ENDF Project Report to WPEC 2014

M. Herman for CSEWG
ENDF Project Pages

- Reorganized the set of ENDF web pages: http://www.nndc.bnl.gov/endf/project.html
- Compiling ENDF history back to ENDF/B-I
  - Data files
  - Lab reports (BNL & others)
  - Formats
- Links to ENDF development pages
  - Includes ADVANCE requirements document
  - Various ENDF QA requirements documents
Post ENDF/B-VII.1 activities

- 2 new thermals scattering law evaluations for SiO2
- New evaluation for 236m1Np
- New RR evaluations for 63,65Cu, 56Fe and 235U
- Numerous but minor fixes to VII.1
- ENDF/B-VII.1 validation
- Modernizing infrastructure
  - Evaluation methodology (reaction codes, PFNS, inelastic scattering, assimilation)
  - Continuous verification and validation
  - New XML format
  - CIELO
Priorities for the next ENDF/B

Highest Priority

- 239-Pu
- 235-U
- 238-U
- 56-Fe
- 16-O
- Standards
- Update covariances

Lower Priority

- CP reactions
- Be
- 12,natC
- 23-Na
- Ca
- V
- Ti?
- Cr
- Ni
- Cu
- Zr
- Mo?
- Ta
- Gd
- Dy

Brookhaven Science Associates
New ENDF/B evaluations
Status Report on ORNL Nuclear Data Evaluations

Luiz Leal, Marco Pigni, Vladimir Sobes, Doro Wiarda, Klaus Guber, Royce Sayer, Goran Arbanas, RQ Wright, and Mike Dunn

Nuclear Data & Criticality Safety Group
<table>
<thead>
<tr>
<th>Energy Range</th>
<th>Resonance Covariance Evaluation</th>
<th>Target date for delivery the evaluation</th>
</tr>
</thead>
<tbody>
<tr>
<td>63,65 Thermal to 300 keV</td>
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<td>Completed</td>
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<tr>
<td>182 Thermal to 10 keV</td>
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<td>Yes</td>
<td>FY2014</td>
</tr>
<tr>
<td>186 Thermal to 10 keV</td>
<td>Yes</td>
<td>FY2014</td>
</tr>
<tr>
<td>56 Thermal to 2 MeV</td>
<td>Yes</td>
<td>CIELO</td>
</tr>
<tr>
<td>16 Thermal to 6.3 MeV</td>
<td>Yes</td>
<td>CIELO</td>
</tr>
<tr>
<td>239 Thermal to 2.5 keV</td>
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<td>Completed</td>
</tr>
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<td>235 Thermal to 2.25 keV</td>
<td>Use ENDF/B-VII. 1 (FILE33)</td>
<td>CIELO</td>
</tr>
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</table>
56Fe Resolved Resonance Region Evaluation

- New high resolution transmission measurements at RPI extending the resonance region up to 5 MeV
- New inelastic cross-section measurements done at GEEL
- Extend the resolved resonance region from 850 keV to 2.0 MeV
- Include new transmission measurements and inelastic cross section data
- Use the extended (RML=7) R-matrix formalism in the SAMMY code for fitting the experimental data
Comparison of SA MMY predictions to differential elastic data of Perry.
235U Resonance Region Evaluation

✓ New data measurements from RPI (capture and fission yields) (kind of alpha measurements)
✓ New capture data from LANL
✓ Use SAMMY code for fitting the new data
✓ Test the new evaluation in benchmark calculations: ZEUS benchmarks (FCA not available)
✓ Use JENDL4 as the template
✓ Benchmark Calculations done with MCNP with everything else from ENDF/B-VII.0
RPI and LANL Capture Data

25.56 m
15 ns

25.45 m
125 ns
Fit of the RPI $^{235}$U Data

- ENDF/B
- RPI - Experiment

Capture Cross Section (barns)

- RPI - Experiment
- Resonance Parameter (SAMMY)

Capture Yield

- RPI - Experiment
- Resonance Parameter (SAMMY)

$^{235}$U fission

$^{235}$U capture
Comparison of $^{235}\text{U}(n,\gamma)$ and $^{235}\text{U}(n,f)$ cross sections … recent ORNL re-evaluation, designated ORNL8, based upon new LANL and RPI data versus the current (ENDF/B-VII.1) evaluation … “a work in progress” per Luiz Leal.
HST Benchmarks

- Regression fit to HST benchmarks versus ATLF has been excellent since ENDF/B-VI.3 (Lubitz).

