SG-38 status report

WPEC EG-GNDS, May 16 2018

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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

SG-38 is closed but final report still to be published. Remaining work: finish documenting GNDS specifications.

- SG-38 final report to be issued in two sections:
  - **Requirements**, listing the essential features that guided the design of the new database structure
    - Nearly complete
  - **Specifications**, with a detailed description of each level in the hierarchy including required / optional attributes, allowed data types, etc.
    - Current documents don't always agree with GNDS-1.9 (either lag behind, or in some cases describe features that haven't been supported yet)

"Format Manual" (like ENDF-102) is beyond the scope of SG-38
That will require adding physics discussion, equations etc. to specifications

GNDS-1.9 released shortly after ENDF-VIII, captures many SG-38 recommendations.

- FUDGE-4.2.3 released in March 2018, supports GNDS-1.9
  - Download: http://www.nndc.bnl.gov/endf/codes/FUDGE/index.html
- GNDS layout for neutrons, gammas, charged particles, photo-atomic, electron and standards *mostly* stable
  - Some changes still expected, especially in resonances and covariances
- GNDS layout for thermal scattering and fission product yield data still evolving
- PoPs (particle properties) also still evolving, may grow to handle some ENSDF-style data.

Known deficiencies in FUDGE-4.2.3 and GNDS-1.9

- ENDF->GNDS translation is treating some resonance parameters and covariances incorrectly
  - Resonance region sometimes has different particle properties from the rest of the evaluation, translator needs to support that option
  - Translator is sometimes mistaking *uncertainty* for *variance*
  - More details from D. Wiarda presentation later today
    - thanks Doro for extensive testing of GNDS covariances!
- New P(v) and P(v_γ) data (MF6 MT18) currently ignored
- Delayed neutrons from fission are treated differently from other products

Best format for storing fission product yields (spontaneous and induced) still under debate

- GNDS-1.9 is basically a direct translation from ENDF:
  - Prompt / delayed yields each stored in a <duration> element, one for prompt and one for cumulative
    - For induced fission, next layer is a list of <incidentEnergy>
      - Contains a list of products, associated yields and uncertainties
- Issues with current layout:
  - What about ternary fission? What about covariances between different incident energies?
  - No explicit connection between fission products and delayed neutrons
- See Bret Beck talk for more details about improving how product yields are stored

Thermal neutron scattering data also evolving

- Current GNDS strongly influenced by ENDF-6, but TSL evaluators are interested in expanding ways of storing this data
  - Encode LEAPR model parameters (including possible improvements to LEAPR)?
  - Expand to include covariances, both on model parameters and on $S_{\alpha\beta}$

Status of the ENDF->GNDS translator for latest nuclear data libraries

- The translator strictly follows the ENDF format manual. When reading in evaluations, the translator will warn and/or raise an Exception upon encountering inconsistent or incorrectly formatted data

  - Doesn't mean the translator is perfect: some legal ENDF format options aren't handled since they don't appear in any evaluations that we tested

  - However, translator can help find and resolve issues in current evaluations

ENDF-VIII testing included translating ENDF-6↔GNDS. After extensive testing + fixing, all ENDF-VIII files can be translated

- ENDF-VIII files in GNDS-1.9 are available for download:

  http://www.nndc.bnl.gov/endf/b8.0/gndsfiles.html

- All sub-libraries can be translated to GNDS, most can be translated back to ENDF-6
  - Writing decay sub-library back to ENDF-6 is incomplete, some sections are missing
  - Writing nfy and sfy back to ENDF-6 still TBD

Most of JENDL-4 can be translated:

- Translator has trouble with 11 / 406 incident neutron evaluations
  - U233, U235, U238, Np237, Pu238, Pu240: discrepancy between MF2 and MF32 resonance parameters
  - Tc129m: incorrect Q-values for inelastic scattering to the ground state (QI should equal QM in MF3 MT51)
  - Am241: MF9 MT102 claims energy level of Am242m = 0 eV
  - B10, U234, Pu242: error may be in the translator
- To be done: test other JENDL-4 sub-libraries

JEFF-3.3 neutron sub-library shares many issues in TENDL

- 276 / 562 evaluations fail to translate. Reasons include:
  - Indices out of range in MF32 LCOMP=2 matrix. Appears to be a problem with 0-based vs. 1-based indexing (Ne10, S32, Ca40, …)
  - Distributions for two-body reactions given in lab frame (e.g. Fe54)
  - May be due to problems with translator: Zn64,

JEFF-3.3 thermal scattering sub-library:

- Tested for the first time: 4 / 20 evaluations fail to translate. All appear to be due to a limitation in the translator (these evaluations use ENDF format option not previously encountered)

TENDL-2017: big improvement over previous TENDL versions

- Many evaluations still fail to translate, but most errors are due to a few common causes
  - Reporting issues to Koning et. al., hopefully fixed soon
- Failures:
  - Neutrons: 655 / 2813
  - Protons: 1027 / 2804
  - Deuterons: 1063 / 2811
  - Tritons: 1059 / 2810
  - Helium-3s: 1039 / 2808
  - Alphas: 967 / 2808
  - Gammas: 705 / 2809

Common problems:

Metastable states with energy = 0

Ground states with energy != 0

MF8 / 9 / 10 / 40 claim different levels are metastable (LIS flags)

WPEC SG-38 guided the development of GNDS through version 1.9. Next steps: continue refining format + start code implementation!

