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The LLNL Interactive System for Nuclear Data Evaluation

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THE LLNL INTERACTIVE SYSTEM FOR NUCLEAR DATA EVALUATION

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ABSTRACT

LLNL's interactive system for nuclear data evaluation uses a general-purpose two-dimensional graphics code, QPX. With simple commands, we access and plot any information in the Livermore evaluated neutron data library (ENDL), activation library (ACTL), or charged-particle library (ECPL), the Livermore experimental cross section information library (ECSIL), or any evaluated data library using the ENDF format. Features of this system important to evaluation work are discussed. The conversion of evaluations from the ENDF format to the ENDL format for use in our system is discussed.

1. Introduction

In a previous paper,[1] we reviewed specific methods used for evaluation of charged-particle reactions. Specific features of the LLNL interactive evaluation system were described as part of that work. In this paper, we concentrate on generalized tools for nuclear data evaluations using the LLNL interactive system.

2. QPX

QPX is our general-purpose, two-dimensional graphics code and serves as the shell for our interactive system. This code is designed to be a user-friendly visualization and evaluation tool. Using simple commands, data files containing (x,y) or (x,y,Δy) space-delimited data can be accessed and plotted. The limits of the axes can be changed interactively as can be many other properties of the plot. Reasonable default values are picked for all plot properties so that quick plots (QP) can be made instantly. It is designed to run on workstations running the UNIX operating system and employing the X-windowing system (hence the name QPX).

An important capability of this code is that while viewing data, an evaluator can use the computer mouse to define the knots of a cubic-spline curve. In this manner, it is extremely easy to draw a smooth curve. The left mouse button places a knot at the location of the mouse cursor and the middle button removes the knot closest to the location of the cursor. Each time, the resulting cubic-spline curve is redrawn on the screen without removing the previous curves. This allows the user to see exactly how the curve changes each time a knot is added or removed. To refresh the screen with only the last curve, the right button is pushed. In Fig. 1 we show cubic-spline curves that have been drawn

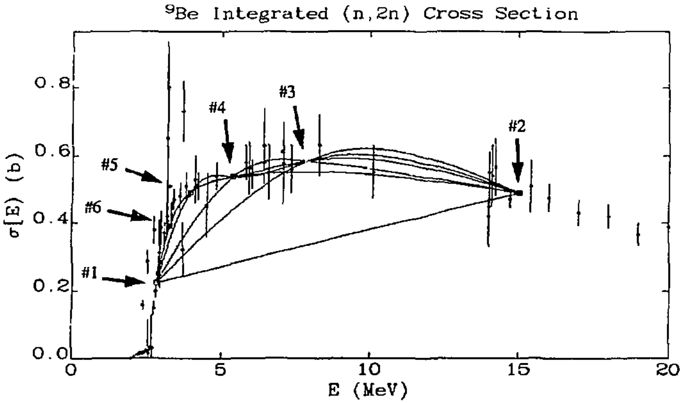

Figure 1: Cubic-spline curves drawn with QPX and the computer mouse. The order of the knot placement is indicated. Note the lowering of the curve near 7 MeV when knot #3 is removed.

through experimental data using QPX and the computer mouse.

2.1. ENDL, ACTL, ECPL

The contents of the Livermore evaluated neutron data library (ENDL), activation library (ACTL), and charged-particle library (ECPL) have been placed into a hierarchial tree structure for easy access on our UNIX workstations. The ENDL library contains evaluations for 109 materials, the ACTL library contains evaluations for 360 materials, and the ECPL library contains evaluations for 14 materials. QPX allows a user to enter simple commands to access and plot any quantities in these libraries. In Fig. 2 we show the integrated fission cross section for ^{235}U that was obtained from the sample QPX session shown in Fig. 3. It is extremely easy for QPX to access this information since *all* of the data in these libraries exist in tabular form using linear-linear interpolation between all points.

2.2. ECSIL

The Livermore experimental cross section information library (ECSIL) is also readily accessible from QPX. This library contains experimental data for neutron-induced reactions from over 6,000 references dating back to 1938. Many of these data were obtained from the National Nuclear Data Center at Brookhaven National Laboratory in the EXFOR format and were translated at LLNL into a common units base and format.

