture.
- $\mathcal{S}^e_{14} = M_g$ contains the maximum number of condensed groups.
- $\mathcal{S}^e_{15} = M_h$ contains the maximum number of homogeneous mixtures.
- $\mathcal{S}^e_{16} = M_F$ contains the total number of ISOTXS files generated.

The list of directory {/micdir/} names EDIDIR will be composed according to the following laws. In the case where the set of keywords `SAVE ON` are used followed by a directory name (see example above), the contents of EDIDIR will be identical the name of the specified directory (here EDIDIR=`EDITCELL2G␣␣`). If the `SAVE` option is used without specifying a directory, then EDIDIR will be created as follows:

`WRITE(`EDIDIR`,'(A8,I4)'), 'REF-CASE',` J

where J is the number of default `SAVE` directory in the current /EDITION/ directory. Finally note that each subdirectory created by the `EDI:` module has the general form of a /MICROLIB/ (see Section 4).

10 CONTENTS OF A /BURNUP/ DIRECTORY

This directory contains the main burnup information including the multigroup flux and the isotopic concentration at each time or burnup step.

10.1 The main directory

The following records and sub-directories will be found in the /BURNUP/ directory:

Table 39: Main records and sub-directories in /BURNUP/

Name	Type	Units	Comment
SIGNATURE␣␣␣	C∗12		parameter SIGNA containing the signature of the data structure.
STATE-VECTOR	I(40)		array $\mathcal{S}_i^b$ containing various parameters that are required to describe this data structure.
EVOLUTION-R␣	R(5)		array R_i containing the various parameters associated with the burnup calculation options.
DEPL-TIMES␣␣	R($\mathcal{S}_3^b$)	10^8 s	array T_i containing the various time steps at which burnup information has been saved.
FUELDEN-INIT	R(2)		array containing the initial density of heavy element in the fuel ρ_f (g cm^{-3}) and the initial mass of heavy element in the fuel m_f (g).
ISOMIXT-EVO␣	R($\mathcal{S}_4^b$)		array M_I containing the mixture number associated with each isotope.
ISONAMES-EVO	C($\mathcal{S}_4^b$) ∗ 12		array NAMI$_I$ containing the name of each isotope.
{*/DEPLDIR/*}	Dir		list of sub-directories that contain the properties associated with each burnup step.

The signature for this data structure is SIGNA=L_BURNUP␣␣␣␣. The array $\mathcal{S}_i^b$ contains the following information:

- $\mathcal{S}_1^b = I_s$ contains the type of solution considered where:

$$I_s = \begin{cases} 1 & \text{fifth order Runge–Kutta method;} \\ 2 & \text{forth order Kaps–Rentrop method.} \end{cases}$$

- $\mathcal{S}_2^b = I_t$ contains the type of burnup considered where:

$$I_t = \begin{cases} 0 & \text{out of core or zero flux/power depletion;} \\ 1 & \text{constant flux depletion;} \\ 2 & \text{constant power depletion.} \end{cases}$$

- $\mathcal{S}_3^b = N_t$ contains the number of time steps for which burnup properties are present in this directory
- $\mathcal{S}_4^b = N_I$ contains the number of isotopes.

- $\mathcal{S}_5^b = G$ contains the number of groups.
- $\mathcal{S}_6^b = N_r$ contains the number of regions.

The list of directory {/DEPLDIR/} names DEPLDIR will be composed using the following FORTRAN instructions:

```
WRITE(DEPLDIR,'(A8,I4)') 'DEPL-DAT', J
```

for time step J (associated time stamp T_J) such that $1 \leq J \leq N_t$. For the case where $N_t = 2$, two such directory would be generated, namely

Table 40: Example of depletion directories

Name	Type	Units	Comment
DEPL-DAT␣␣␣1	Dir		sub-directory that contains the information associated with time step $J = 1$.
DEPL-DAT␣␣␣2	Dir		sub-directory that contains the information associated with time step $J = w$.

10.2 The depletion sub-directory

Inside each depletion directory the following records and sub-directories will be found:

Table 41: Contents of a depletion sub-directory

Name	Type	Units	Comment
ISOTOPESDENS	R(N_I)	(cm b)$^{-1}$	array ρ_i containing the isotopic densities for each of the isotopes.
FLXDIR␣␣␣␣␣␣	R(N_r, G)	cm^{-2} s^{-1}	array ϕ_r^g containing the multiregion and multigroup flux where for each energy group the flux associated with the region are stored successively.
FLUX-NORM␣␣␣	R(1)		parameter K containing the flux normalization constant. It is zero for out of core depletion and represent the normalization that ensures that the cell integrated flux or power are that required when fixed flux or power burnup is requested.
DELTA␣␣␣␣␣␣␣	R(2)		array containing the fuel burnup (MW d T^{-1}) and irradiation (Kb^{-1}) increments between the current time step and the preceding time step.
BURNUP-IRRAD	R(2)		array containing the fuel burnup (MW d T^{-1}) and irradiation (Kb^{-1}) reached at this time step.

