

# **Python software for the conversion of SRAC PDS Neutron Cross Section Sets into PHISICS- compatible format**

Andrea Alfonsi

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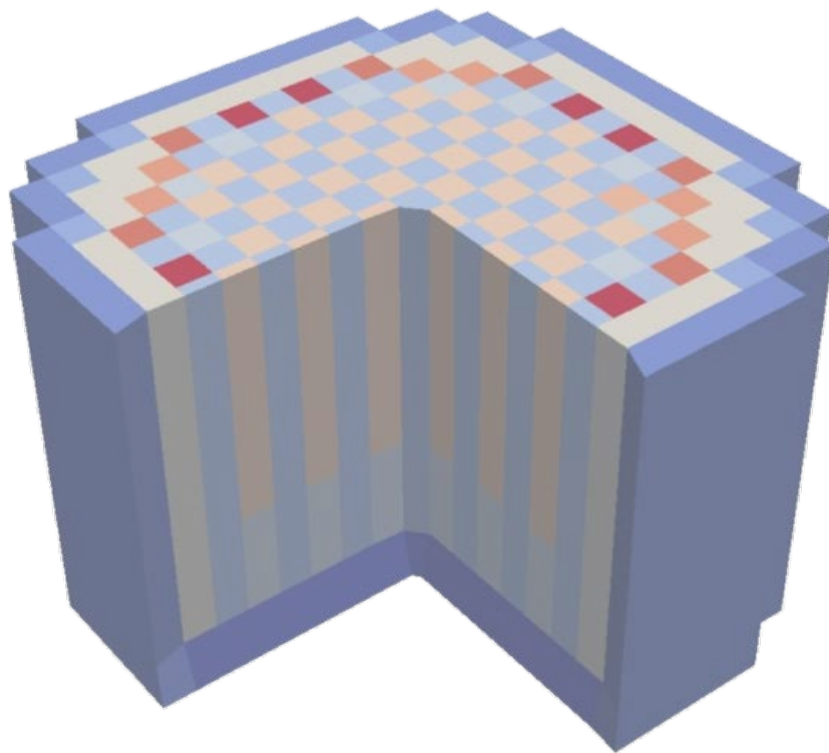
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## **EXECUTIVE SUMMARY**

The goal of this document is about the description on how to use the PDS converter software developed at INL. This short user guide is aimed to describe, in details, how to convert SRAC PDS XS formats into PHISICS-compatible XML cross section set.

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## ACRONYMS

ART	Advanced Reactor Technologies
PHISICS	Parallel and Highly Innovative Simulation for the INL Code System
INL	Idaho National Laboratory
XS	Cross Sections
XML	eXtensible Markup Language



# 1. PDS FORMAT

The SRAC code is a lattice calculation module in use at Japan Atomic Energy Agency (JAEA). This module performs the neutron transport calculation for various types of fuel elements including existing light water reactors, research reactors, etc. based on the collision probability method with a set of the 200 group cross sections generated from the Japanese Evaluated Nuclear Data Library JENDL. Among the different capabilities, the SRAC code is able to generate homogenized set of cross sections aimed to be used in full-core reactor physics codes.

SRAC is able to export homogenized macroscopic (any energy collapsing structure) and microscopic (107 neutron energy groups) cross sections in native unformatted FORTRAN binary files using a proprietary format named PDS.

The PDS XS data set is a unique file system format that is structured as follows:

- MACROSCOPIC (any energy neutron energy structure) homogenized cross sections:
  - o For each homogenized MACROscopic region (e.g. assembly) and tabulation coordinate (e.g. BURN-UP level) a required binary file is provided (optionally Delayed Neutron File), containing the following cross sections:
    - Prompt Cross Sections (1<sup>st</sup> binary file):
      - Total XS
      - Scattering XS
      - Capture and Absorption XS
      - Production XS
      - Fission XS (if fissile region)
      - Total Fission Spectrum (if fissile region)
    - Optional Delayed Cross Sections (2<sup>nd</sup> binary file):
      - Delayed Neutron Families' Fractions (if fissile region)
      - Delayed Neutron Decay Constants (if fissile region)
      - Delayed Neutron Fission Spectrum (if fissile region)
- MICROSCOPIC (**fixed** 107 energy groups' structure) homogenized cross sections:
  - o For each homogenized MICROscopic region (e.g. assembly), tabulation coordinate (e.g. BURN-UP level) and isotope (e.g. U235) two required binary files are provided (optionally Delayed Neutron File), containing the following cross sections:
    - Prompt Fast Groups' Cross Sections (1<sup>st</sup> binary file):
      - Total XS
      - Capture and Absorption XS
      - Production XS
      - Fission XS (if fissile region)
      - Total Fission Spectrum (if fissile region)
    - Prompt Thermal Groups' Cross Sections (2<sup>st</sup> binary file):



- Total XS
- Capture and Absorption XS
- Production XS
- Fission XS (if fissile region)
- Total Fission Spectrum (if fissile region)
- Optional Delayed Cross Sections (3<sup>rd</sup> optional binary file):
  - Delayed Neutron Families' Fractions (if fissile region)
  - Delayed Neutron Decay Constants (if fissile region)
  - Delayed Neutron Fission Spectrum (if fissile region)

## 2. PHISICS XS Format

PHISICS core simulator is able to import cross sections set (tabulated and not) from four different standards:

- 1) Native XML-format
- 2) AMPX code format libraries
- 3) ISOTXS-format
- 4) ECCO/ERANOS code format

The cross-section format that is generated by the PDS converter software here documented is the Native PHISICS XML-format.