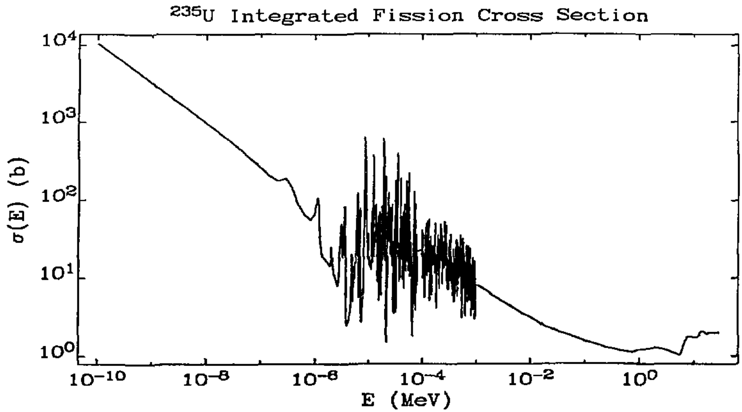

Figure 2: Integrated fission cross section from the LLNL Evaluated Neutron Data Library (ENDL). The QPX commands required to generate this figure are shown in Fig. 3.

3. Conversion of ENDF/B to the ENDL Format

While describing the same basic kinds of data, the formats employed by the Livermore libraries (ENDL) and the U.S. libraries (ENDF/B) are completely different. The ENDL format for a data set consists of two header lines followed by either 2, 3, or 4 columns of linear-linear interpolatable data. The header lines contain the target information and the ENDL 'quantum numbers' (C, I, S, etc.) describing the type of reaction information. An example of the ENDL format is shown in Fig. 4 for the energy distributions of secondary neutrons from ^{113}Cd(n,2n) as translated from ENDF/B-V. The first column gives the incident neutron energy, the second column is the energy of the emitted neutron, and the fourth column is the normalized probability distribution. In the ENDF/B system, the data are expressed in many different formats employing multiple interpolation regions and the possibility of six different interpolation schemes. See Fig. 5 for the original ENDF/B-V information which corresponds to Fig. 4. In this case, the energy distributions are described by a combination of both an arbitrary tabulated function and an evaporation spectrum.

Before using an evaluation in the ENDF/B format, we preprocess the information into pointwise form using D. E. Cullen's suite of codes.[2] The output is then passed through an additional set of codes and translated into the ENDL format. In the ENDL format, the information in ENDF/B formatted evaluations can be accessed and plotted using QPX.