11 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.

11.1 The main directory

The following records and sub-directories will be found in the /CPO/ directory:

Table 42: 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 43: 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.

11.2 The mixture sub-directory

Each mixture directory contains the following records and sub-directories will be found:

Table 44: 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 $\mathcal{P}_i^{\text{cpo}}$ 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($\mathcal{P}_4^{\text{cpo}}$)		MW d T^{-1}	array B_k containing the burnup steps.
`N/KB␣␣␣␣␣␣␣␣`	R($\mathcal{P}_4^{\text{cpo}}$)		Kb^{-1}	array w_k containing the fuel irradiation for the different burnup steps.
`ISOTOPESNAME`	C($\mathcal{P}_2^{\text{cpo}}$) $*$ 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 $\mathcal{P}^{\text{cpo}}$:

- $\mathcal{P}_1^{\text{cpo}} = G$ contains the number of groups for this homogeneous mixture.
- $\mathcal{P}_2^{\text{cpo}} = N_I$ contains the number of isotopes in this mixture.

- $\mathcal{P}_3^{\text{cpo}} = N_L$ 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 FORTRAN instructions:

```
WRITE(BRNDIR,'(A8,I4)'), 'BURN    ', J
```

for $1 \leq J \leq N_B$. For the example given above ($N_B = 2$), two such directories will be generated, namely

Table 45: 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 that contains the information associated with burnup step 2.

11.3 The burnup sub-directory

A burnup sub-directory contains the following records and sub-directories:

Table 46: Contents of a burnup sub-directory in /CPO/

Name	Type	Condition	Units	Comment
ISOTOPESDENS	R(N_I)		(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 (cm b)$^{-1}$. The content of the isotopic multigroup cross section directory is described in Section 14.

12 CONTENTS OF A /FBM/ DIRECTORY

This directory contains a burnup and local parameter dependent hierarchical reactor data base compatible with a CANDU reactor.

12.1 The main directory

The records and sub-directories that will be found in the /FBM/ directory are:

Table 47: Main records and sub-directories in /FBM/

Name	Type	Condition	Units	Comment
SIGNATURE$_{\sqcup\sqcup\sqcup}$	C$*$12			parameter SIGNA containing the signature of the data structure.
INFORMATION$_{\sqcup}$	C$*$72			parameter NAMDB containing the name of the database.
{*/MATDIR/*}	Dir			list of material sub-directories containing a homogeneous material.

The signature variable for this data structure must be SIGNA=REACTOR_XSDB. The list of directory {/matdir/} names MATDIR will be composed using the following FORTRAN instructions:

WRITE(MATDIR,'(A8,I4)'),*DNAME*, J

where *DNAME* in provided when the CFC: module is executed and $1 \leq J \leq N_H$ is the mixture number considered. If $N_H = 2$, and *DNAME*=MATH$_{\sqcup\sqcup\sqcup\sqcup}$, two such directory will be generated, namely

Table 48: Example of homogeneous mixture directories

Name	Type	Condition	Units	Comment
MATH$_{\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup}$1	Dir			is the sub-directory that contains the information associated with homogeneous material 1.
MATH$_{\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup}$2	Dir			is the sub-directory that contains the information associated with homogeneous material 2.

12.2 The material sub-directory

Each material directory will contain the following records and sub-directories:

Table 49: Contents of a material sub-directory in /FBM/

Name	Type	Condition	Units	Comment
PARAM$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	I(4)			array $\mathcal{P}_i^{\text{fbm}}$ containing the various parameters associated with this mixture.
HITAB$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	C($\mathcal{P}_2^{\text{fbm}}$) $*$ 12			array ISO$_i$ containing the name of the various isotopes saved for this mixture.
VOLUME$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R(1)		cm^3	parameter V_i containing the volume of the region associated this homogeneous mixture in the EDITION data structure.
MASS$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R(1)		kg	parameter M containing the initial mass of heavy elements in the fuel.
ENERGY$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R($\mathcal{P}_1^{\text{fbm}}+1$)		eV	array E_g containing the energy groups limits.
BURNUP$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R($\mathcal{P}_4^{\text{fbm}}$)		MW d T^{-1}	array B_k containing the burnup steps.
N/KB$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	R($\mathcal{P}_4^{\text{fbm}}$)		Kb^{-1}	array w_k containing the fuel irradiation for the different burnup steps.
JTAB$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$	I($\mathcal{P}_2^{\text{fbm}}$)			array I_i containing flags to indicate the type of data stored in each isotopic sub-directory.
INFO-NOMINAL	Dir			sub-directory where the information on the nominal local parameters is stored.
{*/BRNDIR/*}	Dir			list of sub-directories that contain the burnup dependent cross sections associated with this homogeneous mixture.

