The LLNL Nuclear Data Processing System

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for the LLNL CNP Group

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

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Motivation and outline

Motivation:

- Make ENDF/B-VI and JEFF-3.1 data available to LLNL application codes.
- Access world's data: JENDL-3.3 (Japan), CENDL-2.1 (China), ENDF/B-VIIβ2, and JEFF-3.0.

Outline of talk:

1. Outline of library preparation
2. Fixes applied and backfilling the data
3. Conclusion

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Library content requirements

	ENDL	ENDF/B
$\sigma_{tot}(E)$, $\sigma_{el}(E)$	Yes	Yes
Other $\sigma(E)$	Yes	Yes
Fission: $\bar{\nu}(E)$	Yes, prompt and delayed	Not required
$P_{n,\gamma}(E\vert\mu,E')$	Yes, for all outgoing n, p, d, t, ^{3}He, α and γ	Yes, only n, γ
$M_\gamma(E)$	Yes	Yes
Capture: $M_\gamma(E)$	Yes	Yes
$P_\gamma(E\vert\mu,E')$	Yes	Not required
All others: $M_\gamma(E)$	Yes	Yes
$P_x(E\vert\mu,E')$	Yes, for all outgoing n, p, d, t, ^{3}He, α and γ	Yes, only n, γ

Extend data translated by fete to support LLNL applications

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How data is prepared

1. Arrange ENDF/B data and preprocess w/ PREPRO2004:
   a) Makes resonance region linearly interpolatable.
   b) Heats data to room temperature.
2. Data translated to ENDL's ascii format using fete.
3. Data fixed and missing data filled.
4. Ascii data processed into MCF (Monte-Carlo) and NDF (deterministic) files using mcfgen and ndfgen.
   a) Monte Carlo and deterministic: 230 groups
   b) Monte Carlo: continuous energy also
5. Ascii and processed data is tested in variety of ways.

Translating data w/ fete

- **F**rom **E**NDF/B **T**o **E**NDL translates:
  - All $\sigma(E)$
  - All outgoing particle distributions: $P(E|\mu)$, $P(E|E')$, $P(E|\mu,E')$, $M_\gamma(E)$ and $\nu(E)$
  - n, p, d, t, ^{3}He, α, γ incident
- Result of heroic, yet tedious, multi-man year effort.
  - D.A. Brown (LLNL), G. Hedstrom (LLNL), T. Hill (LANL)
- Received 2006 PAT PDRP Award
- Released under GNU Public License
- Available at Computational Nuclear Physics website: http://nuclear.llnl.gov

Fixes we applied

- Q values and thresholds fixed.
  - Mass evaluation from Audi, Wapstra, *et al.*
- Filled in missing data when possible
- Converted legacy "breakup" data into ENDL.
  - ENDF/B kludge for legacy $P(E|\mu,E')$ data.
- Bugs fixed in ENDF files when possible
  - Submitted to maintainers of respective libraries.
  - Includes 14 fixes included in ENDF/B-VII.β3 release
- Use `endepC++` for energy depositions.

Filling in the missing data

- (n,f) often missing $\bar{\nu}_p$ or $\bar{\nu}_d$
- (n,γ) often missing outgoing γ data
  - If have P(E|μ) and multiplicity is 1, generate P(E,μ|E') from kinematics
  - Otherwise use `nxgam.py` to do γ cascade
- (n,n') get isotropic angular distributions
- Other reactions often missing outgoing particle distributions:
  - steal from other libraries, starting from ENDF/B-VII, then JEFF-3.1, then JENDL-3.3, then rest.

Simple testing

- Format & Physics testing within fudge:
  - Database Q matches Q value computed from masses and threshold.
  - Check normalization of probabilities.
  - Data completeness.
  - Points are in order, with no steps or double values.
  - Cross sections, multiplicities and probability densities > 0
- Simple sanity checks of processed data files:
  - MCF files using Mercury: dynamic simulation of sphere of material with neutron source in middle
  - NDF files using AMTRAN: k_{eff} calculation with ENDL99's ^{239}Pu as fuel, material of interest as reflector

To Do…

- Release as many processing codes as we can:
  - endepC++, mcfgen, ndfgen, fudge, …
- Propagate fixes back into ENDF/B-VII
  - Requires work on endl2endf code

