FUDGE / GIDIplus development and ENDF-VIII.1 testing

Caleb Mattoon
Nuclear Data and Theory Group, NACS/PHY

CSEWG formats / processing session
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FUDGE-6.4 was released on Github in early October

- Available at https://github.com/LLNL/fudge
  - Requires Python3.7 or later, numpy, matplotlib, C++ compiler for extensions.
  - Release schedule: around 4 public versions per year

- Recent additions:
  - Improvements to URR processing to support multi-temperature processing.
  - Supporting the MT=900 – 999 ENDF-6 format proposal (see Ian's talk later this afternoon).
  - Several fixes to support translating and processing ENDF-VIII.1 candidates.
  - Expanded support for generating ACE files for MCNP.
  - Improved physics checking tools (more later…).

- Expect next release in early 2024. Focus areas:
  - Full support for translating and processing VIII.1
  - Integrating URR treatment into the 'processProtare' script
  - Processing fixes based on user feedback

FUDGE now supports generating URR probability tables (and other URR processing options)

- FUDGE/bin/processURR.py: adds URR style and probability tables for each temperature in a processed GNDS evaluation.
  - Results stored in ‘applicationData’ as GNDS-2.0 does not define a URR probability table container.
- Sample usage to add PTs at 3 temperatures:

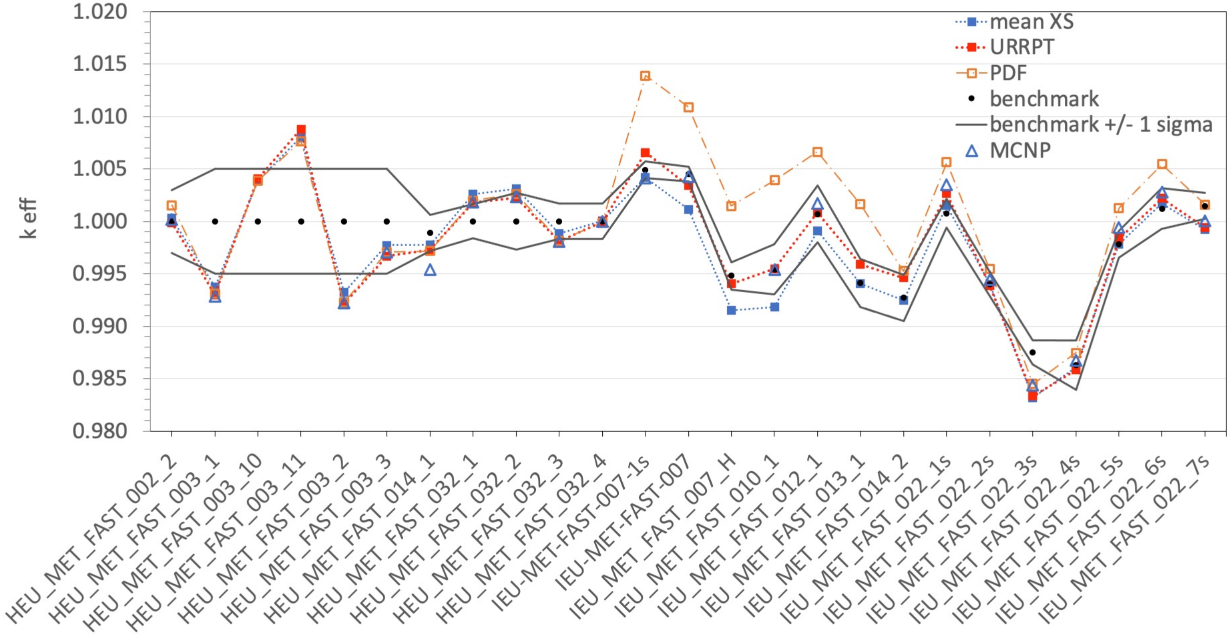
```
python3 processProtare.py <eval>.xml –mc –t 293.6 –t 350 –t 400 –temperatureUnit K
python3 processURR.py <eval>.proc.xml 100 –o <eval>+urr.xml

# also support exporting results to ACE (one temperature at a time):
python3 toACE.py <eval>+urr.xml <eval>.ace –i 80 -s MonteCarlo_000
```