The following information is stored in $\mathcal{P}^{\text{fbm}}$:

- $\mathcal{P}_1^{\text{fbm}} = G$ contains the number of groups for this homogeneous mixture.
- $\mathcal{P}_2^{\text{fbm}} = N_I$ contains the number of isotopes in this mixture.
- $\mathcal{P}_3^{\text{fbm}} = N_L$ contains the order of the scattering anisotropy for this mixture.
- $\mathcal{P}_4^{\text{fbm}} = N_B$ contains the number of burnup steps for this mixture.

The list of directory {/BRNDIR/} names BRNDIR will be composed according to the following FORTRAN instructions:

```
WRITE(BRNDIR,'(A8,I4)'), 'BURN    ', J
```

for $1 \leq J \leq N_B$. If $N_B = 2$, two such directories will be generated, namely BURN$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$1 and BURN$\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup$2. These will contain the information associated with burnup step 1 and 2 respectively.

12.3 The information sub-directory

The information sub-directory /INFO-NOMINAL/ will contain the following records:

Table 50: Contents of the information sub-directory of /FBM/

Name	Type	Condition	Units	Comment
`NOMINALN␣␣␣␣`	C(7) ∗ 12			an array NP_i containing the name of the local and global parameters stored in the database.
`NOMINALP␣␣␣␣`	R(7)			an array NP_i containing the nominal value of the local and global parameters stored in the database.

The local parameters currently programmed are:

- NP_1 =`PW` identifies the power parameter with $P_1 = P$ the burnup power in kW/kg.
- NP_1 =`TCOOL` identifies the coolant temperature with $P_2 = T_c$ the coolant temperature in K.
- NP_3 =`TMOD` identifies the moderator temperature with $P_3 = T_m$ the moderator temperature in K.
- NP_4 =`TFUEL` identifies the fuel temperature with $P_4 = T_f$ the fuel temperature in K.
- NP_5 =`RHOC` identifies the coolant density with $P_5 = \rho_c$ the coolant density in g/cc.
- NP_6 =`RHOM` identifies the moderator density with $P_6 = \rho_m$ the moderator density in g/cc.
- NP_7 =`PUR` identifies the moderator purity with $P_7 = p_m$ the moderator purity in %.

12.4 The burnup sub-directory

The burnup directory contains the following records and sub-directories:

Table 51: Contents of a burnup sub-directory in /FBM/

Name	Type	Condition	Units	Comment
`ISOTOPESDENS`	R(N_I)		(cm b)$^{-1}$	array ρ_i containing the density of each isotopes.
`DCR␣␣␣␣␣␣␣␣␣␣`	R(N_I)		s^{-1}	array λ_i containing the radioactive decay constant 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.
`HISTORY␣␣␣␣␣`	Dir			a sub-directory that contains the pseudo-fissile isotope history coefficients.
{*/FBMISO/*}	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 (cm b)$^{-1}$. The content of the isotopic multigroup cross section directory is described in Section 15.

12.5 The history sub-directory

Inside each history directory the following records and sub-directories will be found:

Table 52: Contents of an history sub-directory /HISTORY/ in /BRNDIR/

Name	Type	Condition	Units	Comment
CHIS␣␣␣␣␣␣␣␣	R(1)		(cm b)$^{-1}$	parameter H_d containing the coolant density history.
FHIS␣␣␣␣␣␣␣␣	R(1)		K	parameter H_T containing the coolant temperature history.
PHIL1␣␣␣␣␣␣␣	R(1)		kW/kg	parameter $H_{1,1}$ containing the first high power level history.
PHIL2␣␣␣␣␣␣␣	R(1)		kW/kg	parameter $H_{1,2}$ containing the second high power level history.
PHIS1␣␣␣␣␣␣␣	R(1)		kW/kg	parameter $H_{2,1}$ containing the first low power level history.
PHIS2␣␣␣␣␣␣␣	R(1)		kW/kg	parameter $H_{2,2}$ containing the second low power level history.