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Backup slides

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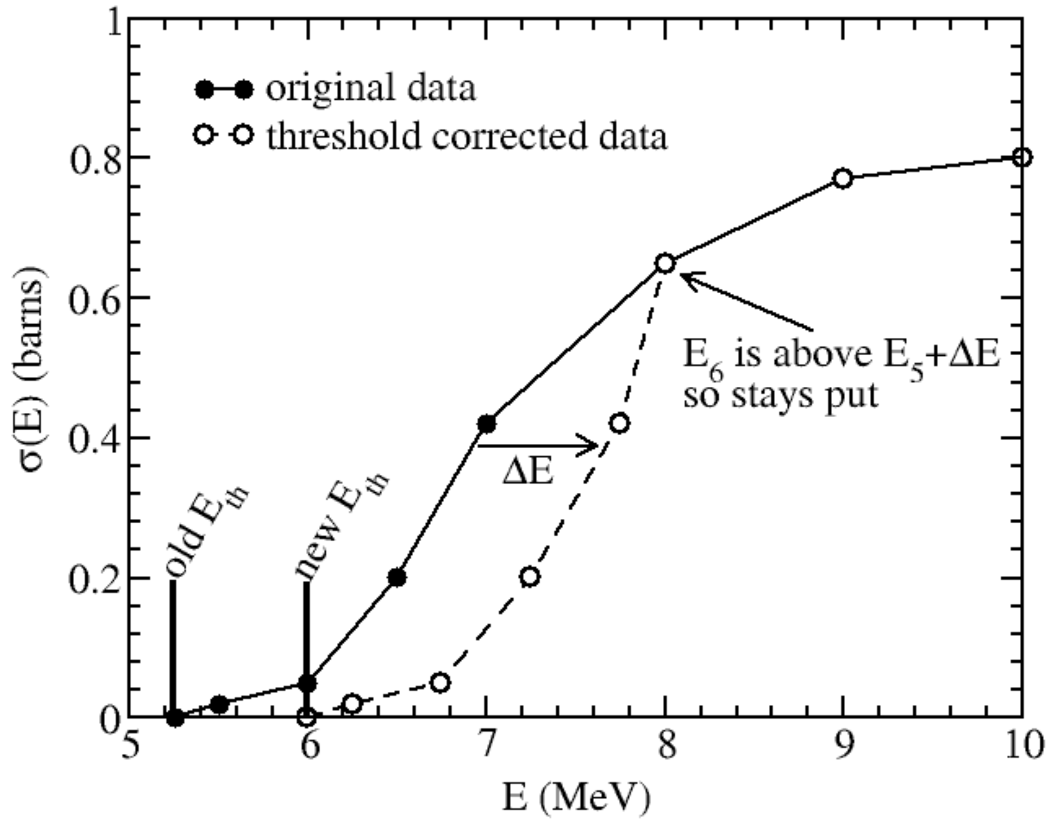
Unfixable problems

- Kalbach systematics for correlated E’-μ distributions requires well defined Z, A. Makes no sense for natural targets
  - Used in CENDL-2.1, JENDL-3.3, BROND-2.2
- Non-standard ENDF formats
  - BROND-2.2’s za030000 uses weird format for γ’s
  - JEFF-3.1’s za004009 uses illegal MT’s
- Stuff not yet implemented in `fete`
  - BROND-2.2 only place several uncommon options used
  - LR=1, 40 flags for break-up cross-sections too tough to implement
- “Hopelessly broken”
  - JEFF-3.1 Ti evals. have bad γ data
  - BROND-2.2’s Z<3 evals.

Fixing Q values & thresholds

- Get best-guess Q
  - Compute from mass tables
  - Use ground-state masses
  - For fission, take from file
- Compute actual threshold
  - Charged particles get real threshold even if have effective threshold
  - Include level excitation
- Check thresholds in data and adjust if outside tolerance and any points below threshold



ΔE = new E_{th} - old E_{th}

Masses changed little, so ΔE typically small

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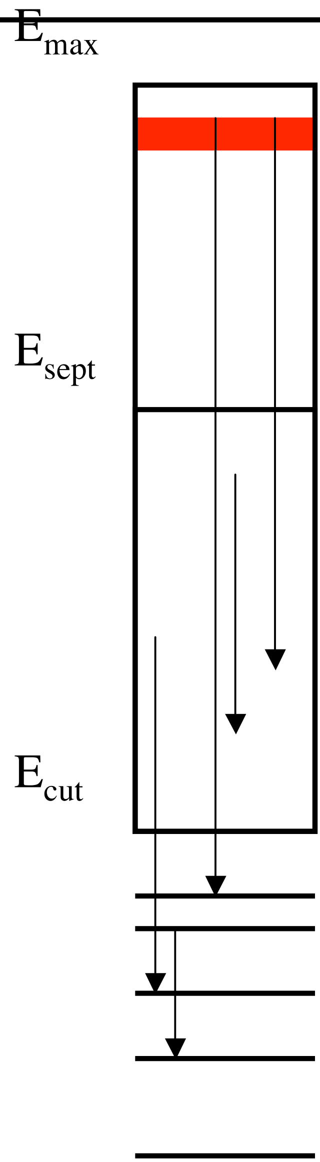
Missing (n,γ) Data: `nxgam.py`



