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TORTSQ – A SCALE Sequence for 3D Discrete Ordinates Calculations

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INTRODUCTION

In an effort to improve the usability of the TORT [1] three-dimensional (3-D) deterministic transport code, a new sequence called TORTSQ (**TORT** S**e**Q**u**ence) has been developed within the SCALE [2] code system.

The new TORTSQ sequence provides

- a user-friendly keyword-based input and a reduced amount of required input data, as compared to the current FIDO format TORT input;
- automated use of point sources (incorporation of GRTUNCL3D, a first collision code);
- built-in angular quadratures; and
- automated, problem-dependent, cross-section library generation, including problem-dependent cross-section self-shielding and collapsing with a fixed source or an eigenvalue calculation.

A major feature of the sequence is the coupling of the SCALE cross-section libraries (or any library in the AMPX master format) and the SCALE cross-section processing codes with TORT, thus eliminating the need for the use of the GIP cross-section mixing program. The option to use a GIP-generated library is retained by the sequence. The possibility of using pointwise cross sections for resonance processing is provided by the incorporation of the CENTRM module in the sequence. It is worth noting that the CSASI sequence in SCALE-5 can also be used to prepare mixed resonance self-shielded cross sections for deterministic codes such as ANISN, DORT, TORT, DANT, and PARTISN.

POINT SOURCES CAPABILITY

The presence of a point source in the input file automatically triggers the generation of a GRTUNCL3D input file and the execution of this code to calculate the uncollided flux and the first collision source throughout the geometry of the problem. This source is passed to the TORT code for calculation of the collided part of the flux. Subsequently, the sequence adds the TORT collided flux with the uncollided flux to determine the total flux.

CROSS-SECTION COLLAPSE

In general, a fine group library with a large number of groups is expected to give better results. However, the use of such a library with a 3-D discrete ordinates code can be impractical, or even prohibitive, because of the large number of phase space variables. As an example, an S8 calculation for a pressurized-water reactor (PWR) model with a 60 × 60 × 48-mesh geometry and a P3 expansion for the cross sections in TORT can lead to a moments file more than 10 GB large when the VITAMIN-B6 library [3] was used. The VITAMIN-B6 library is a 199-group neutron and 42-group photon library containing 120 isotopes, based on ENDF/B-VI, with Bondarenko factors for self-shielding and temperature effects.

A possible remedy for this situation is to use fewer energy groups. The 47-group preshielded BUGLE-96 library [4] is frequently used for light-water reactor (LWR) shielding and hence might be a possibility for the above problem. However, as will be shown in the example below, broad-group libraries like BUGLE-96 are not always appropriate for the problem under consideration and/or may not contain the desired isotopes. The cross-section collapsing capability in TORTSQ can provide adequate, problem-dependent cross sections in fewer groups for this situation. Because the collapsing feature is based on a 1-D transport calculation (using the XSDRN module of SCALE), which is very fast (few minutes compared to hours or days for a 3-D TORT calculation), the burden on the total CPU time is comparatively negligible.

Thermal Response Calculation Example

To support the above discussion, a thermal response, the $B^{10}(n,\alpha)$ reaction rate, is evaluated at the excore detector, which is located in the cavity region of a PWR reactor, by using different libraries. The calculations are carried out on a 1-D model of the PWR at 300K by using the 199-group VITAMIN-B6 library as a reference. The discrepancies between the BUGLE-96 library (with upscattering) and a self-shielded library obtained by collapsing the VITAMIN-B6 library are analyzed. A P3 expansion of the scattering matrices was used for these calculations.

Figure 1 shows the flux spectrum at the location of interest in the cavity obtained with the three libraries. A large discrepancy between the reference calculation and the BUGLE-96 library calculation is apparent in the intermediate and especially thermal ranges. For the problem-dependent library created with TORTSQ, the last ten thermal energy groups of the VITAMIN-B6 were maintained to account for the large $B^{10}(n,\alpha)$ cross section in this energy range, thus resulting in a 57-group collapsed library. It was not the purpose of this study to

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minimize the number of groups of the collapsed library. From Fig. 1, the flux spectrum obtained from the 57-group problem-dependent calculation shows good agreement with the reference result.

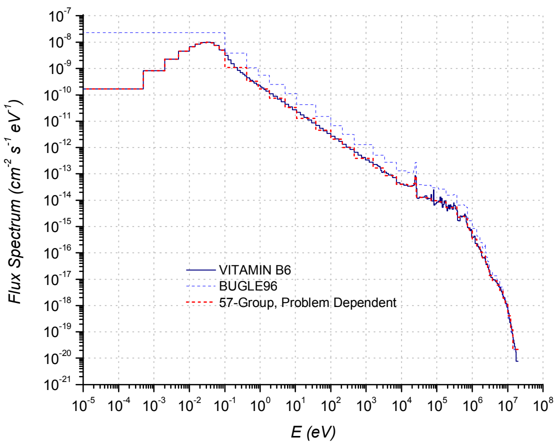

Fig. 1. Flux spectrum at the excore detector (x = 253.5 cm) with different libraries.

Table I contains the $B^{10}(n,\alpha)$ reaction rates per atom calculated as

$$R = \sum_{g=1}^{G} \sigma_g \Phi_g \ , \qquad (1)$$

where σ_g is the group g's (n,α) microscopic cross section (barns), and Φ_g is the scalar flux in group g.

Table I. $B^{10}(n,\alpha)$ Reaction Rates at the Excore Detector (x = 253.5 cm).

Library	R	% Difference	CPU time (min)
VITAMIN-B6	3.2844×10^{-6}	Reference	20.55
BUGLE-96, flat	1.1612×10^{-5}	253.6	3.17
BUGLE-96, 1/4TPV	8.7600×10^{-6}	166.7	3.17
57-Group collapsed	3.2224×10^{-6}	1.9	5.31

As expected, the problem-dependent collapsed library leads to a large improvement for this calculation. The two results corresponding to BUGLE-96 in Table I were obtained with response functions from a flat weighting (ANISN-ID = 7001) and 1/4T PV weighting (ANISN-ID = 7002), respectively, available on the RSICC release. The CPU time for the XSDRN calculation is also provided for comparison.

Although this analysis was performed on a 1-D model, it points out the possible problems one might face when trying to extrapolate the use of existing libraries and the improvements a problem-dependent collapsed library can provide.

CONCLUSIONS AND FUTURE WORK

The present paper introduces a user-friendly, keyword-based TORT sequence under development at ORNL. The sequence includes point source handling and cross sections processing/collapsing capabilities. Future development plans for TORTSQ include

- automated spatial mesh generation based on the SCALE general geometry package, which is also used by KENO-VI and MONACO,
- improvements in the cross-section collapsing methodology for automated determination of problem-dependent group structure, and
- distributed source description independent of the problem's geometry, energy grid, and angular quadrature.

The sequence is currently undergoing internal testing to further improve its reliability, flexibility, and usefulness. The sequence is expected to be incorporated into the next version of the SCALE package.

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