IMPLEMENTATION OF THE RESKR MODULE IN NJOY

POLYTECHNIQUE MONTRÉAL

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Summary

The Blackshaw-Murray 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. 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. Here, we propose an Open-Source implementation of the same module, renamed* RESKR *in NJOY-2012 and NJOY-2016.*

The new RESKR module of NJOY

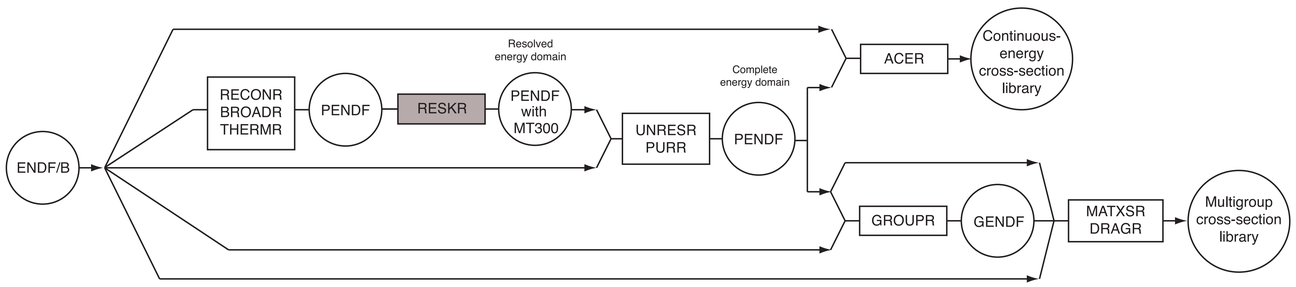
- The new RESKR module of NJOY generates Doppler-broadened resonance elastic scattering kernels (RESKs) in PENDF format starting from piecewise linear cross sections also in PENDF format. The input cross sections are recovered from RECONR *and* from a previous BROADR run.
- The exact Doppler broadened 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 $P_\ell(E \rightarrow E')$. They are written in the output PENDF file as a new `MF6 MT300` reaction type.
- The main entry point is subroutine `reskr` exported by module `reskm`. The coding logic of module `reskm` is similar to the one used by module THERMM.
- In addition to `reskr` new source code, modules `groupr`, `matxsr` and `dragr` were uptated to accomodate the MT300 reaction.
- 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.

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 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 the yellow box 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; `EP` is the 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.

```
[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
```

- 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 MT=300 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.



Conclusion

- The *resonant 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.
- RESKR is an Open-Source contribution distributed under the BSD license.
- The actual implementation is a beta version requiring further validation. Collaboration is welcome.
- The source code is available at `http://merlin.polymtl.ca/pynjoy2012.htm`.

References

1. G. L. Blackshaw and R. L. Murray, "Scattering functions for low-energy neutron collisions in a Maxwellian monoatomic gas," *Nucl. Sci. Eng.*, **27**, 520–532 (1967).
2. M. Ouisloumen and R. Sanchez, "A Model for Neutron Scattering of Heavy Isotopes that Acccounts for Thermal Agitation Effects," *Nucl. Sci. Eng.*, **107**, 189–200 (1991).
3. T. Zu, J. Xu, Y. Tang, H. Bi, F. Zhao, L. Cao and H. Wu, "NECP-Atlas: A new nuclear data processing code," *Ann nucl. Energy*, **123**, 153–161 (2019).
4. J. Xu, T. Zu and L. Cao, "Development and verification of resonance elastic scattering kernel processing module in nuclear data processing code NECP-Atlas," *Progress nucl. Energy*, **110**, 301–310 (2019).
5. R. E. MacFarlane and A. C. Kahler, "Methods for Processing ENDF/B-VII with NJOY," *Nuclear Data Sheets*, **111**, 2739 (2010).
6. Lawrence Livermore Laboratory report UCID-16426 (January 1974).