- This excellent fit is retained with the latest (ORNL8) $^{235}\text{U}$ resolved resonance file.
HMF7 (HEU + CH$_2$) Benchmarks

- HEU + poly system tests xs data over several orders of magnitude.
- E70 & E71 results are near unity at either energy extreme but are biased high in the intermediate energy range.
- This bias is worsened with the latest ORNL8 $^{235}$U evaluated file.
Validation
Data Testing Revised $^{235}\text{U}$ and $^{239}\text{Pu}$ Files with ICSBEP Benchmarks

A. C. (Skip) Kahler
Los Alamos National Laboratory

L. C. Leal
Oak Ridge National Laboratory
Pu – WPEC SG34

- Revised resolved resonance
- Revised $\nu_p(E)$ data, up to 650 eV
- Revised PFNS
- Differences between JEFF and ENDF remain, ☹.

Although the Sub-Group is near an end, this work remains a “work in progress” that will continue under CIELO.
Pu-SOL-THERM Benchmarks - I

- A ~500 pcm bias in calculated PST reactivity is a long-standing issue.

- WPEC Sub-Group 34 was tasked with defining a new (better?) set of resolved resonance parameters for $^{239}$Pu in an attempt to resolve this issue.

- Can define a sub-set of these 150 benchmarks to test revised data files.

Consider benchmark attributes such as (i) ATLF; (ii) $^{239}$Pu atom-% in Pu; (iii) Above-Thermal Fission Fraction (ATFF); (iv) H/Pu number density (or gPu per liter) to define this sub-set.
Analysis of VNIITF Mo Benchmarks

M. L. Zerkle
Bettis Atomic Power Laboratory

Cross Section Evaluation Working Group Meeting
November 20-22, 2013
Brookhaven National Laboratory
VNIITF Mo Benchmarks

- 9Be – new evaluation by G. Hale
- 92Mo – new evaluation by Mughabghab + JENDL-3.3
- 95Mo – new evaluation by Kim, Herman, Mughabghab

New ICSBEP Mo Benchmarks
- HMF092 – fast, Mo reflected
- HMF093 – fast, Mo reflected/diluted
- HMF094 – fast, Mo diluted, Be/BeO mod, DU/Be/BeO Reflected
- HMM020 – mixed, Mo diluted, CH$_2$ mod/reflected

Analyzed with MC21
- ENDF/B-VII.0 cross section
- ENDF/B-VII.1 cross section
- 108 active neutron histories (∼0.0001 Δk 95% CI)
Conclusions

• ENDF/B-VII.0 and ENDF/B-VII.1 results consistent except for Be moderated/reflected cases (HMF094)
  – Implies improvement in ENDF/B-VII.1 Be evaluation
• Positive $k_{\text{calc}}$ bias with Mo reflector thickness
  – Bias grows from +0.4% to +0.6% $\Delta k$ for HMF092
  – Mo elastic ang. distributions insufficiently forward peaked and/or
  – Mo fast capture too low
• Bias increases to +0.7% $\Delta k$ when Mo dilution added (HMF093)
  – Mo fast capture too low
• $k_{\text{calc}}$ biased high in moderated cases
  – +0.6% $\Delta k$ bias for Be/BeO moderated cases (HMF094)
  – +0.64% to 0.74% $\Delta k$ bias for CH$_2$ moderated cases (HMM020)
  – capture too low (RR, fast)
  – Spectral dependence on bias in RR (bias reduced for softer spectrum CH$_2$
    moderated cases)
Investigation of ENDF/B-VII.1 Covariance Data for SCALE-6.2

Mark Williams, B.J. Marshall, Doro Wiarda, Brad Rearden
Oak Ridge National Laboratory
Validation studies performed for 320 benchmark experiments

- Continuous energy (CE), 252g multigroup, and covariance data were processed using AMPX
- Critical eigenvalues computed with Keno Monte Carlo code using both 252g and CE
- Covariance library generated by replacing covariances in SCALE-6.1 with ENDF-VII.1 data, if available. Variations were made in some ENDF-VII.1 values
- S/U calculations with 252g TSUNAMI-3D (Keno)
Uncertainties for LEU-COMP-THERM Benchmarks
Uncertainties for HEU-SOL-THERM Benchmarks
Uncertainties for LEU-SOL-THERM Benchmarks
Uncertainties for HEU-MET-FAST Benchmarks
Uncertainties for PU-SOL-THERM Benchmarks
**Observed Standard Deviations are Less Than Predicted from Nuclear Data Covariances**