The PHISICS XML-format supports three types of cross-sections set:

- *RunMacro*: un-tabulated MACROscopic cross sections:
  - o This cross-section set can be used for eigenvalue, source and time-dependent calculations using the executables *instant* (eigenvalue and source problems) and *time\_dep* (time-dependent standalone calculations). In addition, they can be inputted in RELAP5-3D card system for steady-state or transient problems. An example of this format is reported in the table below:

Table 1. RunMacro XML cross-section set example

RunMacro
<pre> &lt;Macros NG="2"&gt;   &lt;material ID="1" NA="0" fissile="true"&gt;     &lt;name&gt;material1&lt;/name&gt;     &lt;TotalXS&gt;0.22 0.8&lt;/TotalXS&gt;     &lt;NuFissionXS&gt;0.006 0.1&lt;/NuFissionXS&gt;     &lt;ChiXS&gt;1.0 0.0&lt;/ChiXS&gt;     &lt;ScatteringXS&gt;       0.193 0.0       0.017 0.730     &lt;/ScatteringXS&gt;   &lt;/material&gt;   &lt;material ID="2" NA="0" fissile="false"&gt;     &lt;name&gt;material2&lt;/name&gt;     &lt;TotalXS&gt;0.53 0.94&lt;/TotalXS&gt;     &lt;ScatteringXS&gt;       0.526 0.0       0.001 0.83     &lt;/ScatteringXS&gt;   &lt;/material&gt;   &lt;material ID="3" NA="0" fissile="false"&gt;     &lt;name&gt;material3&lt;/name&gt;     &lt;TotalXS&gt;0.701 2.0&lt;/TotalXS&gt;     &lt;ScatteringXS&gt;       0.65 0.0       0.05 1.97     &lt;/ScatteringXS&gt;   &lt;/material&gt; &lt;/Macros&gt; </pre>

- *TabulatedMacro*: tabulated MACROscopic cross sections:
  - o This cross-section set can be used for eigenvalue, source and time-dependent calculations using the executables *instant* (eigenvalue and source problems), *time\_dep* (time-dependent standalone calculations) or coupled with RELAP5-3D (steady state and transient) using the coupled PHISICS/RELAP5-3D executable *relap5.x*. An example of this format is reported in the table below:

Table 2. *TabulatedMacro XML cross-section set example*

<i>TabulatedMacro</i>
<pre> &lt;Macros NG="4"&gt;   &lt;tabulation ID="1" N="3" ND="3"&gt;     &lt;dimension ID="DR" PT="1" REF="0"&gt;0&lt;/dimension&gt;     &lt;dimension ID="Ro_mod_VR_1" PT="2" REF="6.535E+02"&gt;       1.0036E+03 6.535E+02     &lt;/dimension&gt;     &lt;dimension ID="T_stru_HR_1" PT="1" REF="5.3315E+02"&gt;       5.3315E+02     &lt;/dimension&gt;   &lt;/tabulation&gt;   &lt;dim ID="DR" TabID="1" pt="0"&gt;     &lt;dim ID="Ro_mod_VR_1" TabID="1" pt="1.0036E+03"&gt;       &lt;dim ID="T_stru_HR_1" TabID="1" pt="5.3315E+02"&gt;         &lt;matstart N="1"&gt;           &lt;material ID="1" NA="0" fissile="true"&gt;             &lt;TotalXS&gt;1.14E-01 2.05E-01 3.29E-01 3.80E-01&lt;/TotalXS&gt;             &lt;FissionXS&gt;2.06E-02 6.10E-03 6.91E-03 2.60E-02&lt;/FissionXS&gt;             &lt;ScatteringXS&gt;               7.04326E-02 0 0 0               3.47967E-02 1.95443E-01 0 0               1.88282E-03 6.20863E-03 3.20586E-01 0               7.07208E-07 9.92975E-04 3.6236E-01 0             &lt;/ScatteringXS&gt;             &lt;ChiXS&gt;9.7077E-01 2.92301E-02 0 0&lt;/ChiXS&gt;             &lt;ChiDelXS nf="1"&gt;9.7077E-01 2.92301E-02 0 0&lt;/ChiDelXS&gt;             &lt;ChiDelXS nf="2"&gt;9.7077E-01 2.92301E-02 0 0&lt;/ChiDelXS&gt;             &lt;ChiDelXS nf="3"&gt;9.7077E-01 2.92301E-02 0 0&lt;/ChiDelXS&gt;             &lt;ChiDelXS nf="4"&gt;9.7077E-01 2.92301E-02 0 0&lt;/ChiDelXS&gt;             &lt;ChiDelXS nf="5"&gt;9.7077E-01 2.92301E-02 0 0&lt;/ChiDelXS&gt;             &lt;ChiDelXS nf="6"&gt;9.7077E-01 2.92301E-02 0 0&lt;/ChiDelXS&gt;             &lt;beta&gt;               2.1E-04 1.4E-03 1.2E-03 2.5E-03 7.4E-04 2.7E-04             &lt;/beta&gt;           &lt;/material&gt;         &lt;/matstart&gt;       &lt;/dim&gt;     &lt;/dim&gt;   &lt;/dim&gt;   &lt;dim ID="Ro_mod_VR_1" TabID="1" pt="6.535E+03"&gt;     &lt;dim ID="T_stru_HR_1" TabID="1" pt="5.3315E+02"&gt;       &lt;matstart N="1"&gt;         &lt;material ID="1" NA="0" fissile="true"&gt;           &lt;TotalXS&gt;1.14E-01 2.05E-01 3.29E-01 3.80E-01&lt;/TotalXS&gt;           &lt;FissionXS&gt;2.06E-02 6.10E-03 6.91E-03 2.60E-02&lt;/FissionXS&gt;           &lt;ScatteringXS&gt;             7.04326E-02 0 0 0             3.47967E-02 1.95443E-01 0 0             1.88282E-03 6.20863E-03 3.20586E-01 0             7.07208E-07 9.92975E-04 3.6236E-01 0           &lt;/ScatteringXS&gt;           &lt;ChiXS&gt;9.7077E-01 2.92301E-02 0 0&lt;/ChiXS&gt;           &lt;ChiDelXS nf="1"&gt;9.70E-01 2.923E-02 0 0&lt;/ChiDelXS&gt;           &lt;ChiDelXS nf="2"&gt;9.70E-01 2.923E-02 0 0&lt;/ChiDelXS&gt;           &lt;ChiDelXS nf="3"&gt;9.70E-01 2.923E-02 0 0&lt;/ChiDelXS&gt;           &lt;ChiDelXS nf="4"&gt;9.70E-01 2.923E-02 0 0&lt;/ChiDelXS&gt;           &lt;ChiDelXS nf="5"&gt;9.70E-01 2.923E-02 0 0&lt;/ChiDelXS&gt;           &lt;ChiDelXS nf="6"&gt;9.70E-01 2.923E-02 0 0&lt;/ChiDelXS&gt;           &lt;beta&gt;             2.1E-04 1.4E-03 1.2E-03 2.5E-03 7.4E-04 2.7E-04           &lt;/beta&gt;         &lt;/material&gt;       &lt;/matstart&gt;     &lt;/dim&gt;   &lt;/dim&gt; &lt;/dim&gt; &lt;/Macros&gt; </pre>

- *RunMicro and TabulatedMicro*: tabulated and not MICROscopic cross sections:
  - o These cross-section sets can be used for eigenvalue, source, time-dependent, depletion, criticality search, fuel management and control rod movement calculations using the

executables *dpl instant\_run* (PHISICS standalone) and *relap5.x* (PHISICS/RELAP5-3D coupled). An example of this format is reported in the table below:

*Table 3. Microscopic XML cross-section set example*

<i>RunMicro and TabulatedMicro</i>
<pre> &lt;Micro NG="2" n_libraries="4"&gt;   &lt;NeutronEnergyBound&gt;200.0 1 1.0E-6&lt;/NeutronEnergyBound&gt;   &lt;no_tabulation&gt;     &lt;library lib_name="fuel1" n_iso="12" na="0"&gt;       &lt;isotope id="U235" fissile="true"&gt;         &lt;TotalXS&gt;0.0 0.0&lt;/TotalXS&gt;         &lt;ngXS&gt;4.20 42.90&lt;/ngXS&gt;         &lt;nalphaXS&gt;0 0&lt;/nalphaXS&gt;         &lt;npxXS&gt;0 0&lt;/npxXS&gt;         &lt;n2nXS&gt;0 0&lt;/n2nXS&gt;         &lt;NuFissionXS&gt;18.544 582.184&lt;/NuFissionXS&gt;         &lt;FissionXS&gt;7.60 238.60&lt;/FissionXS&gt;         &lt;KappaXS&gt;2.432E-10 7.635E-09&lt;/KappaXS&gt;         &lt;ChiXS&gt;1 0&lt;/ChiXS&gt;         &lt;ScatteringXS&gt;           &lt;XS&gt;             -11.80 0.0             0.0 -282.50           &lt;/XS&gt;         &lt;/ScatteringXS&gt;       &lt;/isotope&gt;       &lt;isotope id="U238" fissile="true"&gt;         &lt;TotalXS&gt;0.0 0.0&lt;/TotalXS&gt;         &lt;ngXS&gt;0.85 1.23&lt;/ngXS&gt;         &lt;nalphaXS&gt;0 0&lt;/nalphaXS&gt;         &lt;npxXS&gt;0 0&lt;/npxXS&gt;         &lt;n2nXS&gt;0 0&lt;/n2nXS&gt;         &lt;NuFissionXS&gt;0.342 0.00&lt;/NuFissionXS&gt;         &lt;FissionXS&gt;0.12 0.00&lt;/FissionXS&gt;         &lt;KappaXS&gt;3.840E-12 0.00&lt;/KappaXS&gt;         &lt;ChiXS&gt;1 0&lt;/ChiXS&gt;         &lt;ScatteringXS&gt;           &lt;XS&gt;             -0.97 0.0             0.0 -1.23           &lt;/XS&gt;         &lt;/ScatteringXS&gt;       &lt;/isotope&gt;       &lt;isotope id="XE135" fissile="false"&gt;         &lt;TotalXS&gt;0.0 0.0&lt;/TotalXS&gt;         &lt;ngXS&gt;0.0 1.20E+6&lt;/ngXS&gt;         &lt;nalphaXS&gt;0 0&lt;/nalphaXS&gt;         &lt;npxXS&gt;0 0&lt;/npxXS&gt;         &lt;n2nXS&gt;0 0&lt;/n2nXS&gt;         &lt;ScatteringXS&gt;           &lt;XS&gt;             0.0 0.0             0.0 -1200000.00           &lt;/XS&gt;         &lt;/ScatteringXS&gt;       &lt;/isotope&gt;     &lt;/library&gt;     &lt;library lib_name="reflector" n_iso="1" na="0"&gt;       &lt;isotope id="STRM" fissile="false"&gt;         &lt;TotalXS&gt;0.257 1.31&lt;/TotalXS&gt;         &lt;ngXS&gt;9.80E-4 0.138&lt;/ngXS&gt;         &lt;n2nXS&gt;0 0&lt;/n2nXS&gt;         &lt;ScatteringXS&gt;           &lt;XS&gt;             0.23232 0.0             2.37E-2 1.172           &lt;/XS&gt;         &lt;/ScatteringXS&gt;       &lt;/isotope&gt;     &lt;/library&gt;   &lt;/no_tabulation&gt; &lt;/Micro&gt; </pre>

The detailed input specifications of the native PHISICS XML cross-section structure can be found in the PHISICS manuals.

## 3. PDS Converter Software

The PDS Converter Software is a Python code that has been developed in order to convert PDS cross-section format into PHISICS-compatible XML structures. This software is able to process any PDS XS binary file, such as MACROscopic, MICROscopic and Delayed Neutron files.

In the following sections, the software requirements and a brief user guide is reported.

### 3.1 PDS Converter Software Requirements

As already mentioned, the PDS Converter Software has been coded in Python. The following software requirements and dependencies need to be installed before using the Software:

- Python 2.7, available at <https://www.python.org/download/releases/2.7/>
- NumPy library, available at <http://www.numpy.org/>
- SciPy library, available at <https://www.scipy.org/index.html>
- lxml library, available at <http://lxml.de/>

Once the installation of the requirements and libraries is performed, the PDS Converter Software can be used.

### 3.2 PDS Converter Software User Guide

#### 3.2.1 Where to download the PDS Converter

The PDS Converter software can be downloaded either from the INL share-point collaborative portal (reachable at <https://usjapanecwg.inl.gov/SitePages/Home.aspx>) or from the PHISICS GITLAB repository (reachable at <https://hpcgitlab.inl.gov/Phisics/PHISICS>) in the directory *./PHISICS/scripts/XS\_converters/PDS\_SRAC\_converter*.

#### 3.2.2 How to run the PDS Converter Software

The PDS Converter Software is named “*PDS\_converter.py*” and can be executed with the following command:

```
python PDS_converter.py -t XXX input_file_name.xml
```

Where:

- *XXX*, is the type of conversion that needs to be performed:
  - o *run\_macro*, for converting PDS macroscopic XS set into the *RunMacro* XML format
  - o *tabulated\_macro*, for converting PDS tabulated macroscopic XS set into *TabulatedMacro* XML format
  - o *micro*, for converting PDS microscopic XS set (or mixed) into *RunMicro* or *TabulatedMicro* XML format
- *input\_file\_name.xml*, is the templated XML input file that will be converted (user defined name), whose format depends on the flag *XXX*.

The output file name of the Software is *input\_file\_name\_CONVERTED.xml*.

#### 3.2.3 Content and Formats of the XML input file

Depending on the value assumed by the flag *XXX*, the templated XML input file changes following the Native PHISICS XML formats reported in section 2. In the following, examples for each of the templated input files are reported.