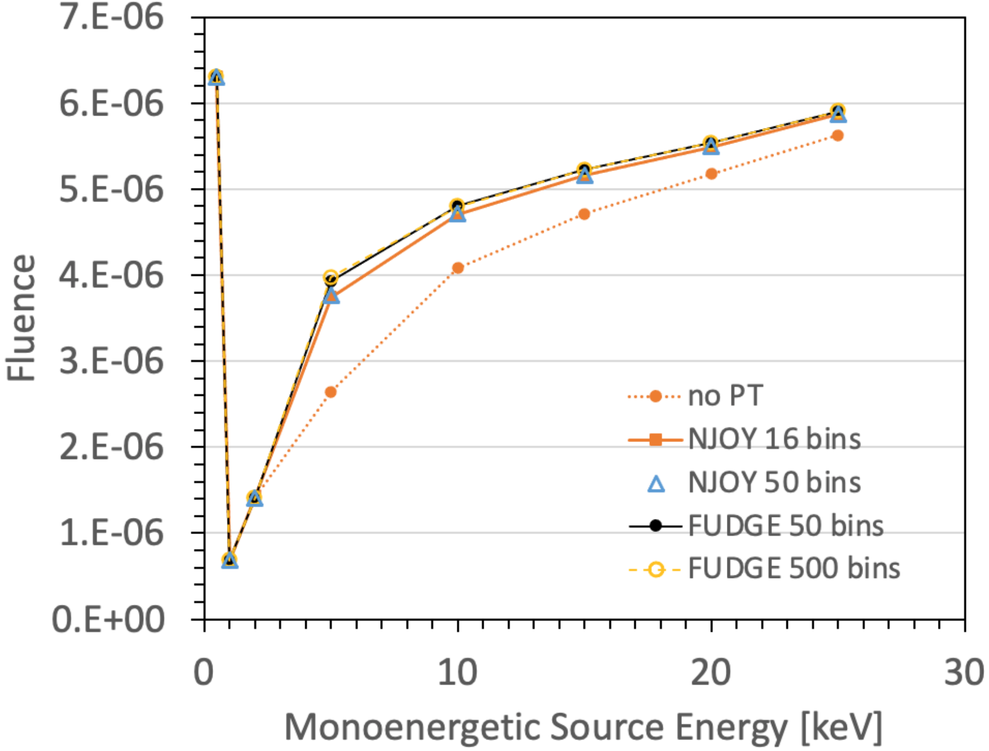
URR probability tables were compared against NJOY & FRENDY, and tested on critical assemblies and shielding benchmarks

- Paper on methods and testing was submitted to PHYSOR 2024:

ICSBEP benchmark comparison



Simulated neutron leakage through 20 cm Pu239 slab



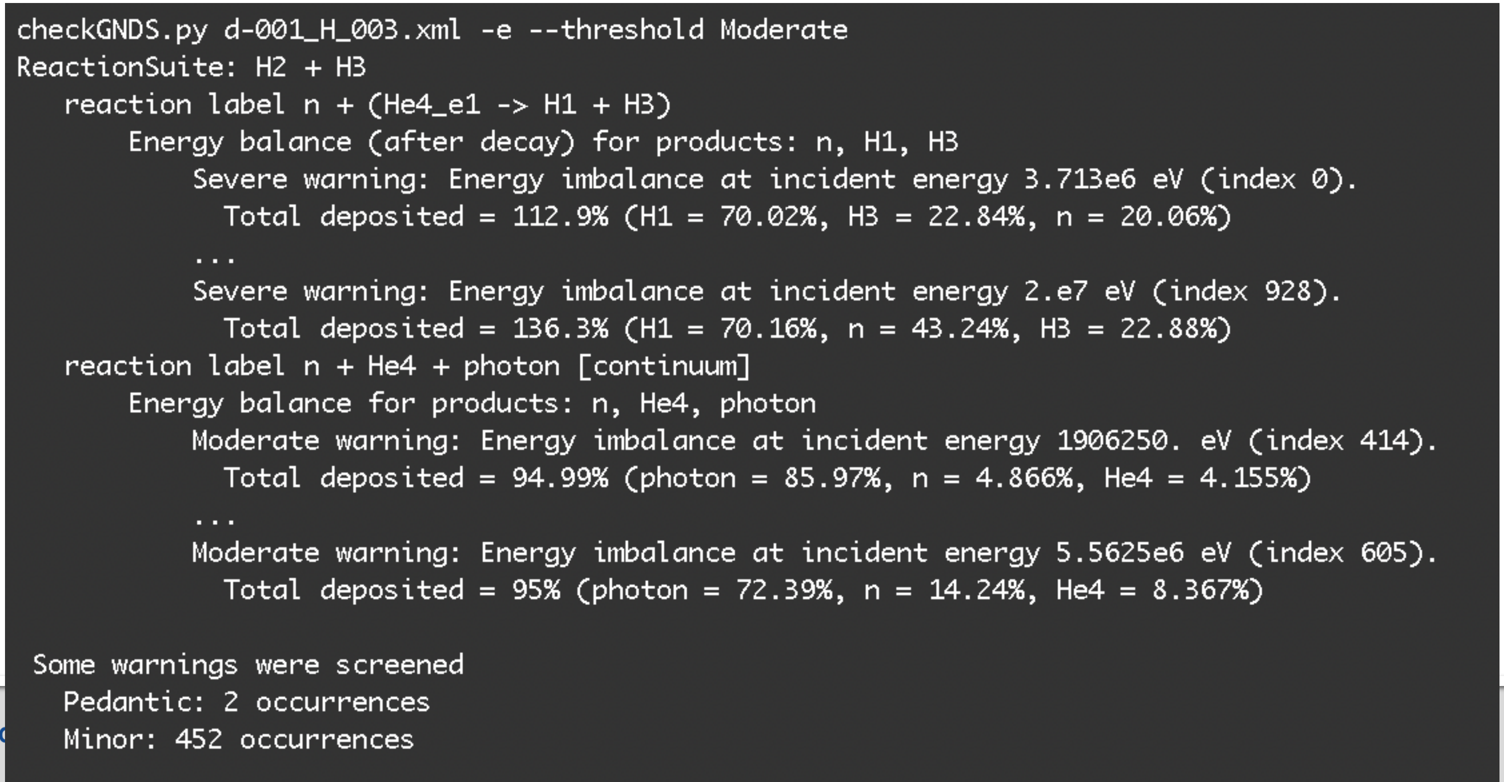
Several recent updates focused on supporting new TNSL evaluations

- For TNSL files, ENDF-6 - GNDS translator uses the file name to determine TNSL material, must be updated when new materials are added.
  - MAT number is not sufficient since ENDF/JEFF/JENDL use different conventions
- Various TNSL processing issues fixed
  - ~1 year old bug in the ENDF-GNDS translator: GNDS-2.0 switched to storing the *bound* atom cross section, but free-bound conversion was not updated properly.
  - Secondary scattering atoms with free-gas approximation incorrectly contributing to incoherent inelastic cross section
  - Updates to support processing large number of Bragg edges in VIII.1 candidate evaluations

Updated the FUDGE physics checker to focus on most important warnings

- Each warning now has a severity level (Pedantic / Minor / Moderate / Severe / Fatal)
  - checkGNDS.py supports filtering by severity and/or by warning types.
  - Default warning threshold = Moderate

- checkGNDS used extensively to test ENDF-VIII.1 candidates:



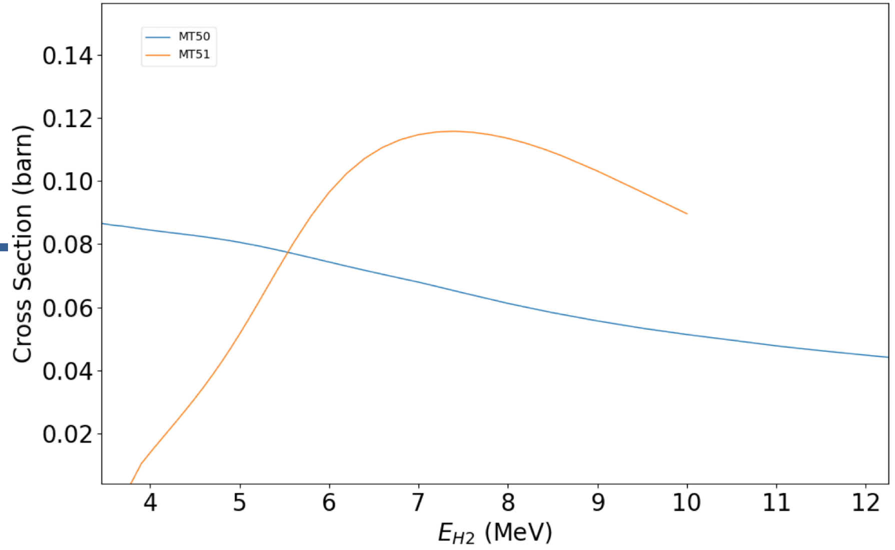
```
checkGNDS.py d-001_H_003.xml -e --threshold Moderate
ReactionSuite: H2 + H3
   reaction label n + (He4_e1 -> H1 + H3)
       Energy balance (after decay) for products: n, H1, H3
           Severe warning: Energy imbalance at incident energy 3.713e6 eV (index 0).
             Total deposited = 112.9% (H1 = 70.02%, H3 = 22.84%, n = 20.06%)
           ...
           Severe warning: Energy imbalance at incident energy 2.e7 eV (index 928).
             Total deposited = 136.3% (H1 = 70.16%, n = 43.24%, H3 = 22.88%)
   reaction label n + He4 + photon [continuum]
       Energy balance for products: n, He4, photon
           Moderate warning: Energy imbalance at incident energy 1906250. eV (index 414).
             Total deposited = 94.99% (photon = 85.97%, n = 4.866%, He4 = 4.155%)
           ...
           Moderate warning: Energy imbalance at incident energy 5.5625e6 eV (index 605).
             Total deposited = 95% (photon = 72.39%, n = 14.24%, He4 = 8.367%)

 Some warnings were screened
   Pedantic: 2 occurrences
   Minor: 452 occurrences
```

ENDF-VIII.1 GNDS translation failures (phase2 branch as of Monday Nov. 13)

- Neutron sublibrary:
  - La139 (inconsistent resonance parameters in MF2 / MF32)
  - Pb206-208 (FUDGE translation issue for L-dependent scattering radius uncertainty)
- Thermal scattering sublibrary:
  - Be-metal, CinC8H8, HinC8H8, HinH2O, OinSiO2-alpha, OinUO2-HEU (minor formatting issues)
  - CinC5O2H8, OinC5O2H8 (temperatures not monotonically increasing)
- Deuteron sublibrary:
  - d + t: discrepancies in MT=51. Is it 3-body reaction d + t -> n + p + t? Or d + t -> n + (He4* -> p+t)?
  - d + a: minor format issue
- Helion sublibrary:
  - h + Li7: move MT=801 to MT=802 (2nd excited state in Li6) and use 2-body kinematics for Li6?

More details on d+t



- VIII.0 (based on 1995 Hale and Drosg work)
  - MT=2 Coulomb elastic scattering, 10 keV – 10 MeV
  - MT=50 d + t -> n + α, 100 eV – 30 MeV
  - MT=51 d + t -> n + (He4* -> p + t), 3.7 MeV – 10 MeV
    - p / t distributions described as N-body phase space. Not appropriate for 2-body breakup
    - 2-step reaction going through He4* should have threshold at 4.3 MeV. 3.7 MeV threshold is consistent with 3-body breakup instead.

- VIII.1 candidate attempts to merge LLNL ECPL with VIII.0… but still has issues:
  - MT=2 Coulomb elastic, 72 keV – 20 MeV
  - MT=50 d + t -> n + a, 16 eV – 20 MeV
  - MT=51 or 28?? d + t -> n + p + t, 3.7 MeV – 20 MeV
    - But still trying to use 2-body kinematics for outgoing neutron distribution
  - MT=91 d + t -> n + He4 + photon, 20 eV – 20 MeV
    - Includes 16.7 MeV photon production. Much smaller cross section than MT 50 / 51

Other issues on phase1 branch (from Monday Nov 13)