<table>
<thead>
<tr>
<th>Cases</th>
<th>St. Dev (pcm) from C/E Values</th>
<th>St. Dev (pcm) from S/U</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>HST</strong></td>
<td>590</td>
<td>800</td>
</tr>
<tr>
<td><strong>LST</strong></td>
<td>259</td>
<td>556</td>
</tr>
<tr>
<td><strong>LCT</strong></td>
<td>185</td>
<td>583</td>
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Modernizing infrastructure
CGMF and CoH3
Nuclear Reaction Codes

Toshihiko Kawano, Ionel Stetcu, Patrick Talou

T-2, Nuclear Physics Group
Los Alamos National Laboratory
CoH3

**What is it?**
- Optical model and coupled-channels calculations (spherical and deformed)
- Exciton pre-equilibrium model
- Direct and semi-direct capture model
- Hauser-Feshbach statistical model
- Calculates nuclear reaction cross sections for medium and heavy targets
- keV and MeV energy regions

**Written in C++**

**Input files** or… “super-lazy mode”: coh –z 26 –a 56 -e 10.0

**Newest addition:**
- **prompt fission neutron spectrum** calculated with the Los Alamos model equations.
- Pre-fission neutrons included
CoH3 calculations of PFNS

Kornilov, 1980 (7.02 MeV)
Lovchikova, 2004
ENDF/B-VII.1
present work
new

n (7 MeV) + $^{238}\text{U}$

Outgoing Neutron Energy (MeV)

Prompt Fission Neutron Spectrum

$E_{\text{inc}} = \text{Thermal}$
$E_{\text{inc}} = 5 \text{ MeV}$
$E_{\text{inc}} = 7 \text{ MeV}$
$E_{\text{inc}} = 10 \text{ MeV}$
$E_{\text{inc}} = 15 \text{ MeV}$
$E_{\text{inc}} = 20 \text{ MeV}$

Outgoing Neutron Energy (MeV)

Unclassified

USNDP Meeting, BNL, Nov. 19, 2013
Cascading Gamma Multiplicities


- Monte Carlo Hauser-Feshbach code

**Fig. 6** Inelastic scattering neutron energy spectra from $^{56}$Fe by 20-MeV incident neutron. The outgoing neutrons are virtually gated by a $\gamma$-ray transition from 847 keV $2^+$ state to the $0^+$ ground state, as well as a fixed number of $\gamma$-ray multiplicities. The spectra are shown alternately by solid and dotted lines.
Summary

- New in CoH3: prompt fission neutron spectrum with the Los Alamos model, including pre-fission neutron emissions.
- CGMF code: Monte Carlo Hauser-Feshbach approach to the prompt fission neutrons and gamma-rays, applied to:
  - Cf-252 spontaneous fission neutrons,
  - fission gamma-rays, and
  - other observables.
- Integration with MCNP6 is planned for near future.
Multilevel Breit-Wigner (MLBW) elastic angular distributions

D.A. Brown, NNDC
Leakage from a critical assembly depends greatly on angular dists.

- A forward peaked distribution lets more particles escape from collision events on boundaries than an isotropic one.
- Most evident in small critical systems.
What angular distributions are available in the resonance region?

<table>
<thead>
<tr>
<th>Format</th>
<th>Number occurrences</th>
<th>Number with angular distributions enabled</th>
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<tr>
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<tr>
<td>SLBW</td>
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<td>0</td>
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<tr>
<td>MLBW</td>
<td>270</td>
<td>0</td>
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<tr>
<td>Reich Moore (LRF=3)</td>
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<td>46</td>
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<tr>
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</table>

**can we salvage these guys?**

D. Brown
BNL
MLBW is not unitary - Is this a problem?

\|U\|_r/\sqrt{\dim(U)}

D. Brown
BNL
ENDF’s MLBW capture is clearly different

Capture

ENDF’s \(^{18}\text{O}\)
This naturally impacts the total too

\[ \sigma_{\text{tot}}(b) \]

\begin{align*}
E (\text{eV}) & \quad 0 \quad 5.0 \times 10^5 \quad 1.0 \times 10^6 \quad 1.5 \times 10^6 \quad 2.0 \times 10^6 \quad 2.5 \times 10^6 \quad 3.0 \times 10^6 \quad 3.5 \times 10^6 \\
\sigma_{\text{tot}} (b) & \quad 0 \quad 2 \quad 4 \quad 6 \quad 8 \quad 10 \quad 12
\end{align*}

- Full MLBW (Re(U))
- Full MLBW (\(\sigma_{\text{el}} + \sigma_{\gamma}\))
- ENDF MLBW (Fudge)

ENDF’s \(^{18}\text{O}\)

D. Brown
BNL
ENDF MLBW elastic is the same as the R matrix MLBW elastic

![Graph showing elastic scattering cross-sections as a function of energy (E) in eV. The x-axis represents energy in eV, ranging from 0 to 3.5x10^6, and the y-axis represents the cross-section in barns (b), ranging from 0 to 12. The graph includes data for Full MLBW (U), ENDF MLBW (Fudge), and Full MLBW (BB).]
We can get MLBW angular distributions!!!