### 3.2.3.1 run\_macro

The templated XML input file for the `run_macro` option is very similar to the PHISICS XML *RunMacro* input file, but replacing the cross-section XML nodes in the `<material>` sections (e.g. `<ScatteringXS>`, `<TotalXS>`, etc.) with the following XML nodes:

- `<pds_macro_xs_file>`, string, **required**, path to the location of the macro XS PDS file associated with this MACRO region.
- `<pds_betas_file>`, string, **optional**, path to the location of the Delayed Neutron PDS file associated with this MACRO region. **Note:** if this file is provided, among the others, an XML node named `<lambda>` will be generated in the output file; this node must be removed from the XS set and added in either the *time\_dep* input file or the RELAP5-3D input file.

If only the `<pds_macro_xs_file>` is provided, the cross-sections set will be usable in *instant* standalone calculations. If also `<pds_betas_file>` is provided, the cross-sections set will be usable in *instant* and *time\_dep* standalone calculations.

An example of the templated input file is reported in table below.

Table 4. RunMacro templated XML input file

RunMacro
<pre> &lt;Macros NG="4"&gt;   &lt;material ID="1" NA="0" fissile="true"&gt;     &lt;name&gt;Core&lt;/name&gt;     &lt;pds_macro_xs_file&gt;       TAKEDA_4g_material_1.pds     &lt;/pds_macro_xs_file&gt;     &lt;pds_betas_file&gt; test_betas_material_1.pds&lt;/pds_betas_file&gt;   &lt;/material&gt;   &lt;material ID="2" NA="0" fissile="false"&gt;     &lt;name&gt;Reflector&lt;/name&gt;     &lt;pds_macro_xs_file&gt;       TAKEDA_4g_material_2.pds     &lt;/pds_macro_xs_file&gt;     &lt;pds_betas_file&gt; test_betas_material_2.pds&lt;/pds_betas_file&gt;   &lt;/material&gt;   &lt;material ID="3" NA="0" fissile="false"&gt;     &lt;name&gt;Control rod&lt;/name&gt;     &lt;pds_macro_xs_file&gt;       TAKEDA_4g_material_3.pds     &lt;/pds_macro_xs_file&gt;     &lt;pds_betas_file&gt;test_betas_material_3.pds&lt;/pds_betas_file&gt;   &lt;/material&gt;   &lt;material ID="4" NA="0" fissile="false"&gt;     &lt;name&gt;Empty&lt;/name&gt;     &lt;pds_macro_xs_file&gt;       TAKEDA_4g_material_4.pds     &lt;/pds_macro_xs_file&gt;   &lt;/material&gt; &lt;/Macros&gt; </pre>

To execute the PDS converter with this format, the following command must be launched:

```
python PDS_converter.py -t run_macro input_file_name.xml
```

### 3.2.3.2 *tabulated\_macro*

The templated XML input file for the *tabulated\_macro* option is very similar to the PHISICS XML *TabulatedMacro* input file, but replacing the cross-section XML nodes in the *<material>* sections (e.g. *<ScatteringXS>*, *<TotalXS>*, etc.) with the following XML nodes:

- *<pds\_macro\_xs\_file>*, string, **required**, path to the location of the macro XS PDS file associated with this MACRO region.
- *<pds\_betas\_file>*, string, **optional**, path to the location of the Delayed Neutron PDS file associated with this MACRO region. **Note:** if this file is provided, among the others, an XML node named *<lambda>* will be generated in the output file; this node must be removed from the XS set and added in either the *time\_dep* input file or the RELAP5-3D input file.

If only the *<pds\_macro\_xs\_file>* is provided, the cross-sections set will be usable in *instant* standalone calculations and in *relap5.x* coupled calculations (steady state). If also *<pds\_betas\_file>* is provided, the cross-sections set will be usable in *instant*, *time\_dep* standalone and in *relap5.x* coupled (transient and steady state) calculations.

An example of the templated input file is reported in table below.

Table 5. *TabulatedMacro* templated XML input file

<i>TabulatedMacro</i>
<pre> &lt;Macros NG="4"&gt;   &lt;tabulation ID="1" N="3" ND="3"&gt;     &lt;dimension ID="DR" PT="1" REF="0"&gt;0&lt;/dimension&gt;     &lt;dimension ID="Ro_mod_VR_1" PT="2" REF="6.535E+02"&gt;       1.0036E+03 6.535E+02     &lt;/dimension&gt;     &lt;dimension ID="T_stru_HR_1" PT="1" REF="5.3315E+02"&gt;       5.3315E+02     &lt;/dimension&gt;   &lt;/tabulation&gt;   &lt;dim ID="DR" TabID="1" pt="0"&gt;     &lt;dim ID="Ro_mod_VR_1" TabID="1" pt="1.0036E+03"&gt;       &lt;dim ID="T_stru_HR_1" TabID="1" pt="5.3315E+02"&gt;         &lt;matstart N="1"&gt;           &lt;material ID="1" NA="0" fissile="true"&gt;             &lt;pds_macro_xs_file&gt;               TAKEDA_4g_material_tab1.pds             &lt;/pds_macro_xs_file&gt;             &lt;pds_betas_file&gt;               test_betas_material_tab1.pds             &lt;/pds_betas_file&gt;           &lt;/material&gt;         &lt;/matstart&gt;       &lt;/dim&gt;     &lt;/dim&gt;     &lt;dim ID="Ro_mod_VR_1" TabID="1" pt="6.535E+03"&gt;       &lt;dim ID="T_stru_HR_1" TabID="1" pt="5.3315E+02"&gt;         &lt;matstart N="1"&gt;           &lt;material ID="1" NA="0" fissile="true"&gt;             &lt;pds_macro_xs_file&gt;               TAKEDA_4g_material_tab2.pds             &lt;/pds_macro_xs_file&gt;             &lt;pds_betas_file&gt;               test_betas_material_tab2.pds             &lt;/pds_betas_file&gt;           &lt;/material&gt;         &lt;/matstart&gt;       &lt;/dim&gt;     &lt;/dim&gt;   &lt;/dim&gt; &lt;/Macros&gt; </pre>