- Completing SG-38 report is high priority. It should capture the state of GNDS-1.9 plus identify areas where improvement needed
  - See talks later this morning
- SG-43: develop code infrastructure for generating and using GNDS data
  - Afternoon session

Status of GNDS documentation

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XML schema (included with FUDGE) can be used multiple ways, including checking GNDS/xml files for format errors

- Check files using 'xmllint' utility:

  > xmllint -huge --noout --schema gnds.xsd ENDF-VIII/neutrons/*
  ENDF-VIII/neutrons/n-000_n_001.endf.gnds.xml validates
  ENDF-VIII/neutrons/n-001_H_001.endf.gnds.xml validates
  ENDF-VIII/neutrons/n-001_H_002.endf.gnds.xml validates
  ENDF-VIII/neutrons/n-001_H_003.endf.gnds.xml validates
  …

- Schema coverage not yet complete. Missing:
  - fission yields
  - thermal neutron scattering
  - some decay sub-library evaluations
  - covarianceSuite

Dave Brown has a proposal to keep schema and documentation synchronized

Current schema has limited documentation, but we could use xs:annotation to add in-line comments

- Example:

```
<xs:element name="crossSection">
  <xs:annotation>
    <xs:documentation>
      Insert description here…
    </xs:documentation>
  </xs:annotation>
  <xs:complexType>
    <xs:choice maxOccurs="unbounded">
      <xs:element name="XYs1d" type="xData_XYs1d_primary"/>
      <xs:element name="regions1d" type="xData_regions_1d_primary"/>
      …
    </xs:choice>
  </xs:complexType>
</xs:element>
```

- Annotations can also be used inside attributes and child elements

PoPs update

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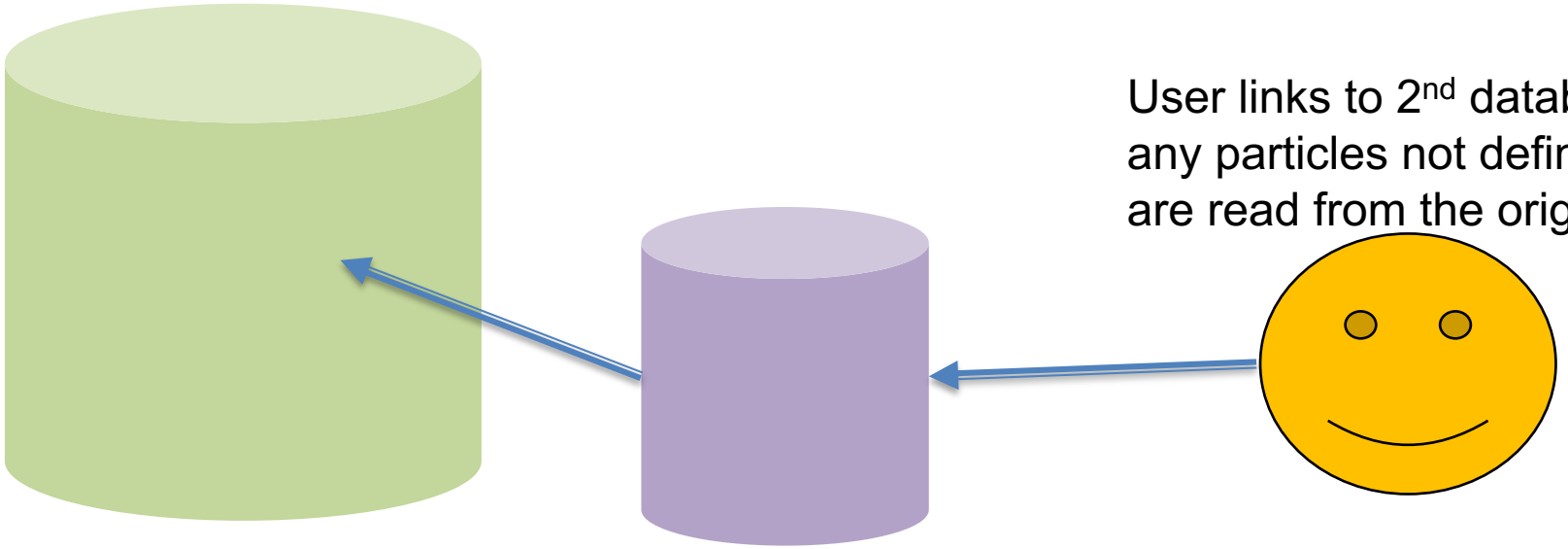
Goal of PoPs: describe all relevant properties for every particle appearing in a transport problem

- Any properties that are reaction-independent belong in PoPs
  - Basic particle properties like mass, spin, parity, charge
  - Excitation energy for excited nuclear states
  - Half-life, decay modes and probabilities
  - Uncertainties and correlations!

PoPs can already handle all particle data that appears in ENDF transport and decay sub-libraries.

- Main sources of information:
  - Masses come from translating AWR, AWP
  - Excited level energies come from translating Q-values, i.e. for MTs 51-90
  - Spin / parity from resonances
  - Gamma decay branching ratios from transition probability arrays (MF12 LO=2)
  - Half-lives, decay modes and spectra come from the decay sub-library

One PoPs database can link to another, overriding particle properties if necessary



User links to 2nd database, any particles not defined there are read from the original

Original database

2nd database links to original but adds or overwrites some particle definitions

Limitations in current implementation of PoPs

- Like the ENDF decay sub-library, PoPs sums decay spectra over all decay modes
  - For example, consider a particle that can decay both via β-delayed n and β-delayed 2n emission. Outgoing neutron energies are likely different in the 2n-emission, but PoPs only stores a single neutron spectrum summed over the two modes
- Correlations between emitted particles aren't currently captured