Status of the NJOY Data Processing System

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The f77 version of NJOY has been upgraded from 99.112 to 99.161 during the last year, and the f90 version has been upgraded to match. Validation testing and a high level of recent use on the new ENDF/B-VII evaluations and on the JEFF-3.1 evaluations suggests that the code is working well.

A large number of the changes are improvements in Fortran compatibility made by running compilers with strong checking turned on or reported by other users using different compilers and operating systems. These included such things as uninitialized variables, missing SAVE statements, and storage outside of array bounds. Few of these problems seemed to affect answers.

We added processing to provide continuous sampling of secondary energies from thermal neutron scattering for MCNP instead of the existing treatment using discrete energies. This requires updated versions of MCNP and MCNPX that are now becoming available. The coding also provides for extended graphing of the neutron energy and angle distributions. In practice, this improvement doesn't make much difference for most criticality problems, which depend on integrated reaction rates, but it strikingly improves calculated flux or leakage spectra in the thermal range for problems where that level of detail might be needed, such as the analysis of experiments.

We modified the LEAPR module in its treatment of discrete lines at low values of alpha and beta, and we added a treatment of the Skold Approximation as used for heavy water intermolecular coherence in the new evaluation used in JEFF-3.1 and END/B-VII. We also changed cutoff values to allow smaller S(alpha,beta) numbers in the output files.

The END/B-VII evaluation for H-1 provides a detailed angular distribution for the emitted photon for the capture reaction. This photon should properly be treated relativistically. Because MCNP cannot handle this effect as yet, we have made temporary patches to handle this photon in an approximate way.

Some of the new END/B-VII actinide evaluations include new beta-delayed gamma emission data (MF12/MT460). We have made patches to allow

these evaluations to pass through NJOY OK, but the data are not processed at this time.

We made a change in the handling of energy-dependent fission energy release. There was an error in the formula used to estimate the energy dependence of the fission-fragment energy as taken from the format description for MF1,MT458. NJOY does not use the other energy dependences for neutrons and photons specified in the format manual, instead it computes those directly from other ENDF data. The effect of this error is small for fission spectra, but gets larger at fusion energies.

We fixed a problem with setting the MCNP TYR variable for fission that showed up for the new Th-232 evaluation. It was the first to put the fission spectrum in File 6, causing a small confusion. This problem did affect criticality results for Th-bearing assemblies.

Some of the new JEFF and ENDF/B evaluations borrowed from JENDL used "unit-base" interpolation in File 5, which has not previously been supported by NJOY. This has now been patched.

A number of changes were made in ERRORR and COVR as recommended by users and to pass evaluations using the new compact representation for resonance-parameter covariances through the processing stream. In order to actually process the new resonance covariances, an extended version of ERROR called ERRORJ developed in Japan has now been adapted to fit gracefully into NJOY.

Finally, a number of smaller changes were made to increase various sizes to handle bigger modern evaluations and to handle other specific problems noted during ENDF/B-VII processing. The details are available at http://t2.lanl.gov/codes/njoy99 in the up161 file or the Readme161 file.

The new changes in NJOY were validated by running the standard testing suite and by running all of the neutron evaluations for the ENDF/B-VII beta versions through the codes. In addition, most of the thermal evaluations and a subset of the photonuclear evaluations were tried. The evaluations needed for critical-assembly tests were processed in full detail and used to compute a substantial subset of the ICSBEP benchmarks with good and consistent results. This also provides evidence that NJOY is working well.

An additional project of cross-code comparisons was also carried out this year to validate the LANL NJOY+MCNP methods, the CEA NJOY-CALENDF/TRIPOLI methods, and the LLNL TART/COG/Mercury methods. Runs were made for water spheres (and hydrogen spheres at high density) with a 14-MeV source. This tests high energy cross sections and distributions, thermal cross sections and distributions, and transport methods at a simple limit. After some fixes to some of the codes and after some converging of energy grids used between the LANL and CEA methods, we were able to get very good agreement between the MCNP and TRIPOLI computed fluxes at the 1% level, except for one small glitch at high energies. The LANL and LLNL results came into good agreement at high energies, but some slightly larger differences showed up in the thermal treatment that are being explored. We are looking forward to seeing this test done with other processing and transport systems. Comparisons of criticality results using ENDF/B-VII cross sections with MCNP at Los Alamos and TRIPOLI and Cadarache seem to show agreement to better than 0.1% with a common base of NJOY processing, which provides encouraging evidence that the transport part of the two different methods is working consistently and the variations in the use of NJOY at the two labs is not causing problems.