Comparison of URR Implementations in GNDS Format

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The Generalized Nuclear Database Structure (GNDS) is an international nuclear data format meant to replace the half-century-old Evaluated Nuclear Data Format (ENDF-6). The current version of the specifications as defined by the Working Party on Evaluation Co-operation (OECD/NEA/WPEC) Expert group on GNDS (EGGNDS), includes specifications for the treatment of the unresolved resonances region (URR) and of thermal neutron scattering laws. However, the URR specifications in the current and upcoming GNDS specifications do not fully support the data format and constructs for the URR probability tables required by ACE files and the Monte Carlo transport codes that use them.

Lawrence Livermore National Laboratory has developed a suite of codes to handle GNDS formatted data, a processing code named FUDGE (For Updating Data and Generating Evaluations), and GIDI+. FUDGE supports translation of ENDF-6 formatted data to and from GNDS. It processes GNDS data for use in Monte Carlo and deterministic transport codes, including reconstructing cross sections and angular distributions from resonance parameters. Finally, FUDGE can also translate data from GNDS into the ACE format, for use in Monte Carlo transport codes that use ACE formatted data (e.g., MCNP6). GIDI+ consists of two C++ libraries named GIDI (General Interaction Data Interface) and MCGIDI (Monte Carlo GIDI) for accessing nuclear data from the Generalized Nuclear Database Structure. GIDI directly accesses the GNDS data and is implemented in LLNL’s Monte Carlo and deterministic particle transport codes named Mercury and Ardra, respectively. The MCGIDI library extracts data from a GIDI instance and puts the data into a form better suited for Monte Carlo transport. MCGIDI also provides routines to look up and sample from the data. MCGIDI is implemented in Mercury.

The implementation of URR has implications in terms of data format specifications, processing codes and processed data files, and transport codes. FUDGE has recently been updated to support two different methods of computing and sampling cross sections in the URR. One option is to produce a cross section probability density function (pdf) for each open reaction. Another option, similar to the PURR module in NJOY, is to produce a probability table for the total cross section at each incident energy along with conditional probabilities for each open reaction. Both options condense the variability of URR cross sections into a form that can be easily integrated in Monte Carlo transport, but the two options must be stored and sampled differently.

We previously demonstrated the first implementation of the processing and simulations capabilities for the URR probability tables in GNDS/GIDI/MCGIDI, and we observed discrepancies between the MCNP and Mercury Monte Carlo codes for some of the criticality benchmarks that are sensitive to the URR cross sections. Here, we present results from criticality benchmark simulations using ENDF/B-VIII.0 evaluated nuclear data to test and compare the original implementation of the Unresolved Resonance Region probability tables in NJOY to FUDGE and GIDI/MCGIDI results using both options outlined above. We also compare k-effective values obtained with the Mercury code (with cross section data in the GNDS format) to those calculated using MCNP6 (with cross section data in the ACE format). For the MCNP cases comparisons are made with ACE files that were generated with both NJOY and FUDGE.

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