13 CONTENTS OF A /HISTORY/ DIRECTORY

This data structure contains the information required to ensure a smooth coupling of DRAGON with DONJON when a history based full reactor calculation is to be performed.

13.1 The main directory

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

Table 53: Main records and sub-directories in /HISTORY/

Name	Type	Condition	Units	Comment
SIGNATURE$_{\sqcup\sqcup\sqcup}$	C$*12$			parameter SIGNA containing the signature of the data structure.
STATE-VECTOR	I(40)			array $\mathcal{S}_i^h$ containing various parameters that are required to describe this data structure.
BUNDLELENGTH	R(1)		cm	parameter L_z containing the fuel bundle length.
NAMEGLOBAL$_{\sqcup\sqcup}$	C($\mathcal{S}_1^h$)$*12$			array $\mathcal{G}_j$ containing the names of the global parameters.
PARAMGLOBAL$_{\sqcup}$	R($\mathcal{S}_1^h$)			array G_j containing the value of the global parameters.
NAMELOCAL$_{\sqcup\sqcup\sqcup}$	C($\mathcal{S}_2^h$)$*12$			array $\mathcal{L}_j$ containing the names of the local parameters.
CELLID$_{\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup}$	I($\mathcal{S}_3^h, \mathcal{S}_4^h$)			array $C_{i,j}$ containing an identification number associated with bundle i and channel j.
FUELID$_{\sqcup\sqcup\sqcup\sqcup\sqcup\sqcup}$	I($\mathcal{S}_3^h, \mathcal{S}_4^h$)			array $F_{i,j}$ containing the fuel type associated with bundle i and channel j.
{*/FUELDIR/*}	Dir			list of sub-directories FUEL$_{i,j}$ that contain the properties associated with the fuel type $F_{i,j}$.
{*/CELLDIR/*}	Dir			list of sub-directories CELL$_{i,j}$ that contain the properties associated with the cell $C_{i,j}$.

The signature for this data structure is SIGNA=L_HISTORY$_{\sqcup\sqcup\sqcup}$. The array $\mathcal{S}_i^h$ contains the following information:

- $\mathcal{S}_1^h = N_g$ contains the number of global parameters.
- $\mathcal{S}_2^h = N_l$ contains the number of local parameters.
- $\mathcal{S}_3^h = N_b$ contains the number of bundles per channel.
- $\mathcal{S}_4^h = N_c$ contains the number of channels in the core.
- $\mathcal{S}_5^h = N_s$ contains the number of bundle shift.
- $\mathcal{S}_6^h = T_s$ contains the type of depletion solution used.
- $\mathcal{S}_7^h = T_b$ contains the type of burnup considered.
- $\mathcal{S}_8^h = N_I$ contains the number of isotopes.

- $\mathcal{S}_9^h = G$ contains the number of transport groups.
- $\mathcal{S}_{10}^h = N_r$ contains the number of regions.
- $\mathcal{S}_{11}^h = N_F$ contains the number of fuel types.

The fuel directory name $\mathsf{FUEL}_{i,j}$ associated with fuel type $F_{i,j}$ is composed using the following FORTRAN instruction:

`WRITE(`FUEL`,'(A4,I8.8)') 'FUEL',`$F_{i,j}$

This directory will contain the initial isotopic content of this fuel type. The cell directory name $\mathsf{CELL}_{i,j}$ associated with $C_{i,j}$ is composed using the following FORTRAN instruction:

`WRITE(`CELL`,'(A4,I8.8)') 'CELL',`$C_{i,j}$

This directory will contain the value of the local parameters associated with cell $C_{i,j}$ as well as the current isotopic content of this cell.

The identification number $C_{i,j}$ associated with channel j and bundle i can be seen as the serial number of the bundle located at a position in space identified by (i, j). It is automatically managed by the `HST:` module.[8] For a fresh core $C_{i,j} = n$ where n represents the cell order definition in the input file. Upon refueling, some bundles in channel k of the core are displaced from region (l, k) to (m, k), new bundles are introduced at location (l, k) and old bundles removed from location (m, k). If one assumes that C^{NEW} and C^{OLD} represents the value of C after and before refueling then we will have:

$$C_{m.k}^{\mathrm{NEW}} = C_{l,k}^{\mathrm{OLD}}$$
$$C_{l,k}^{\mathrm{NEW}} = C_{m,k}^{\mathrm{FRESH}}$$

where $C_{m,k}^{\mathrm{FRESH}}$ represent a fresh fuel cell. The local parameters and burnup power density of the fuel cell previously located at (m, k) are preserved and the fresh fuel isotopic densities is that provided in $F_{m,k}$, the fuel type associated with $C_{m,k}^{\mathrm{FRESH}}$.

