Covariances in ENDF/B-VII.1

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ENDF/B-VII.1 was released on Dec. 22, 2011

- Many more full evaluations in neutron sublibrary than in any other release
  - ENDF/B-VII.0 contains 393 evaluations
  - ENDF/B-VII.1 contains 423 evaluations
- Extensive collection of covariance data (190 evaluations)
- Library summarized in Dec. 2011 issue of Nuclear Data Sheets
- See also http://www.nndc.bnl.gov/exfor/endfb7.1.jsp
ENDF/B-VII.1 was the combined effort of collaborators from across the US...
... and the world.
One of the main thrusts was the addition of covariance data; they are detailed in 3 papers.
An overview of the library

Sources of covariance data

<table>
<thead>
<tr>
<th>Category</th>
<th>Materials</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light nuclei</td>
<td>12</td>
<td>6 evaluated by R-matrix; 6 low fidelity estimates</td>
</tr>
<tr>
<td>Structural + FP</td>
<td>105</td>
<td>38 evaluated for COMMARA-2.0; 40 updated low fidelity estimates; 15 for criticality safety programs; 12 for other purposes</td>
</tr>
<tr>
<td>Priority Actinides</td>
<td>20</td>
<td>13 evaluated for COMMARA-2.0; 1 from ENDF/B-VII.0; 6 from JENDL-4.0</td>
</tr>
<tr>
<td>Minor Actinides</td>
<td>53</td>
<td>All from JENDL-4.0</td>
</tr>
</tbody>
</table>

ENDF.B-VII.1 (with covariance data)

Stable nuclei

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ENDF
B-VII.1
ENDF/B VII.1 covariance materials

184 materials: 12 Light, 99 structural, 73 Actinides

- $^1$H, $^2$H, $^4$He, $^6$Li, $^7$Li, $^9$Be, $^{10}$B, $^{11}$B, $^{0}$C, $^{15}$N, $^{16}$O, $^{19}$F, $^{24}$Mg, $^{25}$Mg, $^{26}$Mg, $^{27}$Al, $^{28}$Si, $^{29}$Si, $^{30}$Si, $^{35}$Cl, $^{37}$Cl, $^{39}$K, $^{41}$K, $^{46}$Ti, $^{47}$Ti, $^{48}$Ti, $^{49}$Ti, $^{50}$Ti, $^{50}$Cr, $^{52}$Cr, $^{53}$Cr, $^{54}$Cr, $^{55}$Mn, $^{54}$Fe, $^{56}$Fe, $^{57}$Fe, $^{59}$Co, $^{58}$Ni, $^{60}$Ni, $^{89}$Y, $^{90}$Zr, $^{91}$Zr, $^{92}$Zr, $^{93}$Zr, $^{94}$Zr, $^{95}$Zr, $^{96}$Zr, $^{95}$Nb, $^{92}$Mo, $^{94}$Mo, $^{95}$Mo, $^{96}$Mo, $^{97}$Mo, $^{98}$Mo, $^{100}$Mo, $^{99}$Tc, $^{101}$Ru, $^{102}$Ru, $^{103}$Ru, $^{104}$Ru, $^{106}$Ru, $^{105}$Pd, $^{107}$Pd, $^{108}$Pd, $^{109}$Ag, $^{127}$I, $^{129}$I, $^{131}$Xe, $^{132}$Xe, $^{134}$Xe, $^{133}$Cs, $^{135}$Cs, $^{139}$La, $^{141}$Ce, $^{141}$Pr, $^{143}$Nd, $^{145}$Nd, $^{146}$Nd, $^{148}$Nd, $^{147}$Pm, $^{149}$Sm, $^{151}$Sm, $^{142}$Sm, $^{153}$Eu, $^{155}$Eu, $^{152}$Gd, $^{153}$Gd, $^{154}$Gd, $^{155}$Gd, $^{156}$Gd, $^{157}$Gd, $^{158}$Gd, $^{160}$Gd