To execute the PDS converter with this format, the following command must be launched:

```
python PDS_converter.py -t tabulated_macro input_file_name.xml
```

### 3.2.3.3 *micro*

The templated XML input file for the *micro* option is very similar to the PHISICS XML *RunMicro* and *TabulatedMicro* input file, but replacing the cross-section XML nodes in the *<isotope>* sections (e.g. *<ScatteringXS>*, *<TotalXS>*, etc.) with the following XML nodes:

- *<pds\_micro\_xs\_file>*, comma separated string, **required**, path to the location of the micro XS PDS files associated with this ISOTOPE:
  - o First filename is the PDS file containing XS for the Fast Groups (whose number is inputted with the attribute **NGF** in the *<Micro>* XML node)
  - o Second filename is the PDS file containing XS for the Thermal Groups
- *<pds\_betas\_file>*, string, **optional**, path to the location of the Delayed Neutron PDS file associated with this ISOTOPE. **Note:** if this file is provided, among the others, an XML node named *<lambda>* will be generated in the output file; this node must be removed from the XS set and added in either the *time\_dep* input file or the RELAP5-3D input file. If delayed neutron information is available at the MACRO level only, a new *<isotope>* XML node needs to be created containing the *<pds\_betas\_file>* XML node (see example below, isotope named "macro").

The conversion of the MICROscopic XS in PDS format is slightly different than the one for MACROscopic PDS files. Indeed, the PDS MICROscopic format has two drawbacks:

- 1) Homogenized microscopic cross sections can be exported in a fixed fine-energy structure (107 groups) only (no collapsing is performed to get coarse-group XS)
- 2) Only 1D cross sections (e.g. Fission, Total, etc.) are provided (no Scattering XS is present)

The first issue (fixed 107 group fine-energy structure) is optionally addressed as follows:

- I) The user can request to collapse the 1D cross sections into a coarse energy structure. For achieving this, in each *<library>* XML node, a new node, named *<for\_collapsing>*, needs to be inputted. This node will contain two additional XML nodes:
  - a. *<flux>*, space separated value, **required**, the flux for each fine energy structure must be inputted (107 values)
  - b. *<NeutronEnergyBound>*, space separated value, **required**, the energy bounds of the fine energy structure (108 values)

If is inputted, the 1D microscopic cross sections will be collapsed to the coarse energy structure defined by the attribute **NG** and the node *<NeutronEnergyBound>* in the *<Micro>* XML node.

The second issue (1D cross sections only) is addressed in two mutual exclusive ways:

- I) Within each *<isotope>* XML node, the *<ScatteringXS>* must be manually inputted, or
- II) A new *<isotope>* XML node needs to be created containing the *<pds\_macro\_xs\_file>* XML node (see example below, isotope named "macro"). **Note:** The macroscopic XS here inputted is assumed to have been preprocessed removing the other isotope contributions

It is important to notice that if no collapsing is requested, the *<ScatteringXS>* or the MACRO XS contained in the specified *<pds\_macro\_xs\_file>* must have the fixed fine-energy structure of the MICROscopic XS (i.e. 107 groups).

If only the *<pds\_micro\_xs\_file>* (s) are provided, the cross-sections set will be usable in *dpl\_instant\_run* standalone calculations and in *relap5.x* coupled calculations (steady state, depletion evolution with feedback,



etc.). If also `<pds_betas_file>` (s) are provided, the cross-sections set will be usable in `dpl_instant_run`, `time_dep` standalone and in `relap5.x` coupled (transient and steady state) calculations.

An example of the templated input file is reported in table below.