For ENDF/B-V, we have completed a full translation to the ENDL format. For

```
X QP  --  Version:  2.7, 92/08/10 11:12:36

Enter QP command:  endl

     0001 n          14000 Si       40000 Zr       79197 Au197      94239 Pu239
     1001 H1         15031 P31      41093 Nb93     80000 Hg         94240 Pu240
     1002 H2         16032 S32      42000 Mo       82000 Pb         94241 Pu241
     1003 H3         17000 Cl       47107 Ag107    83209 Bi209      94242 Pu242
     2003 He3        18000 Ar       47109 Ag109    90231 Th231      94243 Pu243
     2004 He4        19000 K        48000 Cd       90232 Th232      95241 Am241
     3006 Li6        20000 Ca       49000 In       90233 Th233      95242 Am242
     3007 Li7        22000 Ti       50000 Sn       91233 Pa233      95243 Am243
     4007 Be7        23051 V51      51000 Sb       92233 U233       96242 Cm242
     4009 Be9        24000 Cr       53127 I127     92234 U234       96243 Cm243
     5010 B10        25055 Mn55     54000 Xe       92235 U235       96244 Cm244
     5011 B11        26000 Fe       54134 Xe134    92236 U236       96245 Cm245
     6012 C12        27059 Co59     56138 Ba138    92237 U237       96246 Cm246
     6013 C13        28000 Ni       63000 Eu       92238 U238       96247 Cm247
     7014 N14        28058 Ni58     64000 Gd       92239 U239       96248 Cm248
     7015 N15        29000 Cu       67165 Ho165    92240 U240       97249 Bk249
     8016 O16        30000 Zn       72000 Hf       93235 Np235      98249 Cf249
     9019 F19        31000 Ga       73181 Ta181    93236 Np236      98250 Cf250
    10020 Ne20       33074 As74     74000 W        93237 Np237      98251 Cf251
    11023 Na23       33075 As75     75185 Re185    93238 Np238      98252 Cf252
    12000 Mg         39088 Y88      75187 Re187    94237 Pu237      99120 fp120
    13027 Al27       39089 Y89      78000 Pt       94238 Pu238

Enter isotope descriptor:  u235

  C short &  long reaction type descriptors

   1 tot      total
  10 elas     elastic scattering
  11 n        n
  12 2n       2n
  13 3n       3n
  14 4n       4n
  15 f        fission
  46 g        gamma
  55 xg       xgamma

Enter reaction type descriptor:  f

  I short &  long reaction property descriptors

   0 int      integrated cross-sections and related parameters
   4 ead      energy-angle distributions, normalized legendre coefficients
   7 nubar    average neutrons per fission (prompt or delayed)
   9 mult     multiplicities
  10 aveenyo  average energy deposits to Yo
  11 aveenrn  average energy deposits to residual nucleus

Enter reaction property descriptor:  0

  The following dataset has been selected:

  library(endl)      target(u235)      projectile(n)

    C= 15    fission
    I=  0    integrated cross-sections and related parameters
   Yo=  0    not applicable or none
    S=  0    no x-field data

Enter QP command:  p
```

Figure 3: Sample QPX session showing the four commands required to access and the single command to plot the ^{235}U integrated fission cross section shown in Fig. 2.

```
 48113  1  1  0.000000+0 920930 12  0.000000+0  1.00000+50  2.586000-8
12  4  0  -6.53980+0  0.000000+0  0.000000+0  0.000000+0  0.000000+0
 6.59823000E+00  1.000000E-10  0.000000E+00  1.920040E-10
 6.59823000E+00  1.000000E-02  0.000000E+00  2.919859E+01
 6.59823000E+00  2.000000E-02  0.000000E+00  2.470091E+01
 6.59823000E+00  3.000000E-02  0.000000E+00  1.775450E+01
 6.59823000E+00  4.000000E-02  0.000000E+00  1.365683E+01
 6.59823000E+00  5.000000E-02  0.000000E+00  1.126418E+01
 6.59823000E+00  5.843006E-02  0.000000E+00  1.022340E+01
 7.50000000E+00  1.000000E-10  0.000000E+00  9.235492E-09
 7.50000000E+00  1.000000E-02  0.000000E+00  6.622125E+00
 7.50000000E+00  1.112447E-02  0.000000E+00  7.689136E+00
 7.50000000E+00  1.224894E-02  0.000000E+00  7.180500E+00
...
 7.50000000E+00  4.024014E-01  0.000000E+00  5.573474E-01
 7.50000000E+00  4.400000E-01  0.000000E+00  5.052957E-01
 7.50000000E+00  5.986021E-01  0.000000E+00  1.046834E+00
 7.50000000E+00  7.948028E-01  0.000000E+00  3.747333E-01
 7.50000000E+00  9.602000E-01  0.000000E+00  1.056197E+00
...
 2.00000000E+01  0.000000E+00  0.000000E+00  0.000000E+00
 2.00000000E+01  1.000000E-02  0.000000E+00  2.977437E-01
 2.00000000E+01  2.000000E-02  0.000000E+00  4.266854E-01
 2.00000000E+01  3.000000E-02  0.000000E+00  4.586002E-01
 2.00000000E+01  4.000000E-02  0.000000E+00  4.381352E-01
...
 2.00000000E+01  8.500000E-01  0.000000E+00  9.175333E-02
 2.00000000E+01  8.600000E-01  0.000000E+00  5.192256E-02
 2.00000000E+01  8.700000E-01  0.000000E+00  9.388713E-02
 2.00000000E+01  8.800000E-01  0.000000E+00  5.334506E-02
 2.00000000E+01  1.346020E+01  0.000000E+00  9.602093E-02
                                                                       1
```

