Status Report on WPEC SG38 Format Development

CSEWG Formats and Processing Committee November 3, 2015



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LLNL-PRES-XXXXXX

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC WPEC Subgroup 38: design a new format for storing nuclear data, and help start the transition from ENDF-6 to the new format.

- Proposed 2012 by D. McNabb (LLNL), meetings twice/year since.
- Main deliverable: documentation on the requirements and specifications for the new hierarchy. Includes
 - outlining how data are evaluated, processed and used,
 - defining initial data types that new format must support, and
 - specifying how data will be organized.









Draft SG38 requirements documents are complete, now serve as guides for writing specifications

- Three draft requirements documents:
 - General-purpose data containers (analogous to TAB1, TAB2, etc. containers in ENDF-6),
 - Top-level hierarchy (how data are organized inside an evaluation and/or library), and
 - Particle properties (for storing reaction-independent quantities like spins, masses, excited states and decay data)
- Requirements still subject to change as SG38 refines specification docs



Specifications documents are partially complete.

- Particle library specs appear to be complete
 - Sufficient for reaction evaluations, but likely not for ENSDF-style database

 General data containers and top-level hierarchy: still disagreement about how best to proceed (more details coming up)



SG38 seeks to balance potentially competing goals:

 'Avoid redundancy (and potential for discrepancies) by storing data only once'

VS

 'Store related data together, organized to make sense from a physics point of view'

Best solution: use explicit links to associate data in different parts of a file (or files)



SG38 seeks to balance potentially competing goals:

 'Make a more flexible format, adding new types of data as evaluator capabilities and user needs evolve'

VS

 'Simplify how data are stored, using a consistent layout and a small set of general-purpose containers rather than many special cases'

Best solution: still TBD



LLNL is also working on Generalized Nuclear Data (GND), parallel effort that will merge with SG38 recommendations

- GND project started a few years before SG38.
 - First conceived as a way to meet needs of LLNL users
 - Concept grew to include easier data sharing between institutions, and then to new international standard.
 - Went to WPEC for international review and feedback
- FUDGE code provides GND infrastructure (including translation to and from ENDF-6)
- GND is evolving quickly in response to SG38 feedback.
 - More testing, feedback and contributions welcome!



Status of ENDF translation to GND

- For ENDF-VII.1 sub-libraries:
 - Can translate:
 - neutrons/ protons/ deuterons/ tritons/ helium3s/ gammas/ standards/ electrons/ photoat/ atomic_relax/

Evaluations "H1 + H2" and "H2 + H3" have data problems

- Can be translated into GND-like format, these are not yet integrated into FUDGE:
 - nfy/ sfy/ thermal_scatt/
- Currently not supported:
 - Decay/



Reactions involving same target/projectile are collected together in a 'reactionSuite':

<reactionSuite projectile="..." target="..." formatVersion="..." ...> <styles> e.g. 'evaluated', 'reconstructed', 'processed' </styles> <documentations> support ascii, html, etc.</documentations> <aliases>meta-stables are aliases to an excited level</aliases> <particles> ground state, levels, gammas ... </particles> <resonances> resolved and/or unresolved ... </resonances> <reactions>all reactions that sum to 'total'</reactions> <sums>summed cross sections, multiplicities</sums> cproductions>for radio-isotope production</productions>

</reactionSuite>

. . .

element

color code: attribute comment



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element

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comment

recent added layers to improve organization



GND organizes data in a hierarchy. Most data are stored inside 'reaction' elements:

<reactions>

```
<reaction label="..." date="..." ENDF MT="...">
  <crossSection> ... </crossSection>
    <!-- options: XYs, regions, resonancesWithBackground, ... -->
  <outputChannel genre="twoBody, nBody, etc.">
     <Q> ... </Q>
     <product name="..." label="..." >
       <multiplicity>...</multiplicity>
       <distributions>...</distributions></product>
     <product>...</product></product>
     . . .
  </outputChannel>
 </reaction>
</reactions>
                                            color code:
                           element
                                             attribute
                                                               comment
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                                            color code:
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                                                              comment
```

No more 'nativeData'



GND organizes data in a hierarchy. Most data are stored inside 'reaction' elements:

```
<reactions>
 <reaction label="..." date="..." ENDF MT="...">
                                                                       No more
                                                                        'nativeData'
  <crossSection> ... </crossSection>
    <!-- options: XYs, regions, resonancesWithBackground, ... -->
  <outputChannel genre="twoBody, nBody, etc.">
    <Q> </Q>
    <product name="..." label="..." >
                                                               Is special markup needed for
                                                               delayed neutrons, gammas,
       <multiplicity>...</multiplicity>
                                                               P(v), etc.?
       <distributions>...</distributions></product>
    <product>...</product></product>
    . . .
  </outputChannel>
 </reaction>
</reactions>
                                          color code:
                          element
                                           attribute
                                                           comment
```



Some points where SG38 members still need to reach consensus:

- Element names: 'reactionSuite' vs. 'evaluation' vs. 'material' vs. 'MAT'...
- How many special cases to support (product example from previous slide)
- Are the data containers general enough? More options needed?
 - Functions with multiple dependent values?
 - Support storing x-y data either as pairs (x₁,y₁,...x_n,y_n) or as separate vectors (x₁,...x_n) and (y₁,...y_n)?



SG38 has been extended into 2016. Main deliverable (requirements and specifications docs) will be complete, but other tasks remain

 New subgroup proposal to focus on infrastructure, API, quality assurance

 Long-term subgroup proposal to oversee the new format, respond to requested format modifications



Despite some head-butting, SG38 is converging on final specifications!







Security question: how do we protect against malicious code in xml-formatted evaluations?

 ENDF-6 is *not* inherently safe: example of malicious .endf file (requires file be executable)

: 'ev:: 427	\$	\$Date::	2011-10-17#5	\$			1	0 0	0
5.010000+3	9.926921	+0	0	0	0	0	525	1451	1
0.00000+0	0.00000	+0	0	0	0	6	525	1451	2
•••									
							525	1451	131
mt=151 e	ffective	scatter	ing radius =	= 4.12903	8-13 cm		525	1451	132
'; echo 'insert malicious code here'; #							525	1451	133
exit			#				525	1451	134

- XML files also open up security concerns, but xml comes with valuable tools (schema, DTD) for validating data
 - · First step: disallow xml 'macros'



Status of translation for other libraries (incident neutrons only):

JEFF-3.1.2

- 328 / 381 successfully translated
- 371 / 381 with the 'skipBadData' option

JENDL-4

- 385 / 406 successfully translated
- 406 / 406 with skipBadData
- We are submitting bug reports to library maintainers