13.2 The Fuel Type Sub-directory

Each fuel sub-directory $\mathsf{FUEL}_{i,j}$ contains the following information

Table 54: Fuel type sub-directory

Name	Type	Condition	Units	Comment
`FUELDEN-INIT`	R(2)			array containing the initial density of heavy element in the fuel ρ_f in g/cm^3 and the initial linear density of heavy element in the fuel m_f in g/cm..
`ISOTOPESNAME`	C(N_I)$*$12			array containing the name of isotopes used in this fuel type.
`ISOTOPESMIXT`	I(N_I)			array containing the mixture associated with each isotopes in this fuel type.
`ISOTOPESDENS`	R(N_I)		(cm b)$^{-1}$	array ρ_i containing the density of each isotopes.

13.3 The Cell Type Sub-directory

Each cell isotopic sub-directory $\mathsf{CELL}_{i,j}$ contains the following information

Table 55: Cell sub-directory

Name	Type	Condition	Units	Comment
FUELDEN-INIT	R(2)			array containing the initial density of heavy element in the fuel ρ_f in g/cm^3 and the initial linear density of heavy element in the fuel m_f in g/cm..
PARAMLOCALBR	R(N_l)			array V_l^B containing the value of the local parameters before refueling.
PARAMLOCALAR	R(N_l)			array V_l^A containing the value of the local parameters after refueling.
PARAMBURNTBR	R(2)			array containing the depletion time T^B in days and the burnup power rate P^B in kW/kg before refueling.
PARAMBURNTAR	R(2)			array containing the depletion time T^A in days and the burnup power rate P^A in kW/kg after refueling.
DEPL-PARAM$\sqcup\sqcup$	R(3)			array containing the time step T in days, the burnup B in kWd/kg and the irradiation w in n/kb currently reached by the fuel in this cell.
ISOTOPESDENS	R(N_I)		(cm b)$^{-1}$	array ρ_i containing the density of each isotopes.

14 CONTENTS OF AN /ISOTOPE/ DIRECTORY

Each isotope directory contains a cross section identifier record that must be used to verify if a given cross section type has been saved for this isotope. For the case where the scattering cross section is expanded up to order L in Legendre polynomial, this record has the form:

Table 56: Isotopic cross section identifier record

Name	Type	Condition	Units	Comment
`XS-SAVED␣␣␣␣`	I$(21+L)$			array κ_k that is used to identify the various type of cross sections saved for this isotope.

The first 20 components of κ_k indicate the presence of different vector reaction cross section records while the last $L+1$ components refer to information pertaining to the scattering matrix. Because we can also use this isotopic directory to store time dependent cross sections in the form of a power series expansion:

$$v_k^g(t) = \sum_{i=0}^{I} v_{k,i}^g t^i \tag{14.1}$$

we must be able to specify explicitly presence of these various terms using κ_k. The presence of the record $v_{k,i}^g$ in this directory is ensured if the condition

$$F_i(\kappa_k) = \mathrm{mod}(\frac{\kappa_k}{2^i}, 2) = 1$$

is satisfied. We will describe later in this section how the different terms $v_{k,i}^g$ are stored for $i = 1, I$. Here we will first consider the more usual case where constant vector reactions are stored on the isotopic directory. Moreover, the maximum value of I permitted for each isotope is specified by N_p as defined in Section 4.1.

Table 57: Vector reaction records

Name	Type	Condition	Units	Comment
`TOTAL␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_1) = 1$	b	array σ^g containing the multigroup total cross section.
`TRANC␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_2) = 1$	b	array σ_{tc}^g containing the multigroup transport correction cross section.
`NUSIGF␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_3) = 1$	b	array $\nu\sigma_f^g$ containing the product of σ_f^g, the multigroup fission cross section with ν^g, the averaged number of neutron produced per fission.
`NFTOT␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_4) = 1$	b	array σ_f^g containing the multigroup fission cross section.