- $^{166}$Er, $^{167}$Er, $^{168}$Er, $^{170}$Er, $^{180}$W, $^{182}$W, $^{183}$W, $^{184}$W, $^{186}$W, $^{191}$Ir, $^{193}$Ir, $^{197}$Au, $^{204}$Pb, $^{206}$Pb, $^{207}$Pb, $^{208}$Pb, $^{209}$Bi, $^{225}$Ac, $^{226}$Ac, $^{227}$Ac, $^{227}$Th, $^{229}$Th, $^{230}$Th, $^{231}$Th, $^{232}$Th, $^{233}$Th, $^{234}$Th, $^{229}$Pa, $^{230}$Pa, $^{232}$Pa, $^{230}$U, $^{231}$U, $^{232}$U, $^{233}$U, $^{234}$U, $^{235}$U, $^{236}$U, $^{238}$U, $^{234}$Np, $^{235}$Np, $^{236}$Np, $^{237}$Np, $^{238}$Np, $^{239}$Np, $^{236}$Pu, $^{237}$Pu, $^{238}$Pu, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, $^{242}$Pu, $^{244}$Pu, $^{246}$Pu, $^{240}$Am, $^{241}$Am, $^{242m1}$Am, $^{243}$Am, $^{240}$Cm, $^{241}$Cm, $^{242}$Cm, $^{243}$Cm, $^{244}$Cm, $^{245}$Cm, $^{246}$Cm, $^{248}$Cm, $^{249}$Cm, $^{250}$Cm, $^{245}$Bk, $^{246}$Bk, $^{247}$Bk, $^{248}$Bk, $^{250}$Bk, $^{246}$Cf, $^{249}$Cf, $^{250}$Cf, $^{251}$Cf, $^{252}$Cf, $^{253}$Cf, $^{254}$Cf, $^{251}$Es, $^{252}$Es, $^{253}$Es, $^{254}$Es, $^{254m1}$Es, $^{255}$Es, $^{255}$Fm
Methodology

- Covariance evaluation methodology determined by priorities:
  - Most important materials treated individually
  - Medium importance materials treated with simplified methods
  - Low priority materials (mostly fission products) treated with low-fidelity type approach
Methodology

Thermal and Resonance Region

- Source of data
- Experiments
- ENDF file (retroactive method)
- Atlas of Neutron Resonances (ANR)
- SAMMY analysis
- full analysis (MF32, Exp. data)
- retroactive (MF32, ENDF file)
- EMPIRE Resonance Module (MF32, ANR, scattering radius and thermal point uncertainties reproduced through correlations (if possible)
- “Kernel Approximation” (MF33, ANR)
- MF32 with systematic uncertainties in MF33
- ‘low-fidelity’ (Mark Williams) solution
- Assimilation

Fast neutron range (MF33)

- EMPIRE/KALMAN considering experimental data
- Least Square fitting of experimental data (SOK code)
- EMPIRE/KALMAN without experimental data (Low-Fidelity)
- Dispersion analysis - differences among evaluations (and exp. data)
- Reconsider previous work (ENDF/B-VI. 8, Low-Fidelity)
- Visual analysis of experimental data
- Assimilation
An overview of the library

* Major actinides essentially unchanged,
* New $^{236,237,239}\text{U}$, fixes to $^{235,238}\text{U},^{239}\text{Pu}$
* New $^{237}\text{Np},^{238,240,241}\text{Pu},\text{Am}$
* Rest of minor actinides from JENDL-4
* Most actinides now have covariance
* New fission energy release
* FPY updated
Quality Assurance

- New web-based Sigma-QA (A. Sonzogni) allows visual and also quantitative inspection of:
  - Differential uncertainties (dynamic)
  - Integral uncertainties (static)
- UnCor applied to full library, performs 8 tests, warnings for possible problems including:
  - small uncertainties: \((n,\text{tot})<1\%, \ (n,\text{el})\) and \((n,\gamma)<2\%,\) etc.
  - non-positive-definite matrices
  - PFNS covariance not summing to zero
- non-positive-definite matrices are usually fixable by slightly reducing the off-diagonal elements. If not, more drastic measures may be required.
$^{28}$Si integral quantities from Sigma-QA (A. Sonzogni)
### 28Si elastic integral quantities from Sigma-QA

