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Implementation of the RESKR module in NJOY

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Abstract. The Blackshaw-Murray[1] elastic kernel represents the effect of neutron up-scattering caused by thermal motion of target nuclei and resonance elastic scattering on the multigroup scattering matrices. A first implementation of this model was proposed by Ouisloumen and Sanchez and made available in proprietary cross-sections libraries of the PARAGON and APOLLO lattice codes.[2] Later, the same technique was reimplemented as module RESK in the NECP-Atlas cross-section generating code by J. Xu, T. Zu and L. Cao.[3, 4] The proposed RESKR module in NJOY-2012 and NJOY-2016 is based on the implementation of module RESK in the NECP-Atlas cross-section generating code.[5] The RESKR module is released under the BSD Open-Source license.

1 Introduction

The new RESKR module of NJOY generates Doppler-broadened resonance elastic scattering kernels (RESKs) in PENDF format starting from piecewise linear cross sections also in PENDF format. The input 0K cross sections are recovered from RECONR *and* from a previous BROADR run. The RESKR module is dedicated to deterministic calculations and requires further processing using the GROUPR module so as to produce the output multigroup cross-section data, as depicted in Fig. 1.

The exact Doppler broadened energy transfer kernel produces a strong up-scattering effect in the resolved resonance energy range, above the upper limit where the $S(\alpha, \beta)$ free gas model of the THERMR module is set. The RESKR module is used to pursue Doppler broadening of the elastic kernel for resonant nuclides above the thermal domain considered by THERMR.

The RESKR module implements the Blackshaw-Murray kernel according to the Ouisloumen and Sanchez formulas. Firstly, the resonance elastic scattering kernel (RESK) formulations for anisotropic scattering up to any Legendre order is adopted to represent the exact Doppler broadened energy transfer kernels. A semi-analytical integration method is applied to perform the RESK calculations. Combining with the RESK calculations, a linearization algorithm is proposed to generate the RESK interpolation tables. These interpolation tables are Legendre moments ℓ of the elastic scattering kernels of the form $P_\ell(E \to E')$.

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They are written in the output PENDF file as a new `MF6` `MT300` reaction type.

The main entry point is subroutine `reskr` exported by the Fortran-90 module `reskm`. The coding logic of module `reskm` is similar to the one used by the Fortran-90 module `thermm`.

An unassigned reaction type number `MT300` in ENDF-6 format is assigned to store and output the interpolation table of the RESK data and the `MF3` `MT300` and `MF6` `MT300` reaction types are defined. The incident energy grid of reaction `MF3` `MT300` is a subset of energy grid in `MF3` `MT2` selected between lower (`elo`) and upper (`ehi`) incident energy boundaries for the RESK calculation. The incident energy grid of reaction `MF6` `MT300` is a coarser grid set to reduce computing cost.

2 The new RESKR module of NJOY

At each reconstructed incident energy, the moments of energy transfer kernels for the different orders are linearized simultaneously on a single unionized grid by the conventional interval-halving techniques of Cullen[6]. It ensures that all orders of the moments are reconstructed smoothly. Meanwhile, the moments of energy transfer kernels for the different orders are interpolated simultaneously once the interpolation interval is found.

A data structure in ENDF-6 format is defined as described in Table 1 where `HEAD`, `TAB2`, `TAB1` and `LIST` are the standard types of records; `ZA` and `AWR` are the standard material charge and mass parameters; `NL` is the maximum Legendre order number of this table; `T` is the absolute temperature; `E1` is the primary energy; `EP` is the
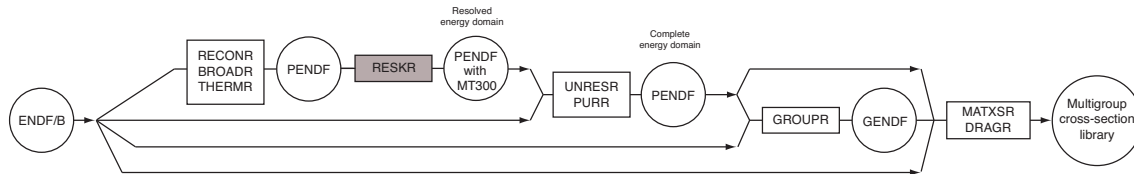
Figure 1. Flow chart of modules in NJOY

Table 1. MF6 MT300 reaction type.

```
[MAT, 6, MT / ZA, AWR, NL, 0, 0, 0 ] HEAD
[MAT, 6, MT / T, 0.0, 0, 0, NR, NE / (INT) ] TAB2
[MAT, 6, MT / 0.0, E1, 0, 0, NRP, NEP / EP / P0(E1->EP) ] TAB1
[MAT, 6, MT / 0.0, 0.0, 0, 0, NW, 0 / P1(E1->EP) ] LIST
Repeat the LIST structure for all NL-1 orders
Repeat the TAB1 structure for all NE incident energies
```

secondary energy; `P0` indicates the 0th moment of energy transfer kernel and `P1` represents the 1st moment of energy transfer kernel. The `TAB1` structure with embedded `LIST` structures is repeated for all `NE` incident energies. Each `TAB1` structure contains $NL-1$ embedded `LIST` structures containing kernel values for P_1, P_2 and higher Legendre moments.

After the processing, the data will be output into derived files which are the point-ENDF (PENDF) files. The reusable PENDF files can be used for generating the different multi-group cross sections and scattering matrices faced with the different requirements of dilutions and energy group structures.

An update of module GROUPR is also required. Subroutine `getrsk` retrieves Legendre-energy data corresponding to the resonance escape scattering kernel and available in the MT300 reaction of the PENDF tape. Subroutine `getrsk` follows the same logic as subroutine `getaed` for thermal scattering data to evaluate the feed function at various incident neutron energies over the panel.

Two multigroup cross section libraries are currently supported: The MATXS format, generated using the MATXSR module and the DRAGLIB format supported by the DRAGR module. The chaining of NJOY modules is depicted in Fig. 1.

3 Conclusion

- The *resonance elastic scattering kernel* (RESK) model is an implementation of Blackshaw-Murray and Sanchez-Ouisloumen elastic kernel consistent with multigroup deterministic calculations.

- The RESK model is the deterministic equivalent of the *Doppler broadening rejection correction* (DBRC) method available in most Monte-Carlo codes.

- Availability of module RESKR is a long-standing request from NJOY community.

- The RESKR module in NJOY is based on the implementation of module RESK in the NECP-Atlas cross-section generating code.

- The new module RESKR is an Open-Source contribution distributed under the BSD license.

- The actual implementation is a beta version requiring further validation. Collaboration is welcome.

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