continued on next page

Vector reaction records continued from last page

Name	Type	Condition	Units	Comment
`CHI␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_5) = 1$		array χ^g containing the multigroup energy spectrum of the neutron emitted by fission.
`NU␣␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_6) = 1$		array ν^g containing the multigroup averaged number of neutron produced per fission.
`NG␣␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_7) = 1$	b	array σ_c^g containing the multigroup neutron capture cross section.
`NHEAT␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_8) = 1$	MeV b	array H_f^g containing the product of σ_f^g, the multigroup fission cross section with H^g, the averaged energy emitted per fission, $H\sigma_f^g$.
`N2N␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_9) = 1$	b	array $\sigma_{(n,2n)}^g$ containing the multigroup cross section for the reaction ${}_Z^AX + n \rightarrow {}_Z^{A-1}X + 2n$.
`N3N␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{10}) = 1$	b	array $\sigma_{(n,3n)}^g$ containing the multigroup cross section for the reaction ${}_Z^AX + n \rightarrow {}_Z^{A-2}X + 3n$.
`N4N␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{11}) = 1$	b	array $\sigma_{(n,4n)}^g$ containing the multigroup cross section for the reaction ${}_Z^AX + n \rightarrow {}_Z^{A-3}X + 4n$.
`NP␣␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{12}) = 1$	b	array $\sigma_{(n,p)}^g$ containing the multigroup cross section for the reaction ${}_Z^AX + n \rightarrow {}_{Z-1}^AX + p$.
`NA␣␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{13}) = 1$	b	array $\sigma_{(n,\alpha)}^g$ containing the multigroup cross section for the reaction ${}_Z^AX + n \rightarrow {}_{Z-2}^{A-3}X + \alpha$.
`GOLD␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{14}) = 1$		array λ^g containing the multigroup Goldstein-Cohen parameters.
`ABS␣␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{15}) = 1$	b	array σ_a^g containing the multigroup absorption cross section.
`NWT0␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{16}) = 1$	$\mathrm{s}^{-1}\mathrm{cm}^{-2}$	array ϕ_w^g containing the multigroup weighted neutron flux spectrum.
`STRD␣␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{17}) = 1$	b	array σ_{tr}^g containing the multigroup transport cross section homogenized over all directions.
`STRD␣X␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{18}) = 1$	b	array $\sigma_{tr,x}^g$ containing the X directed multigroup transport cross section.
`STRD␣Y␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{19}) = 1$	b	array $\sigma_{tr,y}^g$ containing the Y directed multigroup transport cross section.
`STRD␣Z␣␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{20}) = 1$	b	array $\sigma_{tr,z}^g$ containing the Z directed multigroup transport cross section.

Note that the last three characters of each of the records above correspond to the extension `EXT='␣␣␣'` that is associated with term $i = 0$ in the power series expansion for the cross sections (see Eq. (14.1)). 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 58: Additional total cross section records for $I = 2$

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

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

$$\sigma_s^{h\to g}(\vec{\Omega}\to\vec{\Omega}') = \sum_{l=0}^{L}\frac{2l+1}{4\pi}P_l(\vec{\Omega}\cdot\vec{\Omega}')\sigma_l^{h\to g} = \sum_{l=0}^{L}\sum_{m=-l}^{l}Y_l^m(\vec{\Omega})Y_l^m(\vec{\Omega}')\sigma_l^{h\to g}$$

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

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

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

$$\sigma_l^{h\to g} = \int_{4\pi} d^2\Omega\sigma_s^{h\to g}(\vec{\Omega}\to\vec{\Omega}')P_l(\vec{\Omega}\cdot\vec{\Omega}')$$

Note that this definition of $\sigma_l^{h\to g}$ 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 directly these $G\times G$ matrices on the data structure, a compressed storage format will be considered. This choice is justified by the fact that the number of energy groups for which scattering to a specific group does not vanish is generally relatively small compared to the total number of groups in the library. Moreover, the groups with non-zero scattering cross sections are generally clustered around the final energy group. In order to define our compressed storage format we need two different integer indices n_l^g and h_l^g for each order in the scattering cross section and for each final energy group g. These 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:

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

which for the example above leads to

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

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

$$\sigma_l^{h \to g} = \begin{cases} 0 & \text{if } h > h_l^g \\ 0 & \text{if } h < h_l^g - n_l^g + 1 \\ \sigma_{l,c}^k & \text{otherwise} \end{cases}$$

where we have used:

$$k = \sum_{h=1}^{g-1} n_l^h + h_l^g - h + 1$$

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

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

In the case where only the order $l = 0$ moment of scattering cross section is non zero (isotropic scattering) the following records can be found on /ISOTOPE/.