Figure 4: Example of the ENDL format for the energy distributions of secondary neutrons for ^{113}Cd(n,2n). The dots indicate lines which have been omitted. Each section of ENDL starts with two header lines and ends with a line containing only a '1' in column 72.

```
 4.81130+ 4 1.11930+ 2          0          0          2          01318 5 16  506
 6.53980+ 6 0.00000+ 0          0          9          1          41318 5 16  507
          4          2                                            1318 5 16  508
 6.59823+ 6 0.00000+ 0 6.59823+ 6 5.00000- 1 2.00000+ 7 5.00000- 11318 5 16  509
 2.00000+ 7 0.00000+ 0                                            1318 5 16  510
 0.00000+ 0 0.00000+ 0          0          0          1          31318 5 16  511
          3          5                                            1318 5 16  512
 6.59823+ 6 6.47153+ 5 1.50000+ 7 9.75750+ 5 2.00000+ 7 9.75750+ 51318 5 16  513
 0.00000+ 0 0.00000+ 0          0          1          1          41318 5 16  514
          4          2                                            1318 5 16  515
 6.59823+ 6 0.00000+ 0 6.59823+ 6 5.00000- 1 2.00000+ 7 5.00000- 11318 5 16  516
 2.00000+ 7 0.00000+ 0                                            1318 5 16  517
 0.00000+ 0 0.00000+ 0          0          0          1          31318 5 16  518
          3          2                                            1318 5 16  519
 0.00000+ 0 6.59823+ 6          0          0          1          61318 5 16  520
          6          2                                            1318 5 16  521
 1.00000- 4 4.33807-16 1.00000+ 4 1.45486- 5 2.00000+ 4 1.79744- 51318 5 16  522
 4.00000+ 4 2.04983- 5 5.84300+ 4 2.07297- 5 5.84300+ 4 0.00000+ 01318 5 16  523
 0.00000+ 0 7.50000+ 6          0          0          1         171318 5 16  524
         17          2                                            1318 5 16  525
 1.00000- 5 1.00000-16 1.00000+ 4 3.35370- 6 2.00000+ 4 4.14340- 61318 5 16  526
 4.00000+ 4 4.72520- 6 6.00000+ 4 4.78310- 6 8.00000+ 4 4.60920- 61318 5 16  527
 1.00000+ 5 4.31890- 6 1.20000+ 5 3.97090- 6 1.40000+ 5 3.59830- 61318 5 16  528
 1.60000+ 5 3.22120- 6 1.80000+ 5 2.85190- 6 2.00000+ 5 2.49810- 61318 5 16  529
 2.50000+ 5 1.70680- 6 3.00000+ 5 1.06400- 6 3.50000+ 5 5.65100- 71318 5 16  530
 4.00000+ 5 1.89300- 7 4.40000+ 5 1.00000-26                      1318 5 16  531
 0.00000+ 0 2.00000+ 7          0          0          1         171318 5 16  532
         17          2                                            1318 5 16  533
 1.00000- 5 1.00000-16 1.00000+ 4 3.35370- 6 2.00000+ 4 4.14340- 61318 5 16  534
 4.00000+ 4 4.72520- 6 6.00000+ 4 4.78310- 6 8.00000+ 4 4.60920- 61318 5 16  535
 1.00000+ 5 4.31890- 6 1.20000+ 5 3.97090- 6 1.40000+ 5 3.59830- 61318 5 16  536
 1.60000+ 5 3.22120- 6 1.80000+ 5 2.85190- 6 2.00000+ 5 2.49810- 61318 5 16  537
 2.50000+ 5 1.70680- 6 3.00000+ 5 1.06400- 6 3.50000+ 5 5.65100- 71318 5 16  538
 4.00000+ 5 1.89300- 7 4.40000+ 5 1.00000-26                      1318 5 16  539
 0.00000+ 0 0.00000+ 0          0          0          0          01318 5  0  540
```

Figure 5: Example of ENDF/B format for the energy distributions of secondary neutrons from ^{113}Cd(n,2n).