Table 6. RunMicro and TabulatedMicro templated XML input file

RunMicro and TabulatedMicro	
<pre> &lt;Micro NG="4" NGF="61" n_libraries="4"&gt;   &lt;NeutronEnergyBound&gt;     200.0 2.0 1.0 0.0001 1.0E-6   &lt;/NeutronEnergyBound&gt;   &lt;no_tabulation&gt;     &lt;library lib_name="material1" n_iso="3" na="0"&gt;       &lt;for_collapsing&gt;         &lt;flux&gt;           5.000E+06 5.171E+06 5.353E+06 5.549E+06 5.760E+06           5.988E+06 6.234E+06 6.502E+06 6.793E+06 7.112E+06           7.463E+06 7.849E+06 8.278E+06 8.757E+06 9.294E+06           9.901E+06 1.059E+07 1.139E+07 1.232E+07 1.340E+07           1.471E+07 1.629E+07 1.825E+07 2.075E+07 2.404E+07           2.857E+07 3.521E+07 4.587E+07 6.579E+07 1.163E+08           5.000E+08 5.085E+08 5.172E+08 5.263E+08 5.357E+08           5.455E+08 5.556E+08 5.660E+08 5.769E+08 5.882E+08           6.000E+08 6.122E+08 6.250E+08 6.383E+08 6.522E+08           6.667E+08 6.818E+08 6.977E+08 7.143E+08 7.317E+08           7.500E+08 7.692E+08 7.895E+08 8.108E+08 8.333E+08           8.571E+08 8.824E+08 9.091E+08 9.375E+08 9.677E+08           1.000E+09 1.026E+09 1.053E+09 1.081E+09 1.111E+09           1.143E+09 1.176E+09 1.212E+09 1.250E+09 1.290E+09           1.333E+09 1.379E+09 1.429E+09 1.481E+09 1.538E+09           1.600E+09 1.667E+09 1.739E+09 1.818E+09 1.905E+09           2.000E+09 2.105E+09 2.222E+09 2.353E+09 2.500E+09           2.666E+09 2.857E+09 3.076E+09 3.333E+09 3.635E+09           3.999E+09 4.443E+09 4.998E+09 5.712E+09 6.663E+09           7.994E+09 9.991E+09 1.332E+10 1.996E+10 3.984E+10           1.000E+13 1.198E+13 1.493E+13 1.980E+13 2.941E+13           3.636E+13 5.714E+13         &lt;/flux&gt;       &lt;/for_collapsing&gt;     &lt;/library&gt;   &lt;/no_tabulation&gt;   &lt;NeutronEnergyBound&gt;     2.000E+02 1.934E+02 1.868E+02 1.802E+02 1.736E+02     1.670E+02 1.604E+02 1.538E+02 1.472E+02 1.406E+02     1.340E+02 1.274E+02 1.208E+02 1.142E+02 1.076E+02     1.010E+02 9.440E+01 8.780E+01 8.120E+01 7.460E+01     6.800E+01 6.140E+01 5.480E+01 4.820E+01 4.160E+01     3.500E+01 2.840E+01 2.180E+01 1.520E+01 8.600E+00     2.000E+00 1.967E+00 1.933E+00 1.900E+00 1.867E+00     1.833E+00 1.800E+00 1.767E+00 1.733E+00 1.700E+00     1.667E+00 1.633E+00 1.600E+00 1.567E+00 1.533E+00     1.500E+00 1.467E+00 1.433E+00 1.400E+00 1.367E+00     1.333E+00 1.300E+00 1.267E+00 1.233E+00 1.200E+00     1.167E+00 1.133E+00 1.100E+00 1.067E+00 1.033E+00     1.000E+00 9.750E-01 9.500E-01 9.250E-01 9.000E-01     8.750E-01 8.500E-01 8.250E-01 8.000E-01 7.750E-01     7.500E-01 7.250E-01 7.000E-01 6.750E-01 6.500E-01     6.250E-01 6.000E-01 5.750E-01 5.500E-01 5.250E-01     5.001E-01 4.751E-01 4.501E-01 4.251E-01 4.001E-01     3.751E-01 3.501E-01 3.251E-01 3.001E-01 2.751E-01     2.501E-01 2.251E-01 2.001E-01 1.751E-01 1.501E-01     1.251E-01 1.001E-01 7.509E-02 5.010E-02 2.510E-02     1.000E-04 8.350E-05 6.700E-05 5.050E-05 3.400E-05     2.750E-05 1.750E-05 1.000E-06   &lt;/NeutronEnergyBound&gt; &lt;/for_collapsing&gt; &lt;isotope id="U235" fissile="true" capture="true"&gt;   &lt;pds_micro_xs_file&gt;     Material_1_exampleIsotope1.pds,     Material_2_exampleIsotope2.pds   &lt;/pds_micro_xs_file&gt; &lt;/isotope&gt;  &lt;isotope id="XE135" fissile="false" capture="true"&gt;   &lt;pds_micro_xs_file&gt;     Material_1_exampleIsotope2.pds, </pre>	