- Level Scheme made of discrete & continuum:
  - discrete from RIPL
  - continuum from Von Egidy & Bucurescu
- Gamma Branchings:
  - discrete from RIPL
  - continuum from Kopecky & Uhl (RIPL/TALYS)
- Ignore J^{Π} of levels, multipolarity of γ's in first pass
- Cascade done by "collapsing tower" method

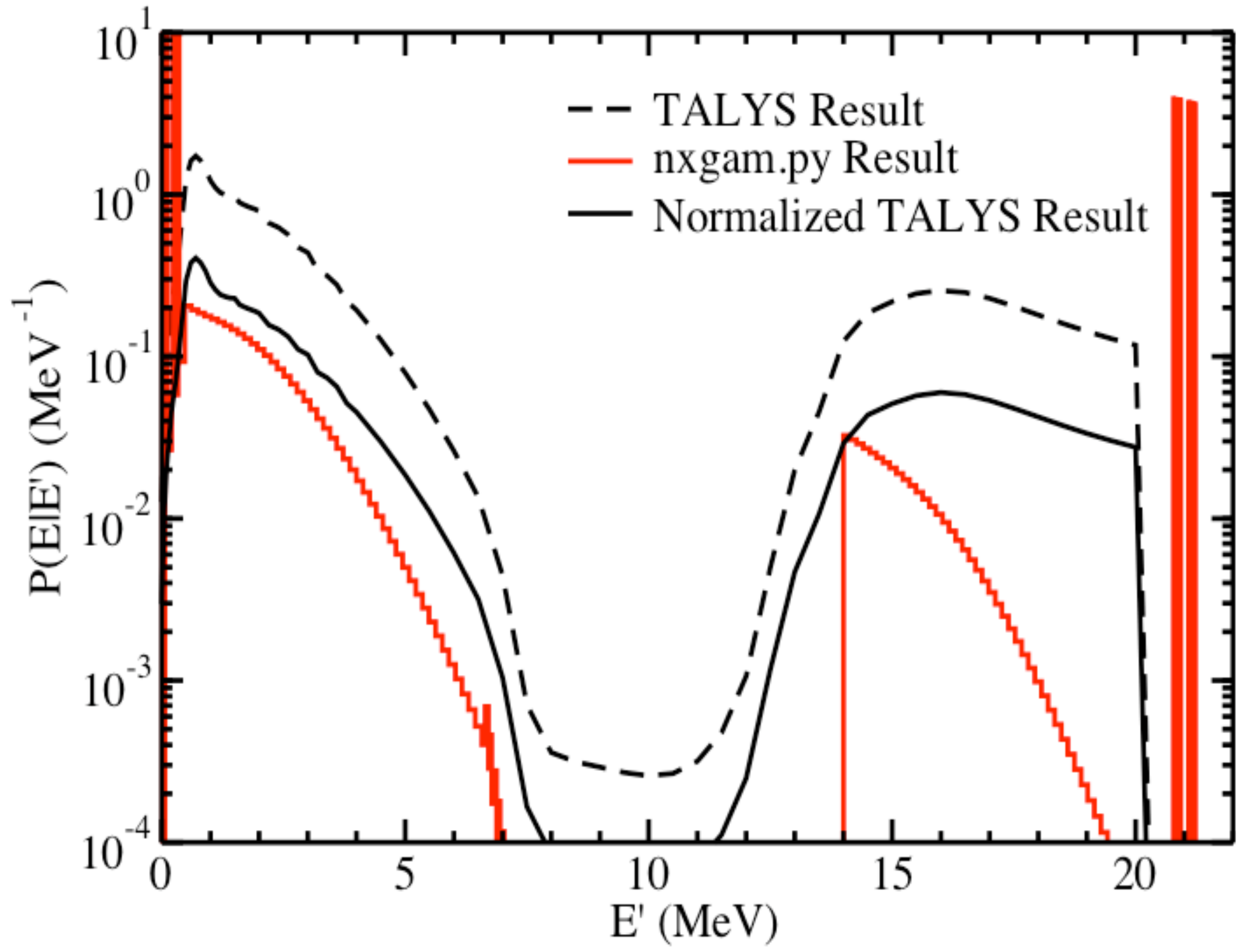
Missing (n,γ) Data: `nxgam.py`, cont.

Construct:

- I=4 (energy-angle distribution)
- I=9 (multiplicity distribution)

Missing E2 peak, neutron competition, High-energy part

Energy balances perfectly (not true of old NXGAM)



Comparison with TALYS for ^{93}Nb surprisingly good!