Table 59: Scattering cross section records

Name	Type	Condition	Units	Comment
`SIGS00␣␣␣␣␣␣`	R(G)	$F_0(\kappa_{21}) = 1$	b	array $\sigma_{0,s}^g$ containing the isotropic component ($l = 0$) of the multigroup total scattering cross section.
`IJJS00␣␣␣␣␣␣`	I(G)	$F_0(\kappa_{21}) = 1$		array h_0^g containing the highest energy group number for which the isotropic component of the scattering cross section to group g does not vanish.
`NJJS00␣␣␣␣␣␣`	I(G)	$F_0(\kappa_{21}) = 1$		array n_0^g containing the number of energy groups for which the isotropic component of the scattering cross section to group g does not vanish.
`SCAT00␣␣␣␣␣␣`	R($\sum_{g=1}^{G} n_0^g$)	$F_0(\kappa_{21}) = 1$	b	array $\sigma_{0,c}^k$ containing the compressed isotropic component of the scattering matrix.

In fact, $\sigma_{l,s}^g$, h_l^g, n_l^g and $\sigma_{l,c}^k$ for $l \leq L$ will be stored respectively on records with names SIGS, IJJ, NJJ and SIGS created using:

```
WRITE(SIGS,'(A4,I2.2,3X,A3)'), 'SIGS',l,EXT
```

```
WRITE(IJJS,'(A4,I2.2,3X,A3)'), 'IJJS',l,EXT
WRITE(NJJS,'(A4,I2.2,3X,A3)'), 'NJJS',l,EXT
WRITE(SCAT,'(A4,I2.2,3X,A3)'), 'SCAT',l,EXT
```

provided that

$$F_0(\kappa_{21+l}) = 1$$

is satisfied. Here EXT is again the extension associated with term i in the power series expansion for the cross sections (see Eq. (14.1)).

Note that most of these cross sections are not required to perform a cell calculation in DRAGON. In fact, transport calculations only use σ^g, σ^g_{tc}, $\nu\sigma^g_f$, χ^g and the isotropic and linearly anisotropic scattering matrix. For burnup calculations, depending on the depletion chain prescribed (either on the WIMS-AECL or WIMS-D4 format libraries or as an input to DRAGON) the following cross sections may be required: σ^g_f, σ^g_c, $\sigma^g_{(n,2n)}$, $\sigma^g_{(n,3n)}$, $\sigma^g_{(n,4n)}$, $\sigma^g_{(n,p)}$, $\sigma^g_{(n,\alpha)}$. 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 DRAGON, this cross section is used to modify the total and isotropic scattering cross section as

$$\begin{aligned}\sigma^g_c &= \sigma^g - \sigma^g_{tc}\\ \sigma^{g\to g}_{c,0} &= \sigma^{g\to g}_0 - \sigma^g_{tc}\end{aligned}$$

On the other hand the so-called homogeneous and directional transport cross section are obtained using

$$\begin{aligned}\sigma^g_{tr} &= (3D^g_h)^{-1}\\ \sigma^g_{tr,x} &= (3D^g_x)^{-1}\\ \sigma^g_{tr,y} &= \left(3D^g_y\right)^{-1}\\ \sigma^g_{tr,z} &= (3D^g_z)^{-1}\end{aligned}$$

where the diffusion coefficients are computed in the editing. If a transport calculation without leakage is performed in DRAGON, an approximate diffusion coefficients given by

$$D^g_h = \frac{1}{3(\sigma^g - \sigma^g_{1,s})}$$

will be used to compute σ^g_{tr}.

15 CONTENTS OF A /ISOFBM/ DIRECTORY

Most of the records found in an /ISOTOPE/ directory now becomes sub-directories in a /ISOFBM/ directory.

Table 60: Isotopic vector reaction sub-directory

Name	Type	Condition	Units	Comment
`TOTAL␣␣␣␣␣␣␣␣`	Dir			the multigroup total cross section sub-directory.
`NUSIGF␣␣␣␣␣␣`	Dir			the sub-directory where the product of σ_f^g, the multigroup fission cross section with ν^g, the averaged number of neutron produced per fission is stored.
`NFTOT␣␣␣␣␣␣␣`	Dir			the multigroup fission cross section sub-directory.
`CHI␣␣␣␣␣␣␣␣␣`	Dir			the sub-directory where the multigroup energy spectrum of the neutron emitted by fission is stored.
`STRD␣␣␣␣␣␣␣␣`	Dir			the multigroup transport cross section sub-directory.
`H-FACTORS␣␣␣␣`	Dir			the sub-directory containing the product of the macroscopic and microscopic fission cross-section times the energy recovered by fission.

