From ENDF to PENDF: NJOY versus PREPRO

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as presented at ND2010 (Jeju Island) by me@marychin.org
Why do we need NJOY and/or PREPRO?

Why can’t we use these direct?

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Does this look like a neutron cross section plot?

somewhat weird:
- absence of resonances
- apparent zero cross sections and discontinuity

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Does this look like a neutron cross section plot?

This looks more like it...

somewhat weird:
- absence of resonances
- apparent zero cross sections and discontinuity

that’s what NJOY and PREPRO are for

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Nuclear data processing does affect Monte Carlo.
Existing Literature


We are not here to add/report any preferred/hardwired processing chain as presented at ND2010 (Jeju Island) by me@marychin.org
but rather to consider the **flexibilities and constraints**

**NJOY**

- module A
  - pendf
  - module B
    - pendf
    - module C
      - pendf
      - module D
        - pendf
        - module E
          - pendf
          - module F

**PREPRO**

- module S
  - pendf
  - module T
  - pendf
  - module U
  - pendf
  - module V
  - pendf
  - module W
  - pendf
  - module X

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the fact that both are modular and i/o by pendfs

opens up the possibility to *interleave*

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that each module

inputs as ‘ingredient’ and

outputs to

different parts (MF-MT pairs) of the

ENDF/PENDF

allows some modules

not to fuss over which goes first

flexibility #2

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how far can we *interleave / swap*

**constraint #1**
unionisation of energy grids

**constraint #2**
inter-module dependencies

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do we want a common energy grid?

extra/‘redundant’ data points, if implemented in a Monte Carlo code, may ‘plague’ every step of every event in every history

Fig. 1. The after-to-before ratio of energy points for MF3 MT1 (total reaction cross section) at a) linearisation; b) unionisation of energy grid. Data are shown for the processing of the 381 materials given in JEFF 3.1.1 incident neutron sub-library.
one of the possible routes to avoid unionisation of energy grids as far as possible

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if we do not mind unionised grids

these could be replaced by RECONR

this could be replaced by BROADR

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complementary physics add-ons / optional modules

lower inter-module dependency, eg:
- ACTIVATE acts on MF9, 10
- LEGEND modifies MF4
- HEATR writes to MT301~450
- UNRESR modifies MF2 MT152
- PURR modifies MF2 MT152, 153
- GASPR writes to MF3 MT203~207
- THERMR writes to MF3, 6 MT211
- SIXPAK doesn’t touch the PENDF

overlapping core modules eg:
- resonance reconstruction
- Doppler broadening & thinning

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<table>
<thead>
<tr>
<th></th>
<th>NJOY</th>
<th>PREPRO</th>
</tr>
</thead>
<tbody>
<tr>
<td>INPUT</td>
<td>active decision from user</td>
<td>defaults available</td>
</tr>
<tr>
<td>OUTPUT</td>
<td>higher verbosity</td>
<td></td>
</tr>
<tr>
<td>PREPRO</td>
<td>NJOY</td>
<td>function</td>
</tr>
<tr>
<td>---------</td>
<td>---------</td>
<td>-----------------------------------------------</td>
</tr>
<tr>
<td>LINEAR</td>
<td>RECONR</td>
<td>linearisation (unionisation)</td>
</tr>
<tr>
<td>RECENT</td>
<td></td>
<td>resolved resonance reconstruction</td>
</tr>
<tr>
<td>SIGMAI</td>
<td>BROADR</td>
<td>Doppler broadening &amp; thinning</td>
</tr>
</tbody>
</table>

functionally equivalent and technically interchangeable modules...

Next question: do the pairs produce equivalent results?
functionally equivalent and technically interchangeable modules... Next question: do the pairs produce equivalent results?

not readily obvious...

most agree some require further investigations

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MAT 7925

Total Cross Section

79-Au-197

-7.829 To 7.829 %

Cross Section (barns)

seq #1

seq #2

Min Ratio

Max Ratio

Ratio

seq #2/seq #1

10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7}

10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6} 10^{7}

1

Incident Energy (eV)

79-Au-197

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1997 negative cross sections detected

indeed they are in the original jeff3.1.1 tape

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but negativity is sometimes intentional. We don’t even need PREPRO/NJOY, detecting negative values is easy. as presented at ND2010 (Jeju Island) by me@marychin.org
ACE files are available everywhere

why mess about with flexibility, constraints, ...?

coz this work is for FLUKA, not MCNP(X)

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FLUKA is different

it is not tied to the ACE format;
it is general-purpose but sub-critical;
most importantly:
it is capable of analog in addition to non-analog transport

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FLUKA vs MCNP(X)

\[ ^{10}\text{B} + ^{1}\text{n} \rightarrow \begin{cases} ^{7}\text{Li} + ^{4}\alpha \\ ^{7}\text{Li}^* + ^{4}\alpha \end{cases} \]

\[ Q\text{-value} \]

- 2.792 MeV (ground state)
- 2.310 MeV (excited state)


From a single collision, MCNP(X) would happily produce one, two or three 0.48 MeV gammas (each of weight=1).

But gets it right when averaged over many histories (one 0.48 MeV gamma 94% of the time).

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FLUKA vs MCNP(X)

\[ ^{10}\text{B} + ^{1}_0\text{n} \rightarrow \begin{cases} \text{\(^{7}\text{Li} + ^{4}_2\text{He}\)} & 2.792 \text{ MeV (ground state)} \\ \text{\(^{3}\text{Li}^* + ^{4}_2\text{He}\)} & 2.310 \text{ MeV (excited state)} \end{cases} \]

0.48 MeV gamma

from a single collision

MCNP(X) would happily produce one, two or three 0.48 MeV gammas (each of weight=1)

but gets it right when averaged over many histories (one 0.48 MeV gamma 94% of the time)

won’t find such aberrations in FLUKA coz FLUKA is analog


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