- Neutron sub-library:
  - Sr88: external R-Matrix only partly implemented in FUDGE
  - Pt190 – 198: inconsistencies in MF= 8 / 10 production cross sections
- Thermal scattering sub-library:
  - ortho-H, para-H, ortho-D, para-D all run into an interpolation rule 'sanity check': files store ln($S_{\alpha\beta}$) instead of $S_{\alpha\beta}$, but also indicate to use log-lin interpolation along α, β and T axes. Need clarification from ESS team on intended interpolation.
- Helion sub-library:
  - h + α is first example of charged-particle evaluation with resonance parameters. ENDF-GNDS translator is now working but needs more checking.
    - Note: evaluation has the LRP=2 flag set: resonance parameters are provided for information only, MF=3 already contains complete cross section.

ENDF-VIII.1 beta-1 and beta-2 were processed with FUDGE for LLNL testing

- Two types of processing
  - 23 ‘standard’ temperatures (300 K to 0.1 MeV/k) without URR / TNSL
  - Room temperature with URR / TNSL
- Tested with Metis V&V suite, see Marie-Anne’s talk tomorrow for details
- Main processing issues were due to unphysical masses for targets or reaction products
  - Kalbach-Mann distributions are especially sensitive to product and residual mass
  - Mass issues were mostly fixed in β-2 (by adopting recent AME values)

GIDIplus: C++ API for reading and sampling processed GNDS data

- GIDIplus is open source, available from https://github.com/LLNL/gidiplus
  - New release will be available soon
- LLNL codes are updating to use GIDIplus by default
  - Effort involves extensive testing and review by Mercury (Monte Carlo) and Ardra (deterministic) transport code teams
- Older version of GIDIplus is used in the GEANT-4 package G4LEND
  - We recently updated G4LEND, still going through internal testing before public release

Shameless advertisement!

- FUDGE / GIDIplus training is scheduled for May 21-24 2024 at the NEA in Paris
  - Week following WPEC
  - Topics to be covered include:
    - Deep look at using GNDS to store evaluated and processed data
    - FUDGE installation and basic use
    - Utilities to help visualize and test nuclear data evaluations
    - Intro to using the GIDIplus API
  - We still have room to adjust the agenda. Please let us know if you are interested in attending and want to hear more about specific topics!

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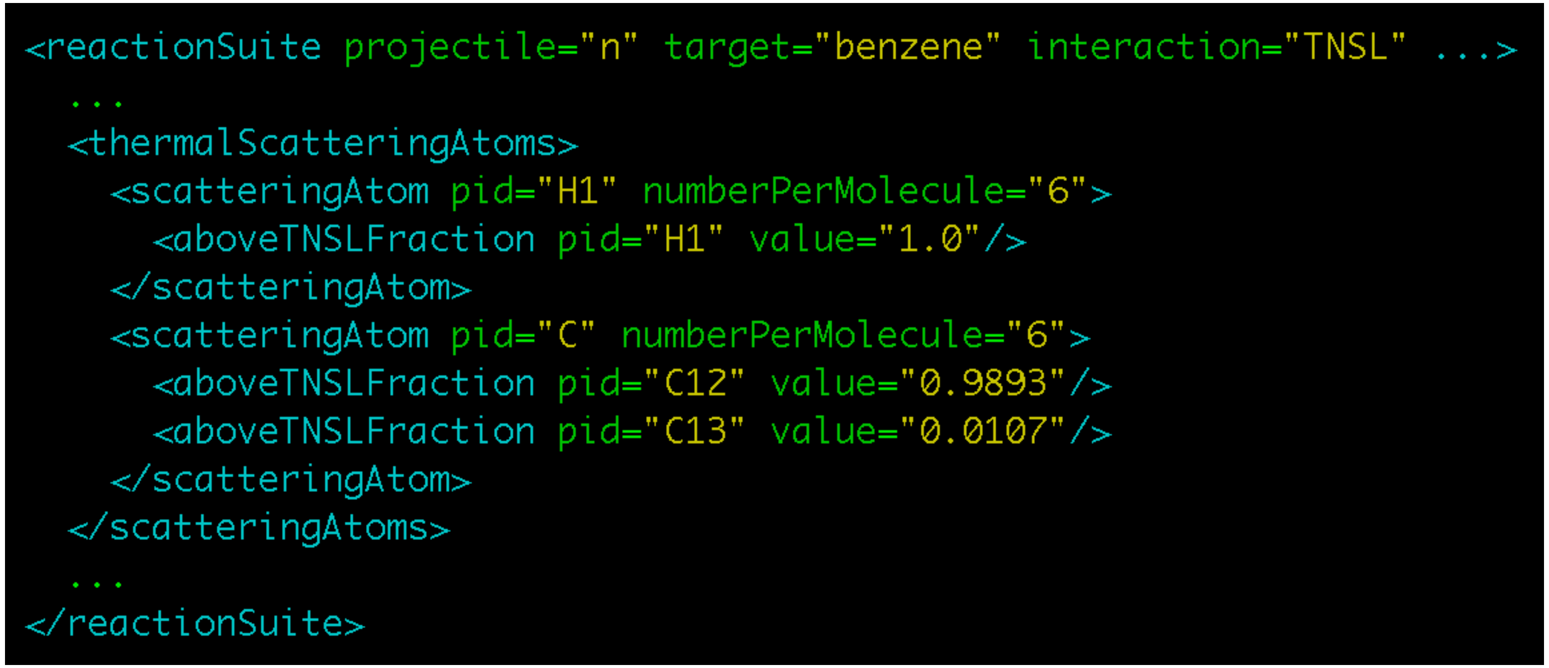
Tentative proposal: move the definition of scattering atoms up to become child of ‘reactionSuite’