The multigroup scattering cross section matrix are again stored in a format similar to that described in Section 14. The main difference here is that `SCAT␣0␣␣␣␣␣␣` and `SCAT␣1␣␣␣␣␣␣` now represent sub-directories rather than records. We will therefore have:

Table 61: Scattering records and sub-directories

Name	Type	Condition	Units	Comment
`IJJ␣0␣␣␣␣␣␣␣`	I(G)			array h_0^g containing the highest energy group number for which the isotropic component of the scattering cross section to group g does not vanish.
`NJJ␣0␣␣␣␣␣␣␣`	I(G)			array n_0^g containing the number of energy groups for which the isotropic component of the scattering cross section to group g does not vanish.
`SCAT␣0␣␣␣␣␣␣`	Dir			the sub-directory containing the compressed isotropic component of the scattering matrix.

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Scattering records and sub-directories continued from last page

Name	Type	Condition	Units	Comment
`IJJ␣1␣␣␣␣␣␣␣`	I(G)	$\mathcal{P}_3 > 1$		array h_1^g containing the highest energy group number for which the linearly anisotropic component of the scattering cross section to group g does not vanish.
`NJJ␣1␣␣␣␣␣␣␣`	I(G)	$\mathcal{P}_3 > 1$		array n_1^g containing the number of energy groups for which the linearly anisotropic component of the scattering cross section to group g does not vanish.
`SCAT␣1␣␣␣␣␣␣`	Dir	$\mathcal{P}_3 > 1$		the sub-directory containing the compressed linearly anisotropic component of the scattering matrix.

Finally each of the above cross section directories will contain the following information:

Table 62: Cross section sub-directories

Name	Type	Condition	Units	Comment
`REF␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the reference cross sections.
`D1C␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the first order coolant density feedback coefficients.
`D2C␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the second order coolant density feedback coefficients.
`D1M␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the first order moderator density feedback coefficients.
`D2M␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the second order moderator density feedback coefficients.
`T1C␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the first order coolant temperature feedback coefficients.
`T2C␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the second order coolant temperature feedback coefficients.
`T1M␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the first order moderator temperature feedback coefficients.
`T2M␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the second order moderator temperature feedback coefficients.
`T1F␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the first order fuel temperature feedback coefficients.
`T2F␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the second order fuel temperature feedback coefficients.

continued on next page

Cross section sub-directories continued from last page

Name	Type	Condition	Units	Comment
`BOR␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the boron concentration feedback coefficients.
`NP239␣␣␣␣␣␣␣`	R(N_x)			array containing the ^{239}Np concentration feedback coefficients.
`SM149␣␣␣␣␣␣␣`	R(N_x)			array containing the ^{149}Sm concentration feedback coefficients.
`XEN␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the ^{135}Xe concentration feedback coefficients.
`FPC1␣␣␣␣␣␣␣␣`	R(N_x)			array containing the first order pseudo-fissile isotope concentration feedback coefficients.
`FPC2␣␣␣␣␣␣␣␣`	R(N_x)			array containing the second order pseudo-fissile isotope concentration feedback coefficients.
`MIXFD␣␣␣␣␣␣␣␣␣`	R(N_x)			array containing the mixed density/temperature feedback coefficients for coolant.

Note that in the above $N_x = G$ when vector cross sections are considered while $N_x = \sum_{g=1}^{G} n_i^g$ for scattering cross sections.

REFERENCES

[1] G. Marleau, A. Hébert, R. Roy, "New Computational Methods Used in the Lattice Code DRAGON," *Topical Meeting on Advances in Reactor Physics*, p. 1.177, Charleston, South Carolina (1992).

[2] G. Marleau, R. Roy, A. Hébert, *DRAGON: A Collision Probability Transport Code for Cell and Supercell Calculations*, Technical Report IGE-157, École Polytechnique de Montréal (1994).

[3] A. Hébert, G. Marleau, R. Roy, "Application of the Lattice Code DRAGON to CANDU Analysis," *Trans. Am. Nucl. Soc.*, **72**, 335 (1995).

[4] G. Marleau, R. Roy, A. Hébert, *A User Guide for DRAGON 3.07*, Technical Report IGE-174 Rev. 8, École Polytechnique de Montréal (2008).

[5] R. Roy, *The CLE-2000 Tool-Box*, Technical Report IGE-163, École Polytechnique de Montréal (1999).

[6] R. Roy, A. Hébert, *The GAN Generalized Driver*, Technical Report IGE-158, École Polytechnique de Montréal (2000).

[7] E. Varin, A. Hébert, R. Roy, J. Koclas, *A User's Guide for DONJON*, Technical Report IGE-208 Rev. 2, École Polytechnique de Montréal (2004).

[8] G. Marleau, E. Varin, *An History Interface Between DRAGON and DONJON: The HST: module*, Technical Report IGE-259 Rev. 1, École Polytechnique de Montréal (2004).

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