<table>
<thead>
<tr>
<th>Library</th>
<th>THERMAL</th>
<th>RI 0.5-2E+7 eV</th>
<th>MACS 30 keV</th>
<th>$^{252}$Cf 14 MeV</th>
<th>$R'$ (fm)</th>
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</thead>
<tbody>
<tr>
<td>ENDF/B-VII.0</td>
<td>1.992</td>
<td>3.882E+1</td>
<td>2.382</td>
<td>2.871</td>
<td>6.620E-1</td>
</tr>
<tr>
<td>JEFF3.1</td>
<td>1.992</td>
<td>3.885E+1</td>
<td>2.382</td>
<td>2.854</td>
<td>6.969E-1</td>
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<tr>
<td>JENDL4.0</td>
<td>1.992</td>
<td>3.904E+1</td>
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<td>ROSFOND</td>
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<td>2.854</td>
<td>6.969E-1</td>
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<td>2.871</td>
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<td>3.879E+1</td>
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<td>6.424E-1</td>
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<tr>
<td>Atlas</td>
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<tr>
<td>Atlas Δ</td>
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<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>AFCI2.0 Δ</td>
<td>1.992E-2</td>
<td></td>
<td>9.587E-1</td>
<td>1.540E-1</td>
<td>5.435E-2</td>
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<tr>
<td>Recommended Δ</td>
<td>6.000E-3</td>
<td></td>
<td>2.46%</td>
<td>6.46%</td>
<td>4.76%</td>
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</tbody>
</table>

Notes:
- RI: Reaction Integral
- MACS: Macroscopic Cross Section
- $R'$: Scattering Length

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Example of Sigma-QA plot

Cursor at: $x = 3.6826E-2$ (eV) $y = 2.0212E-2$ (b)

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Wednesday, May 23, 12
Quality Assurance (continued)

- Code ‘unCor’, (Mattoon, Oblozinsky) checks the library for possible problems in uncertainties and/or correlations
COMMARA-3 (release FY2013)

Using new features of EMPIRE will address cross-correlations, PFNS, and mu-bars

- Extended to include 184 materials with covariances from ENDF/B-VII.1
- Will be applicable to practically any reactor system and associated fuel cycle.
- Will also include new key features:
  - Major cross-correlations among reactions of the same isotope and among selected isotopes
  - Correlations for elastic angular distributions for most important isotopes (Pu-239, U-235, U-238, Fe, Na, O-16)
  - A complete set of prompt fission neutron spectra, including some cross-isotope correlations
$^{19}$F (new ORNL evaluation)

The graph illustrates the uncertainty in the $^{19}$F (n,γ) reaction as a function of incident neutron energy. The data is represented for two different evaluations:

- Commara 3.0
- Commara 2.0

The graph shows the range of uncertainty at various energy levels, with different lines indicating the two evaluations. The y-axis represents the uncertainty in percentage, and the x-axis represents the incident neutron energy in eV.
$^{52}$Cr (New ORNL RRR evaluation)

$^{52}$Cr ($n, \gamma$)

Comarra 3.0

Comarra 2.0

Uncertainty (%) vs. Incident Neutron Energy (eV)
$^{235}\text{U}$ (New MF33 eval by LANL/ORNL)

$^{235}\text{U} (n,f)$

Uncertainty (%) vs. Incident Neutron Energy (eV)
$^{243}\text{Cm (from JENDL-4)}$

$^{243}\text{Cm (n,el)}$

Uncertainty (%) vs Incident Neutron Energy (eV)

- Commara 3.0
- Commara 2.0
Only substantial change to $^{239}$Pu: addition of prompt fission neutron spectrum covariance

- Talou et al (LANL) retrofitted using Madland-Nix model
- Valuable contribution enabling full QMU studies in Pu systems (previously only nubar and cross section covariance available)
$^{228}$Th mu-bar covariance (JENDL-4)

The graph shows the correlation matrix for $^{228}$Th (mt251) with ordinate scales representing % relative standard deviation and mu-bar, and abscissa scales representing energy (eV). The correlation matrix ranges from -1.0 to 1.0, with colors indicating the degree of correlation.
Conclusions

- ENDF/B-VII.1 contains covariances for 190 materials (184 basically complete)
- Several of “High Fidelity” (3 major actinides and 6 R-matrix light nuclei (LANL), 232Th, W, 55Mn (IAEA), RR in recent ORNL evaluations)
- 40 “Medium Fidelity” (fission products and structural materials, coolants)
- Many “Low Fidelity” for low priority materials
- JENDL-4 for minor Actinides (59)
- These covariances are supposed to be at least reasonable :)

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