For example, if benzene should be replaced primarily with C12 but sometimes with C13:



```
<reactionSuite projectile="n" target="benzene" interaction="TNSL" ...>
  ...
  <thermalScatteringAtoms>
    <scatteringAtom pid="H1" numberPerMolecule="6">
      <aboveTNSLFraction pid="H1" value="1.0"/>
    </scatteringAtom>
    <scatteringAtom pid="C" numberPerMolecule="6">
      <aboveTNSLFraction pid="C12" value="0.9893"/>
      <aboveTNSLFraction pid="C13" value="0.0107"/>
    </scatteringAtom>
  </scatteringAtoms>
  ...
</reactionSuite>
```

Provides guidance to user codes for how to replace molecule above thermal region.

TBD: burnup-dependent rule? That may still need to be left to user.

GNDS-2.0 formatted libraries are available now

- ENDF-VIII.0 is available as a ~850 Mb tar.gz file from NNDC
  - Contains all sub-libraries, neutron sub-lib includes reconstructed resonances

- Other libraries also available, but some files fail to translate
  - LLNL regularly translates ENDF, JEFF, JENDL and ENDL libraries as part of testing
  - Translation failures typically show up because of format errors or internal inconsistencies in ENDF-6 data

EG-GNDS (group in charge of GNDS specs) has established milestones for the next GNDS release:

Top Priority: Abstract nodes & JSON schema adoption - foundational for entire code system used to define format & generate API's

2nd Priority: Reduce reduce redundancy redundancy - there is still a lot of duplication in GNDS. Is it needed or not? This is a chance to revisit some early design decisions

3rd Priority: Revisit PoPs - the nuclear structure/decay data in GNDS is awkward to use; ENSDF modernization project gives us chance to rework it

4th Priority: Clean up uncertainties - the uncertainties (inherited from ENDF) are still messy and hard to explain.

Pending evaluator/user needs:

- $P(\nu)$ and $P(\nu_\gamma)$
- Various resonance questions
- Containers for URR processed data to facilitate exchanging processed data?
- Fission product yields
- TSL changes

More detail on 1st goal: migrate GNDS specifications to the new JSON schema language

- GNDS format specification is already stored in JSON files, but their format predates the JSON schema language
- Official JSON schema language is more expressive, and by adopting that we can take advantage of 'off-the-shelf' schema validators and other tools
- G. Gert (LLNL) started migrating the specifications to the official JSON schema
  - Uncovered inconsistencies and ambiguities in current definitions along the way!
- Goal is to make the specifications unambiguous so we can use them to generate documentation, GNDS file validators, code APIs, etc.

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