According to Blatt-Biedenharn formalism, we only need a collision matrix in order to compute an angular distribution:

\[
\frac{d\sigma_{\alpha,\alpha'}(E)}{d\Omega} = \frac{1}{k^2(2i + 1)(2I + 1)} \sum_{s,s'} \sum_{L=0}^{\infty} B_L(\alpha s, \alpha' s'; E) P_L(\mu)
\]

where

\[
B_L(\alpha s, \alpha' s'; E) = \frac{(-)^{s-s'}}{4} \sum_{c_1=\{\alpha \ell_1 s_1 J_1\}} \sum_{c'_1=\{\alpha' \ell'_1 s'_1 J'_1\}} \sum_{c_2=\{\alpha \ell_2 s_2 J_2\}} \sum_{c'_2=\{\alpha' \ell'_2 s'_2 J'_2\}} \tilde{Z}(\ell_1 J_1 \ell_2 J_2 s L) \tilde{Z}(\ell'_1 J'_1 \ell'_2 J'_2 s' L) \\
\times \delta_{s s_1} \delta_{s'_1 s'_1} \delta_{J_1 J'_1} \delta_{s s_2} \delta_{s'_2 s'_2} \delta_{J_2 J'_2} (\delta_{c_1 c'_1} - U_{c_1 c'_1}(E))^* (\delta_{c_2 c'_2} - U_{c_2 c'_2}(E))
\]
The angular distribution directly from ENDF MLBW parameters

\[ \frac{d\sigma_{\text{el}}}{d\Omega} = (4\pi)^{-1} \sum_{L} \sigma_{L} P_{L}(\mu) \]

ENDF's $^{18}\text{O}$
EMPIRE-3.2 (Malta)
Nuclear Reaction Model Code

- Neutron Resonances
- Coupled Channels
- DWBA
  - Optical Model
  - Multistep Direct
  - Multistep Compound
  - Exciton Model
  - Hybrid MC Simulation
  - HRTW
  - Hauser-Feshbach
  - Optical Model for Fission

- ENDF Formatting
- Verification
- Kalman Filter
- Covariances
EMPIRE-3.2 (Malta)

- **A bit more of physics**
  - $T_{ij}$ rather than $T_i$ used for the CN formation & decay
  - Native angular distributions for CN elastic and inelastics
  - Simulation of the Engelbrecht-Weidenmuller transformation.
  - Kalbach parameterizations for breakup and transfer reactions of complex projectiles

- **A bit better numerics**
  - Fixing fluctuations due to the gap between the last level and the continuum
  - Improving x-sec & energy balance
EMPIRE-3.2 (Malta)

- A bit newer FORTRAN
  - HRTW-comp.f90, kalend.f90, kalman.f90, genkal.f90, newinp.f90
  - Improved gfortran compatibility

- A bit more functionality
  - Improved support for assimilation procedure
  - Improved qsubEmpire.py for running on a cluster
  - GUI that applies Kalman results back to Empire input file.

- A bit better formatting
  - Making line numbers in ENDF files optional
FREYA Update

Ramona Vogt (LLNL) & Jørgen Randrup (LBNL)

w/input from C. Hagmann & J. Verbeke (LLNL), M. James (LANL)

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344
Neutron observables: sawtooth $\nu(A)$

Mean neutron multiplicity as a function of fragment mass; agrees with sawtooth shape of data

$\nu(A)$ calculation shows dispersion in Z for a given mass (FREYA ‘error bars’)

\[ \nu(A) \]
Summary

- Event-by-event treatment shows significant correlations between neutrons that are dependent on the fissioning nucleus.
- **FREYA** agrees rather well with most neutron observables for several spontaneously fissioning isotopes and for neutron-induced fission.
- Comparison with n-n correlation data very promising.
- Photon data do not present a very clear picture – clearly more experiments with modern detectors needed to verify older data.
- Refined modeling of photon emission in **FREYA** is planned.
- Plans to incorporate **FREYA** into **MCNP6**, **FREYA1.0** with neutrons released as open source in July 2013.
Optical Model Potential in Rare-earth Region