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Legacy "Breakup" data

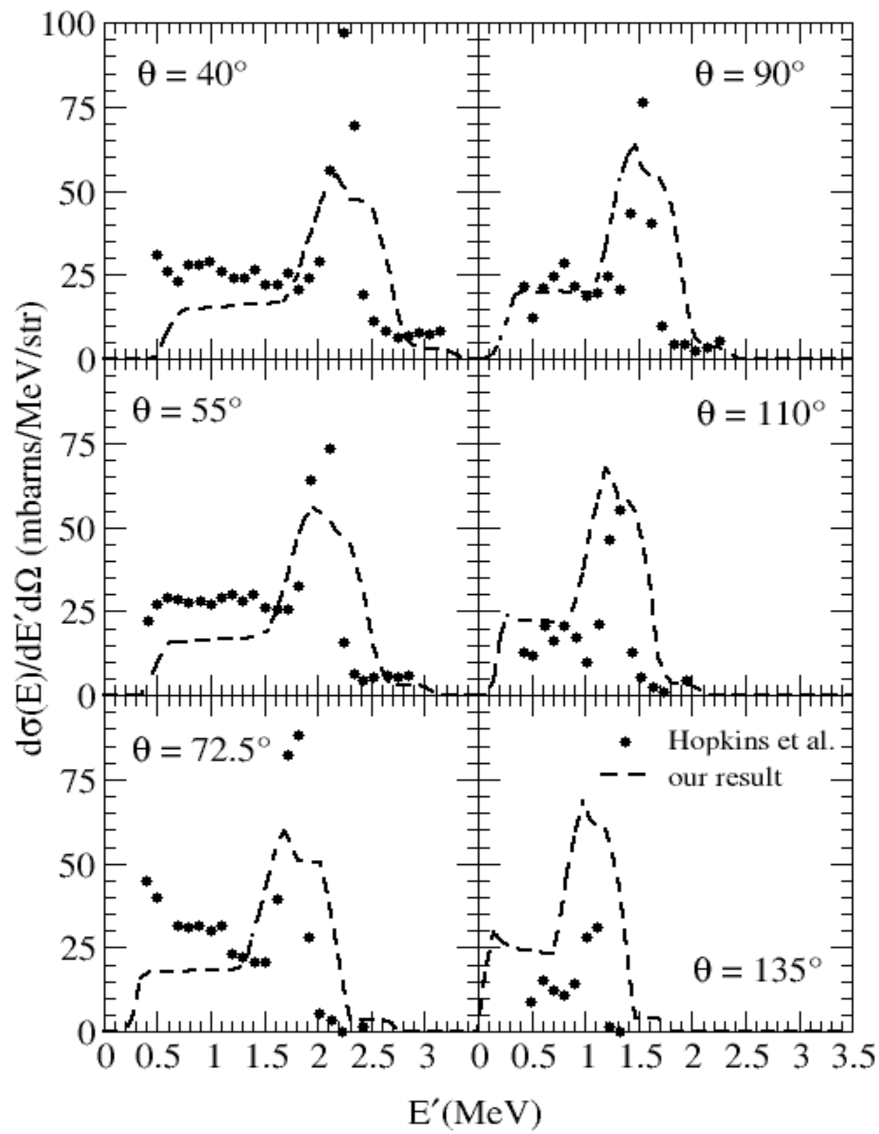
- Back in the old days (1970's), there was no way to represent outgoing particle distributions that exhibit strong E'-μ correlations.
- Typical when light targets go to 3+ body final states
- Still in use in several evaluations:
  - ^{6}Li(n,nd)α: ENDF/B-X, JEFF-3.X, JENDL-3.3
  - ^{7}Li(n,nt)α: ENDF/B-X, JEFF-3.X, JENDL-3.3
  - ^{12}C(n,n2α)α: ENDF/B-X, JEFF-3.X, JENDL-3.3
  - ^{10}B(n,np), (n,nα): ENDF/B-X, JEFF-3.X, JENDL-3.3, CENDL-2.1
  - ^{14}N(n,np): ENDF/B-X, JEFF-3.X, JENDL-3.3
  - ^{16}O(n,n'), (n,np), (n,nα): BROND-2.2

Legacy “Breakup” data, cont.

- Abuse the way we store $d\sigma/d\mu$ for discrete level excitations…
  - Store $\sigma_i(E)$ for series of fake levels *i* as (n,n'_i) data
  - Store $P_i(E|\mu)$, in CM frame, for the emitted neutron from the fake level *i*
  - Pretend each fake level has some width ΔE_i
  - Set LR flag to denote the *real* reaction that occurred
  - Use kinematics, reconstruct $P(E,\mu|E')$ and $P(E|\mu)$ distributions in lab frame
- Scheme has drawbacks:
  - Which Q value? Not documented…
  - Only have the neutron distribution
  - Is a side-effect of NJOY processing

Legacy "Breakup" data, cont.

- Most evaluations are R-matrix fits to small datasets (data skimpy!)
- Most evaluations not documented well
- Validation vs. original data or scans of ancient plots
- Comparisons are fair, but agreement not spectacular



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