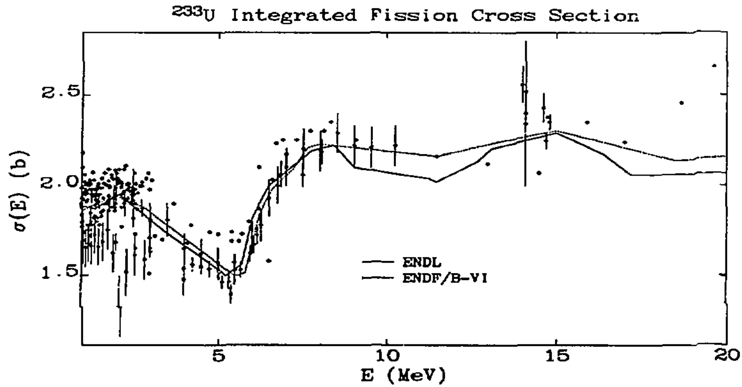

Figure 6: Integrated fission cross section for ^{233}U. Shown are the evaluations from ENDL and ENDF/B-VI along with all of the experimental data available from ECSIL. The QPX commands to generate this plot are shown in Fig. 7.

ENDF/B-VI, we have so far translated the integrated cross sections. In Fig. 6, we show experimental data from ECSIL and the evaluations from ENDL and ENDF/B-VI for the ^{233}U integrated fission cross section. In Fig. 7, we show the QPX command file required to generate the plot shown in Fig. 6. This type of intercomparison of multiple evaluations and the available experimental data will be essential for moving towards a single set of evaluations, i.e., determining the best of the world's evaluations for any isotope.

4. Data Verification—Integral Testing

4.1. *Kerma*

Effects produced by neutron reactions in matter occur principally by the energy loss via ionization and excitation of the charged particles (including residual nuclei) produced. Kerma is defined as the kinetic energy released in matter (per unit mass) and is the sum of all energy transferred to light charged-particles and residual nuclei in a reaction. The neutron kerma factor is defined as the kerma produced per unit neutron fluence.

Because of the importance of neutron kerma factors for both medical applications and in determining heating of materials in fission or fusion power applications, direct measurements of kerma factors have been made. In addition, kerma factors have been calculated from evaluations of reaction data. This is often difficult since many evaluations do not contain all of the requisite information, e.g., the explicit energy distributions of secondary charged particles. The ENDL library does contains explicit energy distributions

```
# retrieve the ENDL and ENDF/B-VI evaluations for U-233(n,f)
#
endl u233 f int
endfb6 u233 f int
#
# draw the ENDF evaluation as a dotted line
#
line10 2
#
# retrieve the experimental information from ECSIL
#
exp u233 f int 0 all
#
# set X axis from 1 to 20 MeV
#
sa 1 20
#
# define the axis labels, main title, and data labels
#
set xtitle $<e (m>e<v)#
set ytitle $*s<(o)> (b)#
set title $&233$<u> <i>ntegrated <f>ission <c>ross <s>ection#
set label 1 1001 5.0 1.5 $<endl# 0.15
set label 2 1010 5.0 1.2 $<endf/b-vi# 0.15
#
# change the X axis length to 10 inches
#
set xlen 10
#
# change the font
#
set font 3
#
# make the plot
p
```

Figure 7: QPX commands used to make the plot of the ^{233}U integrated fission cross section shown in Fig. 6. The lines starting with '#' are QPX comment lines.

for all secondary particles from all neutron-induced reactions and can therefore be used directly to calculate kerma factors using our utility code KERMA. In Fig. 8 we show the neutron kerma factor for ^{12}C as calculated from ENDL along with measured values.

The calculation of neutron kerma factors is one of the *integral* tests we perform on our evaluated data libraries. When a calculation of neutron kerma does not match the experimental measurements of kerma, it is an indication that there is a potential problem with the basic evaluation. Integral tests such as this are not used as the basis for adjusting the evaluations but are used as a guide to what microscopic data we might need to reevaluate. The success of an integral test is satisfying but may only be fortuitous. Therefore, it is only the differences found in integral tests which are significant.