---

```

Material_2_exampleIsotope2.pds
</pds_micro_xs_file>
</isotope>
<isotope id="macro" fissile="true" capture="true">
  <pds_macro_xs_file>
    Material_1_MACRO.pds
  </pds_macro_xs_file>
</isotope>
</library>
<library lib_name="material2" n_iso="3" na="0">
  <for_collapsing>
    <flux>
      5.000E+06 5.171E+06 5.353E+06 5.549E+06 5.760E+06
      5.988E+06 6.234E+06 6.502E+06 6.793E+06 7.112E+06
      7.463E+06 7.849E+06 8.278E+06 8.757E+06 9.294E+06
      9.901E+06 1.059E+07 1.139E+07 1.232E+07 1.340E+07
      1.471E+07 1.629E+07 1.825E+07 2.075E+07 2.404E+07
      2.857E+07 3.521E+07 4.587E+07 6.579E+07 1.163E+08
      5.000E+08 5.085E+08 5.172E+08 5.263E+08 5.357E+08
      5.455E+08 5.556E+08 5.660E+08 5.769E+08 5.882E+08
      6.000E+08 6.122E+08 6.250E+08 6.383E+08 6.522E+08
      6.667E+08 6.818E+08 6.977E+08 7.143E+08 7.317E+08
      7.500E+08 7.692E+08 7.895E+08 8.108E+08 8.333E+08
      8.571E+08 8.824E+08 9.091E+08 9.375E+08 9.677E+08
      1.000E+09 1.026E+09 1.053E+09 1.081E+09 1.111E+09
      1.143E+09 1.176E+09 1.212E+09 1.250E+09 1.290E+09
      1.333E+09 1.379E+09 1.429E+09 1.481E+09 1.538E+09
      1.600E+09 1.667E+09 1.739E+09 1.818E+09 1.905E+09
      2.000E+09 2.105E+09 2.222E+09 2.353E+09 2.500E+09
      2.666E+09 2.857E+09 3.076E+09 3.333E+09 3.635E+09
      3.999E+09 4.443E+09 4.998E+09 5.712E+09 6.663E+09
      7.994E+09 9.991E+09 1.332E+10 1.996E+10 3.984E+10
      1.000E+13 1.198E+13 1.493E+13 1.980E+13 2.941E+13
      3.636E+13 5.714E+13
    </flux>
    <NeutronEnergyBound>
      2.000E+02 1.934E+02 1.868E+02 1.802E+02 1.736E+02
      1.670E+02 1.604E+02 1.538E+02 1.472E+02 1.406E+02
      1.340E+02 1.274E+02 1.208E+02 1.142E+02 1.076E+02
      1.010E+02 9.440E+01 8.780E+01 8.120E+01 7.460E+01
      6.800E+01 6.140E+01 5.480E+01 4.820E+01 4.160E+01
      3.500E+01 2.840E+01 2.180E+01 1.520E+01 8.600E+00
      2.000E+00 1.967E+00 1.933E+00 1.900E+00 1.867E+00
      1.833E+00 1.800E+00 1.767E+00 1.733E+00 1.700E+00
      1.667E+00 1.633E+00 1.600E+00 1.567E+00 1.533E+00
      1.500E+00 1.467E+00 1.433E+00 1.400E+00 1.367E+00
      1.333E+00 1.300E+00 1.267E+00 1.233E+00 1.200E+00
      1.167E+00 1.133E+00 1.100E+00 1.067E+00 1.033E+00
      1.000E+00 9.750E-01 9.500E-01 9.250E-01 9.000E-01
      8.750E-01 8.500E-01 8.250E-01 8.000E-01 7.750E-01
      7.500E-01 7.250E-01 7.000E-01 6.750E-01 6.500E-01
      6.250E-01 6.000E-01 5.750E-01 5.500E-01 5.250E-01
      5.001E-01 4.751E-01 4.501E-01 4.251E-01 4.001E-01
      3.751E-01 3.501E-01 3.251E-01 3.001E-01 2.751E-01
      2.501E-01 2.251E-01 2.001E-01 1.751E-01 1.501E-01
      1.251E-01 1.001E-01 7.509E-02 5.010E-02 2.510E-02
      1.000E-04 8.350E-05 6.700E-05 5.050E-05 3.400E-05
      2.750E-05 1.750E-05 1.000E-06
    </NeutronEnergyBound>
  </for_collapsing>
  <isotope id="U235" fissile="true" capture="true">
    <pds_micro_xs_file>
      Material_2_exampleIsotope1.pds,
      Material_2_exampleIsotope2.pds
    </pds_micro_xs_file>
  </isotope>
  <isotope id="XE135" fissile="false" capture="true">
    <pds_micro_xs_file>
      Material_2_exampleIsotope2.pds,
      Material_2_exampleIsotope2.pds
    </pds_micro_xs_file>
  </isotope>

  <isotope id="macro" fissile="true" capture="true">
    <pds_macro_xs_file>
      Material_2_MACRO.pds

```

---

---

```
    </pds_macro_xs_file>
  </isotope>
</library>
<library lib_name="reflector" n_iso="1" na="0">
  <isotope id="macro" fissile="false" capture="true">
    <pds_macro_xs_file>
      reflector_macro.pds
    </pds_macro_xs_file>
  </isotope>
</library>
</no_tabulation>
</Micro>
```

---

To execute the PDS converter with this format, the following command must be launched:

```
python PDS_converter.py -t micro input_file_name.xml
```