G. P. A. Nobre*, A. Palumbo, M. Herman, D. Brown and S. Hoblit

NNDC, Brookhaven National Laboratory

F. S. Dietrich

Lawrence Livermore National Laboratory

Nuclear Data Week at BNL, USNDP and CSEWG meetings
November 18-22, 2013

gnobre@bnl.gov
Motivation

• Why seek an optical potential for this region?
  • Lack of existing regional OP’s for deformed nuclei
  • Recent work* shows scattering from highly deformed nuclei is near adiabatic limit \( \Rightarrow \) deforming a spherical global potential may be suitable with only minor modifications

We deform the Koning-Delaroche spherical global potential and couple g.s. rotational band

• Another approach (Kunieda et al. §) fitted a global OP considering all studied nuclei as rigid rotors


Comparison between spherical and CC: Total cross sections

Spherical approach fails at low energy and its shape is often in disagreement with experimental data, while deforming KD potential provides a good description of the observed total cross sections.
Angular distributions: Gd, Ho, W

- More detailed analysis on the experimental data sets
- Some elastic ang. dist. data actually contained inelastics
- Ensured convergence regarding number of rotational channels

<table>
<thead>
<tr>
<th>nucleus</th>
<th>$\beta_2^*$</th>
<th>$\beta_4^\S$</th>
<th>$\Delta_R$</th>
<th>$\beta_2^{(sys)}$</th>
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<tbody>
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<td>$^{158}$Gd</td>
<td>0.348</td>
<td>0.056</td>
<td>0.990</td>
<td>0.362</td>
</tr>
<tr>
<td>$^{160}$Gd</td>
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<td>0.056</td>
<td>0.990</td>
<td>0.372</td>
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<tr>
<td>$^{165}$Ho</td>
<td>0.293</td>
<td>-0.020</td>
<td>0.993</td>
<td>0.385</td>
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<tr>
<td>$^{182}$W</td>
<td>0.251</td>
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<td>0.995</td>
<td>0.268</td>
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<tr>
<td>$^{184}$W</td>
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<td>0.996</td>
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<tr>
<td>$^{186}$W</td>
<td>0.226</td>
<td>-0.080</td>
<td>0.996</td>
<td>0.226</td>
</tr>
</tbody>
</table>

* At. Data. Nucl. & Data Tables, 78, (2001) 1
Phys. Lett. 26B (1968) 127;

$^{184}\text{W} – \text{Elastic and inelastic angular distributions}$
Conclusion

- We deformed spherical KD potential in CC calculations to describe statically-deformed nuclei
  - No free parameters (experimental deformations)
  - Radius correction gives (small but) noticeable effect
- This approach provides remarkable results for
  - Total, elastic, inelastic cross sections
  - Elastic and inelastic angular distributions
- Improvement of capture cross sections, in particular their shape

This simple method is a good, consistent and general step towards an OP capable of fully describing the rare-earth region, filling the current lack in this important region.
Continuous verification & validation (ADVANCE system)
ADVANCE system for ENDF quality assurance

- Ensuring that all ENDF files get checked
- Every commit, all changed files subjected to a battery of tests including
  - NNDC checking codes (PSYCHE, CHECKR, FIZCON, STANEF, STAN and INTER)
  - NJOY
  - Fudge
  - PREPRO
ENDF/B Development

The development version of the Evaluated Nuclear Data File (ENDF/B)
Neutrons Sublibrary

ENDF/B Development Library

- General Information:
  - ENDF sublib designator: 10
- Revision Number: 611M
- Last Modified Revision: 532:611M
- Build Status:
  - Build status: ERROR
  - Build time: 2013-04-30 16:52:01.394282
- Listfile: neutrons.list
- Release Notes: neutrons-releaseNotes.pdf
- GForge Links:
  - Browse SVN
  - Browse sublibrary tracker

Latest Updates

- sublib_release_notes: neutrons
  Report sublib_release_notes on neutrons generated. The result was a SUCCESS 2013-04-30 16:57:39.661872

- evaluation_summary: n-098 Cf_251.endf
  Code evaluation_summary completed run on n-098 Cf_251.endf. The result was a SUCCESS 2013-04-30 16:52:41.503573

- sublib_html: neutrons
  Report sublib_html on neutrons generated. The result was a SUCCESS 2013-04-30 16:52:01.501892

Summary of all bugs

RSS activity feed
Comparison between cross section data in this ENDF file and data retrieved from EXFOR

Aggregate channels:

0°K & room temp

Regular channels:

Error band!