4.2. Critical Assemblies and Pulsed-Sphere Experiments

We also perform calculations using our evaluated libraries to compare with our neutron and gamma-ray pulsed-sphere data. These tests check ENDL in the region of 14 MeV and lower. In addition, we have a suite of 69 critical assemblies with which we validate our evaluated libraries. We have started detailed comparisons of using not only ENDL in these integral tests, but our translations of the ENDF/B-V and ENDF/B-VI libraries as well.

In Fig. 9 is a diagram showing the overall picture of the use of nuclear data in applications codes. The integral tests described above make up only one small part of the application calculations. As part of our evaluations, we feel it is critical to close the loop

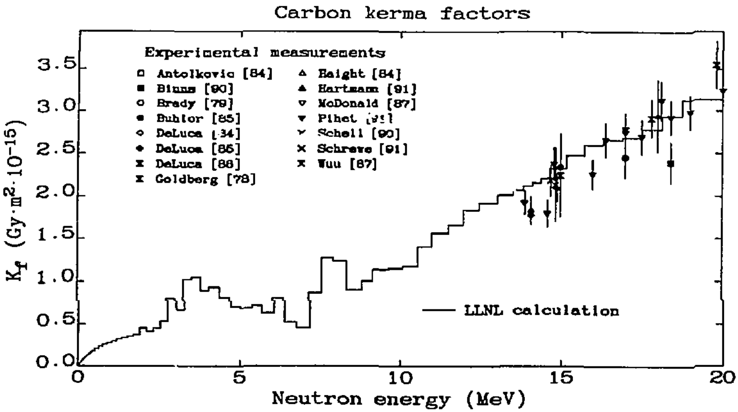

Figure 8: Neutron kerma factors for ^{12}C. The solid line was calculated from ENDL. The references for the experimental data are given elsewhere.[3]

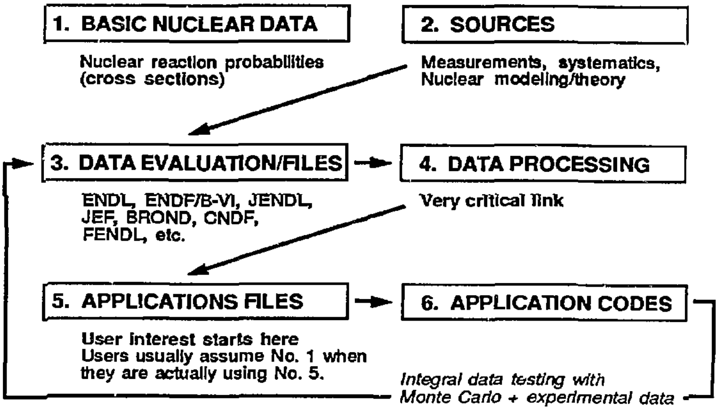

Figure 9: Diagram showing the flow from basic data to applications codes. Our attempt at LLNL has been to close this loop as efficiently as possible so that evaluations and the applications that use them can be improved in a timely manner.

between evaluation, processing, and applications in a timely manner. This is one of the crucial ways that evaluations and the applications that use them can be improved.

5. Conclusions

In this paper we have discussed our general-purpose two-dimensional graphics code QPX and the role it plays in our evaluation methoaology. We have shown the code's ability to :asily and quickly access and plot any information in our evaluated libraries ENDL, ACTL, or ECPL or in our experimental cross section library ECSIL. The conversion of ENDF formatted evaluations to the ENDL format was discussed. Finally, the role of integral testing and its feedback into the evaluation process was presented.

6. Acknowledgments

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7. References

1. D. A. Resler and R. M. White, *Charged-Particle Evaluation Methodology at LLNL*, these proceedings.
2. D. E. Cullen, *The 1992 ENDF Pre-processing Codes*, International Atomic Energy Agency Report IAEA-NDS-39, Rev. 7, February 1992.
3. R. M. White, *Status of Nuclear Data for Use in Neutron Therapy*, Proceedings of The Seventh Symposium on Neutron Dosimetry, *Rad. Prot. Dosimetry*, to be published.